

Supplementary Information 2

Intact live-cell electro-launching ionization mass spectrometry: A novel method for single-cell analysis

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2172 cellular metabolite components were preliminarily identified including 1343 in positive mode and 829 in negative mode from A549 (scan range m/z 100-1000 Da).

Note: Due to the existence of isomers, we have given all species options in the table as preliminary qualitative results for reference.

m/z detected	HMDB ID	Metabolites	Formula	Adduct ions	m/z calculated	Error, ppm
101.0960	HMDB0174748	Cyclohexanol	C6H12O	M+H	101.0961	-0.9
	HMDB0062058	4-Methyl-3-penten-1-ol	C6H12O	M+H	101.0961	-0.9
	HMDB0179350	(E)-4-Hexen-1-ol	C6H12O	M+H	101.0961	-0.9
	HMDB0062792	(2R,3S)-2-methyl-3-propyloxirane	C6H12O	M+H	101.0961	-0.9
	HMDB0165144	3-METHYLPENTANAL	C6H12O	M+H	101.0961	-0.9
	HMDB0165149	3-methylidenepentan-1-ol	C6H12O	M+H	101.0961	-0.9
	HMDB0165150	3-Methyl-4-penten-1-ol	C6H12O	M+H	101.0961	-0.9
	HMDB0165580	2-Penten-1-ol, 2-methyl-, (Z)-	C6H12O	M+H	101.0961	-0.9
	HMDB0176555	3,3-Dimethylbutyraldehyde	C6H12O	M+H	101.0961	-0.9
	HMDB0062034	3-Methyl-2-pentanone	C6H12O	M+H	101.0961	-0.9
	HMDB0061882	3-Methyl-1-penten-3-ol	C6H12O	M+H	101.0961	-0.9
	HMDB0000753	3-Hexanone	C6H12O	M+H	101.0961	-0.9
	HMDB0001318	4-Methylpentanal	C6H12O	M+H	101.0961	-0.9
	HMDB0002939	Methyl isobutyl ketone	C6H12O	M+H	101.0961	-0.9
	HMDB0005842	2-Oxohexane	C6H12O	M+H	101.0961	-0.9
	HMDB0005846	Ethyl isopropyl ketone	C6H12O	M+H	101.0961	-0.9
	HMDB0005994	Hexanal	C6H12O	M+H	101.0961	-0.9
	HMDB0031578	2-Methylpentanal	C6H12O	M+H	101.0961	-0.9
	HMDB0030952	(E)-2-Hexen-1-ol	C6H12O	M+H	101.0961	-0.9
	HMDB0030003	(E)-3-Hexen-1-ol	C6H12O	M+H	101.0961	-0.9
	HMDB0031502	(E)-4-Hexen-1-ol	C6H12O	M+H	101.0961	-0.9
	HMDB0031503	1-Hexen-3-ol	C6H12O	M+H	101.0961	-0.9
	HMDB0031220	2-Ethylbutanal	C6H12O	M+H	101.0961	-0.9
	HMDB0164619	5-Hexenol	C6H12O	M+H	101.0961	-0.9
103.0502	HMDB0014405	Cycloserine	C3H6N2O2	M+H	103.0502	0.0
	HMDB0060739	3-Amino-2-oxazolidone	C3H6N2O2	M+H	103.0502	0.0
103.0751	HMDB0161203	isovalerate	C5H9O2	M+H	103.0754	-2.5
	HMDB0034237	Propyl acetate	C5H10O2	M+H	103.0754	-2.5
	HMDB0041992	Pivalic acid	C5H10O2	M+H	103.0754	-2.5
	HMDB0059678	1-Hydroxy-2-pentanone	C5H10O2	M+H	103.0754	-2.5
	HMDB0061989	2-hydroxy-3-pentanone	C5H10O2	M+H	103.0754	-2.5
	HMDB0167012	1,2-epoxy-3-hydroxy-3-methylbutane	C5H10O2	M+H	103.0754	-2.5
	HMDB0167011	2-methyl-3-butene-1,2-diol	C5H10O2	M+H	103.0754	-2.5
	HMDB0175213	2-ethylidene-propane-1,3-diol	C5H10O2	M+H	103.0754	-2.5
	HMDB0175214	MBDO	C5H10O2	M+H	103.0754	-2.5
	HMDB0032230	2,4-Dimethyl-1,3-dioxolane	C5H10O2	M+H	103.0754	-2.5
	HMDB0000892	Valeric acid	C5H10O2	M+H	103.0754	-2.5
	HMDB0000718	Isovaleric acid	C5H10O2	M+H	103.0754	-2.5
	HMDB0002176	Ethylmethylacetic acid	C5H10O2	M+H	103.0754	-2.5
	HMDB0031516	3-Hydroxy-2-pentanone	C5H10O2	M+H	103.0754	-2.5
	HMDB0031175	Tetrahydro-2-furanmethanol	C5H10O2	M+H	103.0754	-2.5
	HMDB0039799	Tetrahydro-2-methyl-3-furanol	C5H10O2	M+H	103.0754	-2.5
	HMDB0031247	2-Methylpropyl formate	C5H10O2	M+H	103.0754	-2.5
	HMDB0033742	(S)-2-Methylbutanoic acid	C5H10O2	M+H	103.0754	-2.5
	HMDB0040575	Butyl formate	C5H10O2	M+H	103.0754	-2.5
	HMDB0030058	Ethyl propionate	C5H10O2	M+H	103.0754	-2.5
	HMDB0031249	Methyl isobutyrate	C5H10O2	M+H	103.0754	-2.5
	HMDB0031241	Isopropyl acetate	C5H10O2	M+H	103.0754	-2.5
	HMDB0033890	Methyl butyrate	C5H10O2	M+H	103.0754	-2.5
	HMDB0175215	(2,3-Dimethyloxiranyl)methanol	C5H10O2	M+H	103.0754	-2.5
104.0702	HMDB0161316	4-aminobutanoate	C4H8NO2	M+H	104.0701	1.4
105.0544	HMDB0165469	3,4-dihydroxy-2-butanone	C4H8O3	M+H	105.0546	-2.1
	HMDB0165470	2-Butanone, 1,3-dihydroxy-	C4H8O3	M+H	105.0546	-2.1
	HMDB0000011	(R)-3-Hydroxybutyric acid	C4H8O3	M+H	105.0546	-2.1
	HMDB0000023	(S)-3-Hydroxyisobutyric acid	C4H8O3	M+H	105.0546	-2.1
	HMDB0000336	(R)-3-Hydroxyisobutyric acid	C4H8O3	M+H	105.0546	-2.1
	HMDB0000357	3-Hydroxybutyric acid	C4H8O3	M+H	105.0546	-2.1
	HMDB0000442	(S)-3-Hydroxybutyric acid	C4H8O3	M+H	105.0546	-2.1
	HMDB0000710	4-Hydroxybutyric acid	C4H8O3	M+H	105.0546	-2.1
	HMDB0000729	alpha-Hydroxyisobutyric acid	C4H8O3	M+H	105.0546	-2.1
	HMDB0062640	3-Hydroxyisobutyric acid	C4H8O3	M+H	105.0546	-2.1

	HMDB0126088	3-Hydroxyisobutyric acid	C4H8O3	M+H	105.0546	-2.1
	HMDB0031212	Ethoxyacetic acid	C4H8O3	M+H	105.0546	-2.1
	HMDB0059748	2-Methyl-3-hydroxypropanoate	C4H8O3	M+H	105.0546	-2.1
	HMDB0000008	(S)-2-hydroxybutyric acid	C4H8O3	M+H	105.0546	-2.1
105.0697	HMDB0034240	Styrene	C8H8	M+H	105.0699	-1.7
	HMDB0061975	1,3,7-Octatrien-5-yne	C8H8	M+H	105.0699	-1.7
105.0907	HMDB0164607	3-Methyl-1,3-butanediol	C5H12O2	M+H	105.0910	-2.9
	HMDB0164608	2-Methyl-1,4-butanediol	C5H12O2	M+H	105.0910	-2.9
	HMDB0166217	2-Methylbutane-2,3-diol	C5H12O2	M+H	105.0910	-2.9
	HMDB0166218	2-Methyl-1,2-butanediol	C5H12O2	M+H	105.0910	-2.9
	HMDB0166254	2-Methyl-1,3-butanediol	C5H12O2	M+H	105.0910	-2.9
	HMDB0171225	2-Ethylpropane-1,3-diol	C5H12O2	M+H	105.0910	-2.9
	HMDB0171213	pentane-1,5-diol	C5H12O2	M+H	105.0910	-2.9
	HMDB0166253	3-methylbutane-1,2-diol	C5H12O2	M+H	105.0910	-2.9
107.0528	HMDB0171212	pentane-1,4-diol	C5H12O2	M+H	105.0910	-2.9
	HMDB0031716	3-(Methylthio)-1-propanol	C4H10OS	M+H	107.0525	2.7
	HMDB0040185	3-Mercapto-2-butanol	C4H10OS	M+H	107.0525	2.7
	HMDB0041475	4-Mercapto-2-butanol	C4H10OS	M+H	107.0525	2.7
108.0652	HMDB0041929	Methoxyacetic acid	C3H6O3	M+NH4	108.0655	-2.9
	HMDB0001882	Dihydroxyacetone	C3H6O3	M+NH4	108.0655	-2.9
	HMDB0031232	Monoethyl carbonate	C3H6O3	M+NH4	108.0655	-2.9
	HMDB0001311	D-Lactic acid	C3H6O3	M+NH4	108.0655	-2.9
	HMDB0000700	Hydroxypropionic acid	C3H6O3	M+NH4	108.0655	-2.9
	HMDB0000190	L-Lactic acid	C3H6O3	M+NH4	108.0655	-2.9
	HMDB0001051	Glyceraldehyde	C3H6O3	M+NH4	108.0655	-2.9
	HMDB0144295	2-hydroxypropanoic acid	C3H6O3	M+NH4	108.0655	-2.9
	HMDB0029580	Dimethyl carbonate	C3H6O3	M+NH4	108.0655	-2.9
	HMDB0015671	Ammonium lactate	C3H9NO3	M+H	108.0655	-3.0
	HMDB0062492	L-lactate	C3H5O3	M+NH4	108.0650	2.1
110.0808	HMDB0000131	Glycerol	C3H8O3	M+NH4	110.0812	-3.3
111.0437	HMDB0187589	2-Cyclohexene-1,4-dione	C6H6O2	M+H	111.0441	-3.2
	HMDB0032037	1,3-Benzenediol	C6H6O2	M+H	111.0441	-3.2
	HMDB0033002	5-Methyl-2-furancarboxaldehyde	C6H6O2	M+H	111.0441	-3.2
	HMDB0031180	(E,E)-2,4-Hexadienedial	C6H6O2	M+H	111.0441	-3.2
	HMDB0033127	2-Acetylfuran	C6H6O2	M+H	111.0441	-3.2
	HMDB0002434	Hydroquinone	C6H6O2	M+H	111.0441	-3.2
	HMDB0000957	Pyrocatechol	C6H6O2	M+H	111.0441	-3.2
111.0801	HMDB0061891	(E,Z)-2,4-Heptadienal	C7H10O	M+H	111.0804	-3.1
	HMDB0040278	2-Isopropylfuran	C7H10O	M+H	111.0804	-3.1
	HMDB0031541	3-Methyl-2-cyclohexen-1-one	C7H10O	M+H	111.0804	-3.1
	HMDB0029721	2,3,5-Trimethylfuran	C7H10O	M+H	111.0804	-3.1
	HMDB0029728	2-Ethyl-5-methylfuran	C7H10O	M+H	111.0804	-3.1
	HMDB0040277	2-Propylfuran	C7H10O	M+H	111.0804	-3.1
111.1165	HMDB0040966	1,3-Octadiene	C8H14	M+H	111.1168	-2.9
	HMDB0061901	Dimethylhexa-1,4-diene	C8H14	M+H	111.1168	-2.9
	HMDB0061899	2-(Methylenebutyl)-cyclopropane	C8H14	M+H	111.1168	-2.9
	HMDB0061900	2,4-Octadiene	C8H14	M+H	111.1168	-2.9
	HMDB0061902	2,5-Dimethyl-2,4-hexadiene	C8H14	M+H	111.1168	-2.9
112.0008	HMDB0143055	(hydroxymethylidene)carbamic acid	C2H3NO3	M+Na	112.0005	2.6
112.0156	HMDB0062149	Propionamide	C3H7NO	M+K	112.0159	-2.9
	HMDB0001106	3-Aminopropionaldehyde	C3H7NO	M+K	112.0159	-2.9
	HMDB0002134	Aminoacetone	C3H7NO	M+K	112.0159	-2.9
	HMDB0142435	2-(methylamino)acetaldehyde	C3H7NO	M+K	112.0159	-2.9
	HMDB0062210	3-ammoniopropanal	C3H8NO	M+K	112.0159	-2.9
	HMDB0001888	N,N-Dimethylformamide	C3H7NO	M+K	112.0159	-2.9
	HMDB0031331	Chloroacetic acid	C2H3ClO2	M+NH4	112.0160	-3.4
	HMDB0240707	(aminomethyl)phosphonic acid	CH6NO3P	M+H	112.0158	-1.8
112.0424	HMDB0004983	Dimethyl sulfone	C2H6O2S	M+NH4	112.0427	-2.4
112.0502	HMDB0000630	Cytosine	C4H5N3O	M+H	112.0505	-3.0
112.0753	HMDB0000228	Phenol	C6H6O	M+NH4	112.0757	-3.5
	HMDB0062167	2-VINYLFURAN	C6H6O	M+NH4	112.0757	-3.5
	HMDB0037837	2-Ethyl-4-methyloxazole	C6H9NO	M+H	112.0757	-3.5
	HMDB0040148	Trimethyloxazole	C6H9NO	M+H	112.0757	-3.5
	HMDB0039584	5-Imino-2-methyl-1-cyclopenten-1-ol	C6H9NO	M+H	112.0757	-3.5
	HMDB0031308	5-Acetyl-3,4-dihydro-2H-pyrrole	C6H9NO	M+H	112.0757	-3.5

	HMDB0037863	5-Ethyl-4-methyloxazole	C6H9NO	M+H	112.0757	-3.5
	HMDB0031163	N-Acetyl-2,3-dihydro-1H-pyrrole	C6H9NO	M+H	112.0757	-3.5
	HMDB0037858	2-Ethyl-5-methyloxazole	C6H9NO	M+H	112.0757	-3.5
	HMDB0037838	4-Ethyl-2-methyloxazole	C6H9NO	M+H	112.0757	-3.5
	HMDB0037859	5-Ethyl-2-methyloxazole	C6H9NO	M+H	112.0757	-3.5
112.1117	HMDB0031532	1-Methyl-1,3-cyclohexadiene	C7H10	M+NH4	112.1121	-3.3
	HMDB0032395	2-Methyl-1,3-cyclohexadiene	C7H10	M+NH4	112.1121	-3.3
	HMDB0061889	(3E,5Z)-1,3,5-Heptatriene	C7H10	M+NH4	112.1121	-3.3
113.0342	HMDB0000300	Uracil	C4H4N2O2	M+H	113.0346	-3.1
	HMDB0060760	4-Carboxypyrazole	C4H4N2O2	M+H	113.0346	-3.1
113.0594	HMDB0187593	1,4-Cyclohexanedione	C6H8O2	M+H	113.0597	-2.7
	HMDB0179338	(2Z,4E)-6-hydroxyhexa-2,4-dienal	C6H8O2	M+H	113.0597	-2.7
	HMDB0179339	3-[(1E)-prop-1-en-1-yl]oxirane-2-carbaldehyde	C6H8O2	M+H	113.0597	-2.7
	HMDB0179340	(2Z)-3-(3-methyloxiran-2-yl)prop-2-enal	C6H8O2	M+H	113.0597	-2.7
	HMDB0179337	(2Z,4E)-hexa-2,4-dienoic acid	C6H8O2	M+H	113.0597	-2.7
	HMDB0034247	2-(Methoxymethyl)furan	C6H8O2	M+H	113.0597	-2.7
	HMDB0040260	5,5-Dimethyl-2(5H)-furanone	C6H8O2	M+H	113.0597	-2.7
	HMDB0033569	Syovualdehyde	C6H8O2	M+H	113.0597	-2.7
	HMDB0039778	xi-3,5-Dimethyl-2(5H)-furanone	C6H8O2	M+H	113.0597	-2.7
	HMDB0031344	1,2-Cyclohexanedione	C6H8O2	M+H	113.0597	-2.7
	HMDB0001164	trans-1,2-Dihydrobenzene-1,2-diol	C6H8O2	M+H	113.0597	-2.7
	HMDB0031759	(E)-4-Oxo-2-hexen-1-al	C6H8O2	M+H	113.0597	-2.7
	HMDB0031543	3-Methyl-1,2-cyclopentanedione	C6H8O2	M+H	113.0597	-2.7
	HMDB0029581	(2E,4E)-2,4-Hexadienoic acid	C6H8O2	M+H	113.0597	-2.7
	HMDB0032233	2,5-Dimethyl-3(2H)-furanone	C6H8O2	M+H	113.0597	-2.7
113.0957	HMDB0031486	3-Hepten-2-one	C7H12O	M+H	113.0961	-3.5
	HMDB0031540	4-Methylcyclohexanone	C7H12O	M+H	113.0961	-3.5
	HMDB0033667	(R)-3-Methylcyclohexanone	C7H12O	M+H	113.0961	-3.5
	HMDB0033827	(2E)-2-Heptenal	C7H12O	M+H	113.0961	-3.5
	HMDB0031539	2-Methylcyclohexanone	C7H12O	M+H	113.0961	-3.5
	HMDB0031487	(E)-4-Hepten-2-one	C7H12O	M+H	113.0961	-3.5
	HMDB0034372	xi-3-Methyl-3-cyclohexen-1-ol	C7H12O	M+H	113.0961	-3.5
	HMDB0040339	2,5-Heptadien-1-ol	C7H12O	M+H	113.0961	-3.5
	HMDB0061957	(Z)-2-Heptenal	C7H12O	M+H	113.0961	-3.5
	HMDB0031550	5-Methyl-3-hexen-2-one	C7H12O	M+H	113.0961	-3.5
	HMDB0062028	3-Ethylcyclopentanone	C7H12O	M+H	113.0961	-3.5
	HMDB0061994	2-methyl-2-hexenal	C7H12O	M+H	113.0961	-3.5
	HMDB0061985	2-ethylcyclopentan-1-one	C7H12O	M+H	113.0961	-3.5
	HMDB0032301	trans-2-trans-4-Heptadien-1-ol	C7H12O	M+H	113.0961	-3.5
	HMDB0031551	5-Methyl-5-hexen-2-one	C7H12O	M+H	113.0961	-3.5
	HMDB0031488	2-Hepten-4-one	C7H12O	M+H	113.0961	-3.5
	HMDB0031483	(Z)-4-Heptenal	C7H12O	M+H	113.0961	-3.5
113.1322	HMDB0094705	6-methylhept-1-ene	C8H16	M+H	113.1325	-2.4
	HMDB0032449	1-Octene	C8H16	M+H	113.1325	-2.4
	HMDB0061904	(E)-2-Octene	C8H16	M+H	113.1325	-2.4
	HMDB0061903	(Z)-2-Octene	C8H16	M+H	113.1325	-2.4
	HMDB0061906	(E)-3-Octene	C8H16	M+H	113.1325	-2.4
	HMDB0061905	(Z)-3-Octene	C8H16	M+H	113.1325	-2.4
	HMDB0061907	3-Methyleneheptane	C8H16	M+H	113.1325	-2.4
	HMDB0061909	3-Methyl-3-heptene	C8H16	M+H	113.1325	-2.4
	HMDB0061910	(E)-4-Methyl-2-heptene	C8H16	M+H	113.1325	-2.4
	HMDB0061908	3-Methyl-1-heptene	C8H16	M+H	113.1325	-2.4
	HMDB0061911	4-Methyl-3-heptene	C8H16	M+H	113.1325	-2.4
113.9948	HMDB0161401	glycinate	C2H4NO2	M+K	113.9952	-3.4
	HMDB0031239	Ethyl nitrite	C2H5NO2	M+K	113.9952	-3.4
	HMDB0014691	Acetohydroxamic Acid	C2H5NO2	M+K	113.9952	-3.4
	HMDB0000123	Glycine	C2H5NO2	M+K	113.9952	-3.4
114.0910	HMDB0031545	2-Methyl-2-cyclopenten-1-one	C6H8O	M+NH4	114.0913	-3.0
	HMDB0032965	2,4-Dimethylfuran	C6H8O	M+NH4	114.0913	-3.0
	HMDB0040588	3-Ethylfuran	C6H8O	M+NH4	114.0913	-3.0
	HMDB0040587	2-Ethylfuran	C6H8O	M+NH4	114.0913	-3.0
	HMDB0033182	2,5-Dimethylfuran	C6H8O	M+NH4	114.0913	-3.0
	HMDB0034729	(E,E)-2,4-Hexadienal	C6H8O	M+NH4	114.0913	-3.0
	HMDB0031546	3-Methyl-2-cyclopenten-1-one	C6H8O	M+NH4	114.0913	-3.0
	HMDB0062769	Epsilon-caprolactam	C6H11NO	M+H	114.0913	-3.0

	HMDB0037293	2-Acetylpyrrolidine	C6H11NO	M+H	114.0913	-3.0
	HMDB0031199	2,5-Dihydro-2,4,5-trimethyloxazole	C6H11NO	M+H	114.0913	-3.0
	HMDB0031702	1-Piperidinecarboxaldehyde	C6H11NO	M+H	114.0913	-3.0
115.0159	HMDB0001881	(R)-Propylene glycol	C3H8O2	M+K	115.0156	2.7
	HMDB0061973	1,3-Propanediol	C3H8O2	M+K	115.0156	2.7
	HMDB0062150	1,3-Propanediol	C3H8O2	M+K	115.0156	2.7
	HMDB0006213	(S)-Propane-1,2-diol	C3H8O2	M+K	115.0156	2.7
	HMDB0000131	Glycerol	C3H8O3	M+Na	115.0366	-3.1
115.0362	HMDB0060461	cis-Acetylacrylate	C5H6O3	M+H	115.0390	-3.2
115.0386	HMDB0031859	Norfuraneol	C5H6O3	M+H	115.0390	-3.2
	HMDB0163351	(4Z)-6-hydroxyhex-4-enal	C6H10O2	M+H	115.0754	-3.1
115.0750	HMDB0163350	(Z)-hex-4-enoic acid	C6H10O2	M+H	115.0754	-3.1
	HMDB0163353	3-(3-methyloxiran-2-yl)propanal	C6H10O2	M+H	115.0754	-3.1
	HMDB0163354	(4Z)-2-hydroxyhex-4-enal	C6H10O2	M+H	115.0754	-3.1
	HMDB0163352	(4Z)-3-hydroxyhex-4-enal	C6H10O2	M+H	115.0754	-3.1
	HMDB0179351	4-Hexenoic acid	C6H10O2	M+H	115.0754	-3.1
	HMDB0179346	(2Z)-3-(3-methyloxiran-2-yl)prop-2-en-1-ol	C6H10O2	M+H	115.0754	-3.1
	HMDB0179345	{3-[(1E)-prop-1-en-1-yl]oxiran-2-yl}methanol	C6H10O2	M+H	115.0754	-3.1
	HMDB0179344	cis-2,4-hexadien-1,6-diol	C6H10O2	M+H	115.0754	-3.1
	HMDB0179343	(4E)-2-hydroxyhex-4-enal	C6H10O2	M+H	115.0754	-3.1
	HMDB0179342	(4E)-3-hydroxyhex-4-enal	C6H10O2	M+H	115.0754	-3.1
	HMDB0179341	(4E)-6-hydroxyhex-4-enal	C6H10O2	M+H	115.0754	-3.1
	HMDB0169695	(Z)-3-methyl-2-pentenoic acid	C6H10O2	M+H	115.0754	-3.1
	HMDB0169664	(E)-3-Methyl-2-pentenoic acid	C6H10O2	M+H	115.0754	-3.1
	HMDB0165583	2-Methyl-3-ethyloxirane-2-carbaldehyde	C6H10O2	M+H	115.0754	-3.1
	HMDB0165582	(2Z)-4-hydroxy-2-methylpent-2-enal	C6H10O2	M+H	115.0754	-3.1
	HMDB0165581	(2Z)-2-(hydroxymethyl)pent-2-enal	C6H10O2	M+H	115.0754	-3.1
	HMDB0165584	(2Z)-5-hydroxy-2-methylpent-2-enal	C6H10O2	M+H	115.0754	-3.1
	HMDB0163703	(3Z)-5-hydroxy-3-methylpent-3-en-2-one	C6H10O2	M+H	115.0754	-3.1
	HMDB0163702	Pentanal, 3-methyl-4-oxo-	C6H10O2	M+H	115.0754	-3.1
	HMDB0032490	Prenyl formate	C6H10O2	M+H	115.0754	-3.1
	HMDB0039581	Ethyl crotonate	C6H10O2	M+H	115.0754	-3.1
	HMDB0031158	2-Methyl-4-pentenoic acid	C6H10O2	M+H	115.0754	-3.1
	HMDB0031562	2-Methyl-3-pentenoic acid	C6H10O2	M+H	115.0754	-3.1
	HMDB0031559	4-Methyl-2,3-pentanedione	C6H10O2	M+H	115.0754	-3.1
	HMDB0031491	2,3-Hexanedione	C6H10O2	M+H	115.0754	-3.1
	HMDB0031560	2-Methyl-2-pentenoic acid	C6H10O2	M+H	115.0754	-3.1
	HMDB0031501	3-Hexenoic acid	C6H10O2	M+H	115.0754	-3.1
	HMDB0029487	Allyl propionate	C6H10O2	M+H	115.0754	-3.1
	HMDB0033568	5-Oxohexanal	C6H10O2	M+H	115.0754	-3.1
	HMDB0040328	Methyl 4-pentenoate	C6H10O2	M+H	115.0754	-3.1
	HMDB0031492	3,4-Hexanedione	C6H10O2	M+H	115.0754	-3.1
	HMDB0031561	4-Methyl-2-pentenoic acid	C6H10O2	M+H	115.0754	-3.1
	HMDB0010719	Isohydrosorbic acid	C6H10O2	M+H	115.0754	-3.1
	HMDB0003843	Gamma-Caprolactone	C6H10O2	M+H	115.0754	-3.1
	HMDB0060476	epsilon-Caprolactone	C6H10O2	M+H	115.0754	-3.1
	HMDB0240384	4-Hydroxyhexanal	C6H10O2	M+H	115.0754	-3.1
	HMDB0062135	methyl (2E)-2-methylbut-2-enoate	C6H10O2	M+H	115.0754	-3.1
	HMDB0061965	1-methyl-2,3-dioxabicyclo[2.2.1]heptane	C6H10O2	M+H	115.0754	-3.1
	HMDB0061929	Dihydro-4,4-dimethyl-2(3H)-furanone	C6H10O2	M+H	115.0754	-3.1
	HMDB0000453	delta-Hexanolactone	C6H10O2	M+H	115.0754	-3.1
115.0944	HMDB0032303	2-Heptanethiol	C7H16S	M+H-H2O	115.0946	-1.5
	HMDB0032304	Heptane-1-thiol	C7H16S	M+H-H2O	115.0946	-1.5
115.1114	HMDB0003671	2-Heptanone	C7H14O	M+H	115.1117	-3.0
	HMDB0062059	4-methylhexan-3-one	C7H14O	M+H	115.1117	-3.0
	HMDB0166735	trans-2-Hepten-1-ol	C7H14O	M+H	115.1117	-3.0
	HMDB0061896	2-Methyl-3-hexanone	C7H14O	M+H	115.1117	-3.0
	HMDB0004814	4-Heptanone	C7H14O	M+H	115.1117	-3.0
	HMDB0005841	Ethyl isobutyl ketone	C7H14O	M+H	115.1117	-3.0
	HMDB0041320	(2R,4Z)-4-Hepten-2-ol	C7H14O	M+H	115.1117	-3.0
	HMDB0040191	2-Methylhexanal	C7H14O	M+H	115.1117	-3.0
	HMDB0031475	Heptanal	C7H14O	M+H	115.1117	-3.0
	HMDB0031482	3-Heptanone	C7H14O	M+H	115.1117	-3.0

	HMDB0031429	2,4-Dimethyl-3-pentanone	C7H14O	M+H	115.1117	-3.0
	HMDB0031538	3-Methylcyclohexanol	C7H14O	M+H	115.1117	-3.0
	HMDB0031405	(Z)-4-Hepten-1-ol	C7H14O	M+H	115.1117	-3.0
	HMDB0031549	5-Methyl-2-hexanone	C7H14O	M+H	115.1117	-3.0
	HMDB0038052	1-Ethoxy-3-methyl-2-butene	C7H14O	M+H	115.1117	-3.0
	HMDB0032405	3-Methylhexanal	C7H14O	M+H	115.1117	-3.0
	HMDB0059693	1-Methylcyclohexanol	C7H14O	M+H	115.1117	-3.0
	HMDB0175178	6-Hepten-1-ol	C7H14O	M+H	115.1117	-3.0
116.0104	HMDB0000973	Phosphate	H3O4P	M+NH4	116.0107	-2.7
	HMDB0001429	Phosphate	H3O4P	M+NH4	116.0107	-2.7
	HMDB0002105	Phosphate	H3O4P	M+NH4	116.0107	-2.7
	HMDB0002142	Phosphate	H3O4P	M+NH4	116.0107	-2.7
	HMDB0034805	Ammonium dihydrogenphosphate	H6NO4P	M+H	116.0107	-2.8
116.0702	HMDB0062030	3-FURANMETHANOL	C5H6O2	M+NH4	116.0706	-3.5
	HMDB0013742	2-Furanmethanol	C5H6O2	M+NH4	116.0706	-3.5
	HMDB0034245	2-Furanmethanol	C5H6O2	M+NH4	116.0706	-3.5
	HMDB0029609	5-Methyl-2(3H)-furanone	C5H6O2	M+NH4	116.0706	-3.5
	HMDB0040145	5-Hydroxy-4-pentenoic acid d-lactone	C5H6O2	M+NH4	116.0706	-3.5
	HMDB0167281	2,3-dihydroxy-2-methylbutanenitrile	C5H9NO2	M+H	116.0706	-3.5
	HMDB0167283	2,4-dihydroxy-2-methylbutanenitrile	C5H9NO2	M+H	116.0706	-3.5
	HMDB0167282	2-hydroxy-2-(hydroxymethyl)butanenitrile	C5H9NO2	M+H	116.0706	-3.5
	HMDB0177063	1-formyl-pyrrolidin-2-ol	C5H9NO2	M+H	116.0706	-3.5
	HMDB0179973	SCHEMBL55844	C5H9NO2	M+H	116.0706	-3.5
	HMDB0012880	Acetamidopropanal	C5H9NO2	M+H	116.0706	-3.5
	HMDB0030409	4-Amino-2-methylenebutanoic acid	C5H9NO2	M+H	116.0706	-3.5
	HMDB0003411	D-Proline	C5H9NO2	M+H	116.0706	-3.5
	HMDB0034208	Pterolactam	C5H9NO2	M+H	116.0706	-3.5
	HMDB0000162	L-Proline	C5H9NO2	M+H	116.0706	-3.5
116.1067	HMDB0179336	cis,trans-2,4-hexadien-1-ol	C6H10O	M+NH4	116.1070	-2.5
	HMDB0062127	2-methylpent-1-en-3-one	C6H10O	M+NH4	116.1070	-2.5
	HMDB0165587	(2Z)-2-methylpenta-2,4-dien-1-ol	C6H10O	M+NH4	116.1070	-2.5
	HMDB0031496	Hex-trans-2-en-1-al	C6H10O	M+NH4	116.1070	-2.5
	HMDB0176892	Hex-trans-2-en-1-al	C6H10O	M+NH4	116.1070	-2.5
	HMDB0062031	3e-hexene-2-one	C6H10O	M+NH4	116.1070	-2.5
	HMDB0003315	Cyclohexanone	C6H10O	M+NH4	116.1070	-2.5
	HMDB0040264	(Z)-2-Hexenal	C6H10O	M+NH4	116.1070	-2.5
	HMDB0035239	4-Hexen-3-one	C6H10O	M+NH4	116.1070	-2.5
	HMDB0031196	4-Methyl-2-pentenal	C6H10O	M+NH4	116.1070	-2.5
	HMDB0031497	3-Hexenal	C6H10O	M+NH4	116.1070	-2.5
	HMDB0031498	(Z)-3-Hexenal	C6H10O	M+NH4	116.1070	-2.5
	HMDB0033549	(E)-4-Hexenal	C6H10O	M+NH4	116.1070	-2.5
	HMDB0033714	2-Methyl-2-pentenal	C6H10O	M+NH4	116.1070	-2.5
	HMDB0030332	2-Methyl-4-pentenal	C6H10O	M+NH4	116.1070	-2.5
	HMDB0031563	4-Methyl-3-penten-2-one, 9CI	C6H10O	M+NH4	116.1070	-2.5
	HMDB0040271	(Z)-4-Hexenal	C6H10O	M+NH4	116.1070	-2.5
	HMDB0031564	4-Methyl-4-penten-2-one	C6H10O	M+NH4	116.1070	-2.5
	HMDB0144632	diethylamino-acetaldehyde	C6H13NO	M+H	116.1070	-2.5
	HMDB0062041	3,3-Dimethylbutanamide	C6H13NO	M+H	116.1070	-2.5
	HMDB0062140	(1-methylpyrrolidin-2-yl)methanol	C6H13NO	M+H	116.1070	-2.5
	HMDB0031651	N-(3-Methylbutyl)acetamide	C6H13NO	M+H	116.1070	-2.5
	HMDB0034203	N-(2-Methylpropyl)acetamide	C6H13NO	M+H	116.1070	-2.5
116.9767	HMDB0002151	Dimethyl sulfoxide	C2H6OS	M+K	116.9771	-3.4
117.0543	HMDB0129098	2,3-dimethyloxirane-2-carboxylic acid	C5H8O3	M+H	117.0546	-2.7
	HMDB0128943	(2E)-4-hydroxy-3-methylbut-2-enoic acid	C5H8O3	M+H	117.0546	-2.7
	HMDB0129096	(2Z)-2-(hydroxymethyl)but-2-enoic acid	C5H8O3	M+H	117.0546	-2.7
	HMDB0168838	Ethyl 2,3-epoxypropanoate	C5H8O3	M+H	117.0546	-2.7
	HMDB0169666	SCHEMBL4558754	C5H8O3	M+H	117.0546	-2.7
	HMDB0177209	2-Hydroxymethyl-trans-crotonic acid	C5H8O3	M+H	117.0546	-2.7
	HMDB0177210	4-hydroxytiglic acid	C5H8O3	M+H	117.0546	-2.7
	HMDB0003771	2-Methylacetoacetic acid	C5H8O3	M+H	117.0546	-2.7
	HMDB0029172	2-Methylacetoacetic acid	C5H8O3	M+H	117.0546	-2.7
	HMDB0128916	4-hydroxy-3-methylbut-2-enoic acid	C5H8O3	M+H	117.0546	-2.7
	HMDB0128917	dimethyloxirane-2-carboxylic acid	C5H8O3	M+H	117.0546	-2.7
	HMDB0034466	Acetoxyacetone	C5H8O3	M+H	117.0546	-2.7
	HMDB0012233	Glutarate semialdehyde	C5H8O3	M+H	117.0546	-2.7

	HMDB0001865	2-Oxovaleric acid	C5H8O3	M+H	117.0546	-2.7
	HMDB0000310	Methylacetoacetic acid	C5H8O3	M+H	117.0546	-2.7
	HMDB0031643	Ethyl pyruvate	C5H8O3	M+H	117.0546	-2.7
	HMDB0000019	alpha-Ketoisovaleric acid	C5H8O3	M+H	117.0546	-2.7
	HMDB0168839	2-HYDROXYETHYL ACRYLATE	C5H8O3	M+H	117.0546	-2.7
	HMDB0132477	2-(hydroxymethyl)but-2-enoic acid	C5H8O3	M+H	117.0546	-2.7
	HMDB0129097	4-hydroxy-2-methylbut-2-enoic acid	C5H8O3	M+H	117.0546	-2.7
117.0736	HMDB0000720	Levulinic acid	C5H8O3	M+H	117.0546	-2.7
	HMDB0032411	2-Methyl-1-methylthio-2-butene	C6H12S	M+H	117.0732	3.0
	HMDB0040244	1-Propenyl propyl sulfide	C6H12S	M+H	117.0732	3.0
	HMDB0032277	(+/-)-3-(Ethylthio)butanol	C6H14OS	M+H-H2O	117.0738	-2.0
	HMDB0032374	2-Mercapto-2-methyl-1-pentanol	C6H14OS	M+H-H2O	117.0738	-2.0
	HMDB0032375	(+/-)-4-Mercapto-4-methyl-2-pentanol	C6H14OS	M+H-H2O	117.0738	-2.0
	HMDB0036194	4-Methoxy-2-methyl-2-butanethiol	C6H14OS	M+H-H2O	117.0738	-2.0
117.0906	HMDB0034878	3-Mercapto-2-methylpentanol	C6H14OS	M+H-H2O	117.0738	-2.0
	HMDB0040152	3-Mercapto-1-hexanol	C6H14OS	M+H-H2O	117.0738	-2.0
	HMDB0163355	(4Z)-hex-4-ene-1,2-diol	C6H12O2	M+H	117.0910	-3.5
	HMDB0163678	6-hydroxyhexan-2-one	C6H12O2	M+H	117.0910	-3.5
	HMDB0163356	(2Z)-hex-2-ene-1,6-diol	C6H12O2	M+H	117.0910	-3.5
	HMDB0163357	(4Z)-hex-4-ene-1,3-diol	C6H12O2	M+H	117.0910	-3.5
	HMDB0185846	4-(hydroxymethyl)-2-pentanone	C6H12O2	M+H	117.0910	-3.5
	HMDB0176889	SCHEMBL58684	C6H12O2	M+H	117.0910	-3.5
	HMDB0176890	(3-propyloxiran-2-yl)methanol	C6H12O2	M+H	117.0910	-3.5
	HMDB0176888	2-Hexene-1,4-diol	C6H12O2	M+H	117.0910	-3.5
	HMDB0176891	(E)-2-Hexene-1,6-diol	C6H12O2	M+H	117.0910	-3.5
	HMDB0165589	SCHEMBL63629	C6H12O2	M+H	117.0910	-3.5
	HMDB0165586	(2Z)-2-methylpent-2-ene-1,5-diol	C6H12O2	M+H	117.0910	-3.5
	HMDB0165588	2-propylidene-1,3-propanediol	C6H12O2	M+H	117.0910	-3.5
	HMDB0165585	(2Z)-2-methylpent-2-ene-1,4-diol	C6H12O2	M+H	117.0910	-3.5
	HMDB0163715	1567-93-7	C6H12O2	M+H	117.0910	-3.5
	HMDB0163358	3-(3-methyloxiranyl)propan-1-ol	C6H12O2	M+H	117.0910	-3.5
	HMDB0031207	Methyl pentanoate	C6H12O2	M+H	117.0910	-3.5
	HMDB0030059	Propyl propionate	C6H12O2	M+H	117.0910	-3.5
	HMDB0040279	2,4,5-Trimethyl-1,3-dioxolane	C6H12O2	M+H	117.0910	-3.5
	HMDB0033774	3-Methylpentanoic acid	C6H12O2	M+H	117.0910	-3.5
	HMDB0034163	3-Methylbutyl formate	C6H12O2	M+H	117.0910	-3.5
	HMDB0031511	Diacetone alcohol	C6H12O2	M+H	117.0910	-3.5
	HMDB0031580	2-Methylpentanoic acid	C6H12O2	M+H	117.0910	-3.5
	HMDB0030027	Methyl 3-methylbutanoate	C6H12O2	M+H	117.0910	-3.5
	HMDB0037266	2,2,4-Trimethyl-1,3-dioxolane	C6H12O2	M+H	117.0910	-3.5
	HMDB0029762	Methyl (S)-2-Methylbutanoate	C6H12O2	M+H	117.0910	-3.5
	HMDB0062131	Methyl (S)-2-Methylbutanoate	C6H12O2	M+H	117.0910	-3.5
	HMDB0000535	Caproic acid	C6H12O2	M+H	117.0910	-3.5
	HMDB0061883	Caproic acid	C6H12O2	M+H	117.0910	-3.5
	HMDB0033889	Ethyl butyrate	C6H12O2	M+H	117.0910	-3.5
	HMDB0031248	Ethyl 2-methylpropanoate	C6H12O2	M+H	117.0910	-3.5
	HMDB0176566	3,3-dimethylbutyric acid	C6H12O2	M+H	117.0910	-3.5
	HMDB0040327	Pentyl formate	C6H12O2	M+H	117.0910	-3.5
	HMDB0031221	2-Ethylbutanoic acid	C6H12O2	M+H	117.0910	-3.5
	HMDB0030056	Isopropyl propionate	C6H12O2	M+H	117.0910	-3.5
	HMDB0031246	2-Methylpropyl acetate	C6H12O2	M+H	117.0910	-3.5
	HMDB0031325	n-Butyl acetate	C6H12O2	M+H	117.0910	-3.5
	HMDB0000689	Isocaproic acid	C6H12O2	M+H	117.0910	-3.5
117.1010	HMDB0011749	2-Piperidinone	C5H9NO	M+NH4	117.1022	-2.9
	HMDB0162803	3-methyl-2,3-dihydro-1H-pyrrol-2-ol	C5H9NO	M+NH4	117.1022	-2.9
	HMDB0162804	3-methyl-2,3-dihydro-1H-pyrrol-3-ol	C5H9NO	M+NH4	117.1022	-2.9
	HMDB0162806	(2,3-dihydro-1H-pyrrol-3-yl)methanol	C5H9NO	M+NH4	117.1022	-2.9
	HMDB0167280	2-hydroxy-2-methylbutanenitrile	C5H9NO	M+NH4	117.1022	-2.9
	HMDB0040518	2,5-Dihydro-2,4-dimethyloxazole	C5H9NO	M+NH4	117.1022	-2.9

117.1017	HMDB0034587	1-Pyrrolidinecarboxaldehyde	C5H9NO	M+NH4	117.1022	-2.9
	HMDB0060309	(2R)-2-Hydroxy-2-methylbutanenitrile	C5H9NO	M+NH4	117.1022	-2.9
	HMDB0179972	3-Hydroxy-3-methylbutanenitrile	C5H9NO	M+NH4	117.1022	-2.9
	HMDB0012176	5-Aminopentanamide	C5H12N2O	M+H	117.1022	-2.9
	HMDB0062789	1,1,3,3-tetramethylurea	C5H12N2O	M+H	117.1022	-2.9
118.0859	HMDB0163433	N-[(3-methylbutyl)imino]hydroxylamine	C5H12N2O	M+H	117.1022	-2.9
	HMDB0149276	SCHEMBL15659879	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0180166	3-methyl-4-trans-hydroxy-2-butenal	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0163714	1-(2-methyloxiran-2-yl)ethan-1-one	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0132474	2-methylbut-2-enoic acid	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0170858	Isopropenylacetic acid	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0163713	73255-29-5	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0163712	SCHEMBL69133	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0130837	2-methylbut-3-enoic acid	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0129418	3,3-dimethyloxirane-2-carbaldehyde	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0031648	2,4-Pentanedione	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0032459	2-Pentenoic acid	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0032351	Isopropenyl acetate	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0032385	Methyl methacrylate	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0029599	Glutaral	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0000509	Senecioic acid	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0001470	Tiglic acid	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0001862	2-Ethylacrylic acid	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0002167	3-Methylbutyrolactone	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0033978	Ethyl acrylate	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0031598	2,3-Pentanedione	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0031178	2-Methyltetrahydrofuran-3-one	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0033840	Dihydro-5-methyl-2(3H)-furanone	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0031602	4-Pentenoic acid	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0029608	Angelic acid	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0035143	Dihydro-3-methyl-2(3H)-furanone	C5H8O2	M+NH4	118.0863	-3.0
	HMDB0000883	L-Valine	C5H11NO2	M+H	118.0863	-3.0
	HMDB0003355	5-Aminopentanoic acid	C5H11NO2	M+H	118.0863	-3.0
	HMDB0002141	N-Methyl-a-aminoisobutyric acid	C5H11NO2	M+H	118.0863	-3.0
	HMDB0001382	Vaporole	C5H11NO2	M+H	118.0863	-3.0
	HMDB0013716	Norvaline	C5H11NO2	M+H	118.0863	-3.0
	HMDB0061966	1-nitropentane	C5H11NO2	M+H	118.0863	-3.0
	HMDB0062141	N,N-Dimethyl-L-Alanine	C5H11NO2	M+H	118.0863	-3.0
	HMDB0015550	Amyl Nitrite	C5H11NO2	M+H	118.0863	-3.0
119.0699	HMDB0062584	2-Hydroxy-3-methylbutyric acid	C5H10O3	M+H	119.0703	-3.1
	HMDB0161206	2-hydroxy-3-methylbutanoate	C5H9O3	M+H	119.0703	-3.1
	HMDB0041603	Methyl-beta-hydroxybutyrate	C5H10O3	M+H	119.0703	-3.1
	HMDB0130836	4-hydroxy-2-methylbutanoic acid	C5H10O3	M+H	119.0703	-3.1
	HMDB0161204	3-Hydroxy-3-methylbutyrate	C5H9O3	M+H	119.0703	-3.1
	HMDB0161205	4-hydroxy-3-methylbutanoate	C5H9O3	M+H	119.0703	-3.1
	HMDB0172067	2-hydroxypropyl acetate	C5H10O3	M+H	119.0703	-3.1
	HMDB0172068	3-hydroxypropyl Acetate	C5H10O3	M+H	119.0703	-3.1
	HMDB0172069	Propyl glycolate	C5H10O3	M+H	119.0703	-3.1
	HMDB0000410	3-Hydroxy-2-methyl-[S-(R,R)]-butanoic acid	C5H10O3	M+H	119.0703	-3.1
	HMDB0001987	2-Hydroxy-2-methylbutyric acid	C5H10O3	M+H	119.0703	-3.1
	HMDB0001863	2-Hydroxyvaleric acid	C5H10O3	M+H	119.0703	-3.1
	HMDB0000754	3-Hydroxyisovaleric acid	C5H10O3	M+H	119.0703	-3.1
	HMDB0000531	3-Hydroxyvaleric acid	C5H10O3	M+H	119.0703	-3.1
	HMDB0000407	2-Hydroxy-3-methylbutyric acid	C5H10O3	M+H	119.0703	-3.1
	HMDB0000396	2-Ethylhydracrylic acid	C5H10O3	M+H	119.0703	-3.1
	HMDB0000354	2-Methyl-3-hydroxybutyric acid	C5H10O3	M+H	119.0703	-3.1
	HMDB0000351	(2S,3R)-3-Hydroxy-2-methylbutanoic acid	C5H10O3	M+H	119.0703	-3.1
	HMDB0002011	4-Hydroxyisovaleric acid	C5H10O3	M+H	119.0703	-3.1
	HMDB0040735	Ethyl lactate	C5H10O3	M+H	119.0703	-3.1
	HMDB0062057	4-hydroxy-valeric acid	C5H10O3	M+H	119.0703	-3.1
	HMDB0059844	Diethyl carbonate	C5H10O3	M+H	119.0703	-3.1
	HMDB0000642	Erythronilic acid	C5H10O3	M+H	119.0703	-3.1
	HMDB0061927	5-Hydroxypentanoic acid	C5H10O3	M+H	119.0703	-3.1
119.0852	HMDB0059899	alpha-Methylstyrene	C9H10	M+H	119.0855	-2.7
	HMDB0059837	Indane	C9H10	M+H	119.0855	-2.7

	HMDB0062099	cyclopropylbenzene	C9H10	M+H	119.0855	-2.7	
119.0892	HMDB0039806	1-Hexanethiol	C6H14S	M+H	119.0889	2.5	
	HMDB0031431	Dipropyl sulfide	C6H14S	M+H	119.0889	2.5	
	HMDB0029579	Diisopropyl sulfide	C6H14S	M+H	119.0889	2.5	
119.1063	HMDB0164618	Hexane-1,6-Diol	C6H14O2	M+H	119.1067	-3.0	
	HMDB0165148	3-Methyl-1,5-pentanediol	C6H14O2	M+H	119.1067	-3.0	
	HMDB0165146	3-methylpentane-1,3-diol	C6H14O2	M+H	119.1067	-3.0	
	HMDB0165145	3-methyl-1,4-pentanediol	C6H14O2	M+H	119.1067	-3.0	
	HMDB0031490	1,5-Hexanediol	C6H14O2	M+H	119.1067	-3.0	
	HMDB0031327	2-Butoxyethanol	C6H14O2	M+H	119.1067	-3.0	
	HMDB0031644	1,1-Diethoxyethane	C6H14O2	M+H	119.1067	-3.0	
	HMDB0059740	4-Methyl-1,2-dihydroxypentane	C6H14O2	M+H	119.1067	-3.0	
	HMDB0165147	2-ethylbutane-1,4-diol	C6H14O2	M+H	119.1067	-3.0	
119.9384	HMDB0013668	Ruthenium	Ru	M+NH4	119.9382	1.9	
120.0651	HMDB0168831	methyl oxirane-2-carboxylate	C4H6O3	M+NH4	120.0655	-3.5	
	HMDB0171690	ethyl glyoxylate	C4H6O3	M+NH4	120.0655	-3.5	
	HMDB0184570	dihydro-4-hydroxy-3(2h)-furanone	C4H6O3	M+NH4	120.0655	-3.5	
	HMDB0172027	Tocris538	C4H6O3	M+NH4	120.0655	-3.5	
	HMDB0172028	3-Methylloxirane-2-carboxylic acid	C4H6O3	M+NH4	120.0655	-3.5	
	HMDB0178247	5469-16-9	C4H6O3	M+NH4	120.0655	-3.5	
	HMDB0001172	2-Methyl-3-oxopropanoic acid	C4H6O3	M+NH4	120.0655	-3.5	
	HMDB0001259	Succinic acid semialdehyde	C4H6O3	M+NH4	120.0655	-3.5	
	HMDB0003381	4-Hydroxycrotonic acid	C4H6O3	M+NH4	120.0655	-3.5	
	HMDB0000005	2-Ketobutyric acid	C4H6O3	M+NH4	120.0655	-3.5	
	HMDB0002217	(S)-Methylmalonic acid semialdehyde	C4H6O3	M+NH4	120.0655	-3.5	
	HMDB0000060	Acetoacetic acid	C4H6O3	M+NH4	120.0655	-3.5	
	HMDB0031646	Acetic anhydride	C4H6O3	M+NH4	120.0655	-3.5	
	HMDB0159151	alpha-Amino-beta-hydroxybutyric acid	C4H9NO3	M+H	120.0655	-3.5	
	HMDB0004041	L-Allothreonine	C4H9NO3	M+H	120.0655	-3.5	
	HMDB0000719	L-Homoserine	C4H9NO3	M+H	120.0655	-3.5	
	HMDB0159152	L-Homoserine	C4H9NO3	M+H	120.0655	-3.5	
	HMDB0000167	L-Threonine	C4H9NO3	M+H	120.0655	-3.5	
	HMDB0061148	Hydroxyethyl glycine	C4H9NO3	M+H	120.0655	-3.5	
	HMDB0155268	N,N-dimethylhydroxyglycine	C4H9NO3	M+H	120.0655	-3.5	
	HMDB0162440	3-amino-4-hydroxybutanoic acid	C4H9NO3	M+H	120.0655	-3.5	
	HMDB0061877	4-Amino-3-hydroxybutyrate	C4H9NO3	M+H	120.0655	-3.5	
	HMDB0240310	2-methylserine zwitterion	C4H9NO3	M+H	120.0655	-3.5	
	HMDB0060587	Aminoethoxyacetic acid	C4H9NO3	M+H	120.0655	-3.5	
	120.9658	HMDB0000973	Phosphate	H3O4P	M+Na	120.9661	-2.6
		HMDB0001429	Phosphate	H3O4P	M+Na	120.9661	-2.6
HMDB0002105		Phosphate	H3O4P	M+Na	120.9661	-2.6	
HMDB0002142		Phosphate	H3O4P	M+Na	120.9661	-2.6	
121.0256	HMDB0040145	5-Hydroxy-4-pentenoic acid d-lactone	C5H6O2	M+Na	121.0260	-3.3	
	HMDB0062030	3-FURANMETHANOL	C5H6O2	M+Na	121.0260	-3.3	
	HMDB0013742	2-Furanmethanol	C5H6O2	M+Na	121.0260	-3.3	
	HMDB0034245	2-Furanmethanol	C5H6O2	M+Na	121.0260	-3.3	
	HMDB0029609	5-Methyl-2(3H)-furanone	C5H6O2	M+Na	121.0260	-3.3	
121.0644	HMDB0124943	3-ethenylphenol	C8H8O	M+H	121.0648	-3.2	
	HMDB0062765	styrene oxide	C8H8O	M+H	121.0648	-3.2	
	HMDB0013815	2,3-Dihydrobenzofuran	C8H8O	M+H	121.0648	-3.2	
	HMDB0029637	3-Methylbenzaldehyde	C8H8O	M+H	121.0648	-3.2	
	HMDB0029638	4-Methylbenzaldehyde	C8H8O	M+H	121.0648	-3.2	
	HMDB0172088	2-Vinylphenol	C8H8O	M+H	121.0648	-3.2	
	HMDB0029636	2-Methylbenzaldehyde	C8H8O	M+H	121.0648	-3.2	
	HMDB0038997	Lentialexin	C8H8O	M+H	121.0648	-3.2	
	HMDB0004072	4-Hydroxystyrene	C8H8O	M+H	121.0648	-3.2	
	HMDB0033910	Acetophenone	C8H8O	M+H	121.0648	-3.2	
	HMDB0006236	Phenylacetaldehyde	C8H8O	M+H	121.0648	-3.2	
121.0685	HMDB0039781	xi-2-Mercapto-3-methyl-1-butanol	C5H12OS	M+H	121.0682	2.8	
	HMDB0167776	SCHEMBL1376644	C5H12OS	M+H	121.0682	2.8	
	HMDB0041562	4-(Methylthio)-1-butanol	C5H12OS	M+H	121.0682	2.8	
	HMDB0032373	3-Mercapto-2-methyl-1-butanol	C5H12OS	M+H	121.0682	2.8	
	HMDB0036149	3-Mercapto-3-methyl-1-butanol	C5H12OS	M+H	121.0682	2.8	
	HMDB0041476	4-(Methylthio)-2-butanol	C5H12OS	M+H	121.0682	2.8	
	HMDB0167775	2-methyl-4-sulfanylbutan-2-ol	C5H12OS	M+H	121.0682	2.8	

121.1008	HMDB0034029	Isopropylbenzene	C9H12	M+H	121.1012	-3.1
	HMDB0061962	1-ethyl-4-methylbenzene	C9H12	M+H	121.1012	-3.1
	HMDB0059877	Propylbenzene	C9H12	M+H	121.1012	-3.1
	HMDB0059819	o-Ethyltoluene	C9H12	M+H	121.1012	-3.1
	HMDB0059848	m-Ethyl toluene	C9H12	M+H	121.1012	-3.1
	HMDB0041924	Mesitylene	C9H12	M+H	121.1012	-3.1
	HMDB0013733	1,2,4-Trimethylbenzene	C9H12	M+H	121.1012	-3.1
	HMDB0059901	Hemimellitene	C9H12	M+H	121.1012	-3.1
122.0267	HMDB0040458	1,2,4-Tris(methylene)cyclohexane	C9H12	M+H	121.1012	-3.1
	HMDB0000574	L-Cysteine	C3H7NO2S	M+H	122.0270	-2.7
	HMDB0061368	Methyl-S-cystein	C3H7NO2S	M+H	122.0270	-2.7
122.0597	HMDB0003417	D-Cysteine	C3H7NO2S	M+H	122.0270	-2.7
	HMDB0004461	Benzamide	C7H7NO	M+H	122.0600	-2.8
	HMDB0035281	2-Acetylpyridine	C7H7NO	M+H	122.0600	-2.8
122.0961	HMDB0033131	3-Acetylpyridine	C7H7NO	M+H	122.0600	-2.8
	HMDB0061975	1,3,7-Octatrien-5-yne	C8H8	M+NH4	122.0964	-2.6
	HMDB0034240	Styrene	C8H8	M+NH4	122.0964	-2.6
	HMDB0062016	2,4-dimethylaniline	C8H11N	M+H	122.0964	-2.7
	HMDB0001020	N,N-Dimethylaniline	C8H11N	M+H	122.0964	-2.7
	HMDB0002017	1-Phenylethylamine	C8H11N	M+H	122.0964	-2.7
	HMDB0012275	Phenylethylamine	C8H11N	M+H	122.0964	-2.7
	HMDB0060276	Phenylethylamine	C8H11N	M+H	122.0964	-2.7
	HMDB0040041	2-Ethyl-5-methylpyridine	C8H11N	M+H	122.0964	-2.7
	HMDB0029729	5-Ethyl-2-methylpyridine	C8H11N	M+H	122.0964	-2.7
	HMDB0032497	2-Propylpyridine	C8H11N	M+H	122.0964	-2.7
	HMDB0060677	2,6-Dimethylaniline	C8H11N	M+H	122.0964	-2.7
122.1172	HMDB0171225	2-Ethylpropane-1,3-diol	C5H12O2	M+NH4	122.1176	-2.9
	HMDB0164607	3-Methyl-1,3-butanediol	C5H12O2	M+NH4	122.1176	-2.9
	HMDB0164608	2-Methyl-1,4-butanediol	C5H12O2	M+NH4	122.1176	-2.9
	HMDB0166217	2-Methylbutane-2,3-diol	C5H12O2	M+NH4	122.1176	-2.9
	HMDB0166218	2-Methyl-1,2-butanediol	C5H12O2	M+NH4	122.1176	-2.9
	HMDB0166254	2-Methyl-1,3-butanediol	C5H12O2	M+NH4	122.1176	-2.9
	HMDB0171213	pentane-1,5-diol	C5H12O2	M+NH4	122.1176	-2.9
	HMDB0166253	3-methylbutane-1,2-diol	C5H12O2	M+NH4	122.1176	-2.9
123.0298	HMDB0171212	pentane-1,4-diol	C5H12O2	M+NH4	122.1176	-2.9
	HMDB0041492	1,2-Butanedithiol	C4H10S2	M+H	123.0297	1.1
	HMDB0033552	1,3-Butanedithiol	C4H10S2	M+H	123.0297	1.1
	HMDB0031872	Methyl propyl disulfide	C4H10S2	M+H	123.0297	1.1
	HMDB0031708	1,2-Bis(methylthio)ethane	C4H10S2	M+H	123.0297	1.1
	HMDB0029572	Diethyl disulfide	C4H10S2	M+H	123.0297	1.1
123.0437	HMDB0031157	2,3-Butanedithiol	C4H10S2	M+H	123.0297	1.1
	HMDB0186744	3-hydroxybenzaldehyde	C7H6O2	M+H	123.0441	-2.9
	HMDB0034170	2-Hydroxybenzaldehyde	C7H6O2	M+H	123.0441	-2.9
	HMDB0032918	3-(2-Furanyl)-2-propenal	C7H6O2	M+H	123.0441	-2.9
	HMDB0001870	Benzoic acid	C7H6O2	M+H	123.0441	-2.9
123.0549	HMDB0011718	4-Hydroxybenzaldehyde	C7H6O2	M+H	123.0441	-2.9
	HMDB0001406	Niacinamide	C6H6N2O	M+H	123.0553	-3.2
123.0801	HMDB0031861	2-Acetylpyrazine	C6H6N2O	M+H	123.0553	-3.2
	HMDB0033944	2-Phenylethanol	C8H10O	M+H	123.0804	-2.8
	HMDB0062024	2,7-Dimethyloxepine	C8H10O	M+H	123.0804	-2.8
	HMDB0041609	4-Methylbenzyl alcohol	C8H10O	M+H	123.0804	-2.8
	HMDB0059873	3-Ethylphenol	C8H10O	M+H	123.0804	-2.8
	HMDB0032151	3,4-Dimethylphenol	C8H10O	M+H	123.0804	-2.8
	HMDB0029306	4-Ethylphenol	C8H10O	M+H	123.0804	-2.8
	HMDB0032148	2,3-Dimethylphenol	C8H10O	M+H	123.0804	-2.8
	HMDB0032619	1-Phenylethanol	C8H10O	M+H	123.0804	-2.8
	HMDB0032076	1-Methoxy-4-methylbenzene	C8H10O	M+H	123.0804	-2.8
	HMDB0032074	1-Methoxy-2-methylbenzene	C8H10O	M+H	123.0804	-2.8
	HMDB0032150	2,6-Dimethylphenol	C8H10O	M+H	123.0804	-2.8
	HMDB0030540	2,5-Dimethylphenol	C8H10O	M+H	123.0804	-2.8
123.1165	HMDB0038140	Santene	C9H14	M+H	123.1168	-2.6
	HMDB0061784	3-Allyl-1-cyclohexene	C9H14	M+H	123.1168	-2.6
124.0390	HMDB0060665	Isonicotinic acid	C6H5NO2	M+H	124.0393	-2.5
	HMDB0041950	Nitrobenzene	C6H5NO2	M+H	124.0393	-2.5
	HMDB0031713	2-Hydroxy-4-imino-2,5-cyclohexadienone	C6H5NO2	M+H	124.0393	-2.5

	HMDB0002243	Picolinic acid	C6H5NO2	M+H	124.0393	-2.5
	HMDB0001488	Nicotinic acid	C6H5NO2	M+H	124.0393	-2.5
124.0583	HMDB0040068	2-Ethyl-4,5-dimethylthiazole	C7H11NS	M+H-H2O	124.0585	-1.8
	HMDB0040070	5-Ethyl-2,4-dimethylthiazole	C7H11NS	M+H-H2O	124.0585	-1.8
	HMDB0038436	6-Isothiocyanato-1-hexene	C7H11NS	M+H-H2O	124.0585	-1.8
	HMDB0040101	2,4-Diethylthiazole	C7H11NS	M+H-H2O	124.0585	-1.8
	HMDB0037156	4-Methyl-2-(1-methylethyl)thiazole	C7H11NS	M+H-H2O	124.0585	-1.8
	HMDB0040069	4-Ethyl-2,5-dimethylthiazole	C7H11NS	M+H-H2O	124.0585	-1.8
	HMDB0040097	2,5-Diethylthiazole	C7H11NS	M+H-H2O	124.0585	-1.8
	HMDB0040100	2-Methyl-4-(1-methylethyl)thiazole	C7H11NS	M+H-H2O	124.0585	-1.8
	HMDB0031862	2-(2-Methylpropyl)thiazole	C7H11NS	M+H-H2O	124.0585	-1.8
	HMDB0037140	2-(1-Methylpropyl)thiazole	C7H11NS	M+H-H2O	124.0585	-1.8
	HMDB0059892	Isothiocyanatocyclohexane	C7H11NS	M+H-H2O	124.0585	-1.8
124.0732	HMDB0012815	5-Aminopentanal	C5H11NO	M+Na	124.0733	-0.7
	HMDB0172632	2-Piperidinol	C5H11NO	M+Na	124.0733	-0.7
	HMDB0062600	N-butylformamide	C5H11NO	M+Na	124.0733	-0.7
124.0965	HMDB0061944	Trihydroxybutane	C4H10O3	M+NH4	124.0968	-2.6
	HMDB0240298	1,2,4-butanetriol	C4H10O3	M+NH4	124.0968	-2.6
	HMDB0034778	(2R*,3R*)-1,2,3-Butanetriol	C4H10O3	M+NH4	124.0968	-2.6
124.9223	HMDB0012190	Arsenate	AsH3O4	M+H-H2O	124.9220	2.2
124.9995	HMDB0010720	But-2-enoic acid	C4H6O2	M+K	124.9999	-3.5
	HMDB0167139	3-Methyloxirane-2-carbaldehyde	C4H6O2	M+K	124.9999	-3.5
	HMDB0174868	but-3-enoic acid	C4H6O2	M+K	124.9999	-3.5
	HMDB0000549	gamma-Butyrolactone	C4H6O2	M+K	124.9999	-3.5
	HMDB0002523	Oxolan-3-one	C4H6O2	M+K	124.9999	-3.5
	HMDB0003407	Diacetyl	C4H6O2	M+K	124.9999	-3.5
	HMDB0031209	Ethenyl acetate	C4H6O2	M+K	124.9999	-3.5
	HMDB0034439	Isocrotonic acid	C4H6O2	M+K	124.9999	-3.5
	HMDB0033977	Methyl acrylate	C4H6O2	M+K	124.9999	-3.5
	HMDB0167138	(2Z)-4-hydroxybut-2-enal	C4H6O2	M+K	124.9999	-3.5
125.0594	HMDB0135619	3-methoxyphenol	C7H8O2	M+H	125.0597	-2.4
	HMDB0001398	Guaiacol	C7H8O2	M+H	125.0597	-2.4
	HMDB0059709	2-Hydroxybenzyl alcohol	C7H8O2	M+H	125.0597	-2.4
	HMDB0059712	3-Hydroxybenzyl alcohol	C7H8O2	M+H	125.0597	-2.4
	HMDB0000873	4-Methylcatechol	C7H8O2	M+H	125.0597	-2.4
	HMDB0011724	4-Hydroxybenzyl alcohol	C7H8O2	M+H	125.0597	-2.4
	HMDB0038963	4,6-Heptadiyne-1,3-diol	C7H8O2	M+H	125.0597	-2.4
	HMDB0035226	2-Acetyl-5-methylfuran	C7H8O2	M+H	125.0597	-2.4
	HMDB0029696	Mequinol	C7H8O2	M+H	125.0597	-2.4
	HMDB0034877	2-Acetyl-3-methylfuran	C7H8O2	M+H	125.0597	-2.4
	HMDB0032917	1-(2-Furanyl)-2-propanone	C7H8O2	M+H	125.0597	-2.4
	HMDB0040280	1-(2-Furanyl)-1-propanone	C7H8O2	M+H	125.0597	-2.4
	HMDB0031686	(E,E)-2,4-Octadienal	C8H12O	M+H	125.0961	-3.1
125.0957	HMDB0039844	(E,E)-2,6-Octadienal	C8H12O	M+H	125.0961	-3.1
	HMDB0031582	6-Methyl-3,5-heptadien-2-one	C8H12O	M+H	125.0961	-3.1
	HMDB0040272	2-Butylfuran	C8H12O	M+H	125.0961	-3.1
	HMDB0033238	2-Isopropyl-5-methylfuran	C8H12O	M+H	125.0961	-3.1
	HMDB0031414	2,3-Dimethyl-2-cyclohexen-1-one	C8H12O	M+H	125.0961	-3.1
	HMDB0040246	3,5,5-Trimethyl-2-cyclopenten-1-one	C8H12O	M+H	125.0961	-3.1
	HMDB0032446	trans, trans-3,5-Octadien-2-one	C8H12O	M+H	125.0961	-3.1
	HMDB0032447	1,5-Octadien-3-one	C8H12O	M+H	125.0961	-3.1
	HMDB0061898	Methyl-1-cyclopenten-1-yl)-ethanone	C8H12O	M+H	125.0961	-3.1
	HMDB0062073	5-Octen-2-yn-4-ol	C8H12O	M+H	125.0961	-3.1

126.0158	HMDB0011602	3-Oxoalanine	C3H5NO3	M+Na	126.0162	-2.9
	HMDB0002455	Pyruvatoxime	C3H5NO3	M+Na	126.0162	-2.9
126.0216	HMDB0000251	Taurine	C2H7NO3S	M+H	126.0219	-2.7
126.0312	HMDB0142479	2-(dimethylamino)acetaldehyde	C4H9NO	M+K	126.0316	-3.0
	HMDB0031581	Morpholine	C4H9NO	M+K	126.0316	-3.0
	HMDB0001080	4-Aminobutyraldehyde	C4H9NO	M+K	126.0316	-3.0
	HMDB0060247	4-Aminobutyraldehyde	C4H9NO	M+K	126.0316	-3.0
	HMDB0033870	Butyramide	C4H9NO	M+K	126.0316	-3.0
	HMDB0031215	N-Ethylacetamide	C4H9NO	M+K	126.0316	-3.0
	HMDB0172016	(1Z)-3-chloroprop-1-ene-1,2-diol	C3H5ClO2	M+NH4	126.0316	-3.4
	HMDB0172017	1-chloro-2,3-epoxypropanol	C3H5ClO2	M+NH4	126.0316	-3.4
	HMDB0062085	benzonitrile	C7H5N	M+Na	126.0314	-1.7
127.0386	HMDB0011747	Ciliatine	C2H8NO3P	M+H	126.0315	-2.0
	HMDB0013674	1,2,3-Trihydroxybenzene	C6H6O3	M+H	127.0390	-2.9
	HMDB0187592	5-hydroxycyclohex-2-ene-1,4-dione	C6H6O3	M+H	127.0390	-2.9
	HMDB0187591	7-Oxabicyclo[4.1]heptane-2,5-dione	C6H6O3	M+H	127.0390	-2.9
	HMDB0059735	5-Methylfuran-2-carboxylic acid	C6H6O3	M+H	127.0390	-2.9
	HMDB0124831	benzene-1,2,4-triol	C6H6O3	M+H	127.0390	-2.9
	HMDB0034355	5-Hydroxymethyl-2-furancarboxaldehyde	C6H6O3	M+H	127.0390	-2.9
	HMDB0013675	1,3,5-Trihydroxybenzene	C6H6O3	M+H	127.0390	-2.9
	HMDB0030776	Maltol	C6H6O3	M+H	127.0390	-2.9
	HMDB0029750	Methyl 2-furoate	C6H6O3	M+H	127.0390	-2.9
	HMDB0031256	4-Hydroxy-2H-pyran-3-carboxaldehyde	C6H6O3	M+H	127.0390	-2.9
	HMDB0032651	(Z)-Tamarindienal	C6H6O3	M+H	127.0390	-2.9
127.0750	HMDB0033629	xi-4-Hydroxy-4-methyl-2-cyclohexen-1-one	C7H10O2	M+H	127.0754	-2.8
	HMDB0041474	xi-5-Isopropyl-2(5H)-furanone	C7H10O2	M+H	127.0754	-2.8
	HMDB0031222	3-Ethyl-1,2-cyclopentanedione	C7H10O2	M+H	127.0754	-2.8
	HMDB0034835	3-(3-Ethylloxiranyl)-2-propenal	C7H10O2	M+H	127.0754	-2.8
	HMDB0031223	Enol-3-Ethyl-1,2-cyclopentanedione	C7H10O2	M+H	127.0754	-2.8
	HMDB0040445	2-(Ethoxymethyl)furan	C7H10O2	M+H	127.0754	-2.8
	HMDB0037026	3,4-Dimethyl-1,2-cyclopentanedione	C7H10O2	M+H	127.0754	-2.8
	HMDB0037027	3,5-Dimethyl-1,2-cyclopentanedione	C7H10O2	M+H	127.0754	-2.8
	HMDB0034080	3-Methyl-1,2-cyclohexanedione	C7H10O2	M+H	127.0754	-2.8
	HMDB0029582	Methyl sorbate	C7H10O2	M+H	127.0754	-2.8
	HMDB0032067	Allyl crotonate	C7H10O2	M+H	127.0754	-2.8
	HMDB0032333	4-Hydroxy-4-methyl-5-hexenoic acid gamma lactone	C7H10O2	M+H	127.0754	-2.8
127.1114	HMDB0181106	7-Octen-3-one	C8H14O	M+H	127.1117	-2.7
	HMDB0062529	3,5-Dimethyl-1-hexyn-3-ol	C8H14O	M+H	127.1117	-2.7
	HMDB0040151	(2E,4E)-2,4-Octadien-1-ol	C8H14O	M+H	127.1117	-2.7
	HMDB0031197	2,4,4-Trimethylcyclopentanone	C8H14O	M+H	127.1117	-2.7
	HMDB0039769	6-Octenal	C8H14O	M+H	127.1117	-2.7
	HMDB0031301	2-Octen-4-one	C8H14O	M+H	127.1117	-2.7
	HMDB0031591	5-Methyl-5-hepten-2-one	C8H14O	M+H	127.1117	-2.7
	HMDB0030966	(3xi,5Z)-1,5-Octadien-3-ol	C8H14O	M+H	127.1117	-2.7
	HMDB0030961	2-Octenal	C8H14O	M+H	127.1117	-2.7
	HMDB0035915	Sulcatone	C8H14O	M+H	127.1117	-2.7
	HMDB0031309	1-Octen-3-one	C8H14O	M+H	127.1117	-2.7
	HMDB0035242	(S,E)-Filbertone	C8H14O	M+H	127.1117	-2.7
	HMDB0040149	(3E,5Z)-3,5-Octadien-1-ol	C8H14O	M+H	127.1117	-2.7
	HMDB0033547	3-Octen-2-one	C8H14O	M+H	127.1117	-2.7
	HMDB0037152	2-Ethylidenehexanal	C8H14O	M+H	127.1117	-2.7
	HMDB0031590	3-Methyl-3-hepten-2-one	C8H14O	M+H	127.1117	-2.7
	HMDB0163322	7-octen-2-one	C8H14O	M+H	127.1117	-2.7
	HMDB0061945	2-Ethyl-2-hexenal	C8H14O	M+H	127.1117	-2.7
	HMDB0013809	(E)-2-octenal	C8H14O	M+H	127.1117	-2.7
	HMDB0032451	4-Octen-3-one	C8H14O	M+H	127.1117	-2.7
	HMDB0032403	6-Methyl-3-hepten-2-one, trans-	C8H14O	M+H	127.1117	-2.7
	HMDB0039770	(Z)-5-Octenal	C8H14O	M+H	127.1117	-2.7
	HMDB0040146	2,5-Octadien-1-ol	C8H14O	M+H	127.1117	-2.7
	HMDB0035390	5-Octen-2-one	C8H14O	M+H	127.1117	-2.7
128.0105	HMDB0154887	beta-alaninate	C3H6NO2	M+K	128.0108	-2.6
	HMDB0000161	L-Alanine	C3H7NO2	M+K	128.0108	-2.6
	HMDB0061370	L-Alanine	C3H7NO2	M+K	128.0108	-2.6
	HMDB0000056	beta-Alanine	C3H7NO2	M+K	128.0108	-2.6
	HMDB0031219	Ethyl carbamate	C3H7NO2	M+K	128.0108	-2.6

	HMDB0000271	Sarcosine	C3H7NO2	M+K	128.0108	-2.6
	HMDB0001310	D-Alanine	C3H7NO2	M+K	128.0108	-2.6
	HMDB0062251	Alanine	C3H7NO2	M+K	128.0108	-2.6
128.0702	HMDB0187589	2-Cyclohexene-1,4-dione	C6H6O2	M+NH4	128.0706	-3.1
	HMDB0032037	1,3-Benzenediol	C6H6O2	M+NH4	128.0706	-3.1
	HMDB0033002	5-Methyl-2-furancarboxaldehyde	C6H6O2	M+NH4	128.0706	-3.1
	HMDB0031180	(E,E)-2,4-Hexadienedial	C6H6O2	M+NH4	128.0706	-3.1
	HMDB0033127	2-Acetylfuran	C6H6O2	M+NH4	128.0706	-3.1
	HMDB0000957	Pyrocatechol	C6H6O2	M+NH4	128.0706	-3.1
	HMDB0002434	Hydroquinone	C6H6O2	M+NH4	128.0706	-3.1
	HMDB0001084	1-Piperidine-2-carboxylic acid	C6H9NO2	M+H	128.0706	-3.2
	HMDB0062778	1-Piperidine-2-carboxylic acid	C6H9NO2	M+H	128.0706	-3.2
	HMDB0062589	1-piperidine-6-carboxylate	C6H9NO2	M+H	128.0706	-3.2
	HMDB0029434	4-Methylene-2-pyrrolidinecarboxylic acid	C6H9NO2	M+H	128.0706	-3.2
	HMDB0012130	鈇?,3,4,5-Tetrahydro-2-pyridinecarboxylic acid	C6H9NO2	M+H	128.0706	-3.2
	HMDB0059657	鈇?,3,4,5-Tetrahydro-2-pyridinecarboxylic acid	C6H9NO2	M+H	128.0706	-3.2
128.1067	HMDB0029728	2-Ethyl-5-methylfuran	C7H10O	M+NH4	128.1070	-2.2
	HMDB0040277	2-Propylfuran	C7H10O	M+NH4	128.1070	-2.2
	HMDB0029721	2,3,5-Trimethylfuran	C7H10O	M+NH4	128.1070	-2.2
	HMDB0031541	3-Methyl-2-cyclohexen-1-one	C7H10O	M+NH4	128.1070	-2.2
	HMDB0040278	2-Isopropylfuran	C7H10O	M+NH4	128.1070	-2.2
	HMDB0061891	(E,Z)-2,4-Heptadienal	C7H10O	M+NH4	128.1070	-2.2
	HMDB0145117	1-(2-hydroxyethyl)-2,3,4,5-tetrahydropyridin-1-ium	C7H14NO	M+H	128.1070	-2.3
	HMDB0040030	1-(1-Pyrrolidinyl)-2-propanone	C7H13NO	M+H	128.1070	-2.3
	HMDB0031667	Nor-psi-tropine	C7H13NO	M+H	128.1070	-2.3
128.9946	HMDB0041929	Methoxyacetic acid	C3H6O3	M+K	128.9949	-2.0
	HMDB0031232	Monoethyl carbonate	C3H6O3	M+K	128.9949	-2.0
	HMDB0029580	Dimethyl carbonate	C3H6O3	M+K	128.9949	-2.0
	HMDB0144295	2-hydroxypropanoic acid	C3H6O3	M+K	128.9949	-2.0
	HMDB0001051	Glyceraldehyde	C3H6O3	M+K	128.9949	-2.0
	HMDB0000190	L-Lactic acid	C3H6O3	M+K	128.9949	-2.0
	HMDB0000700	Hydroxypropionic acid	C3H6O3	M+K	128.9949	-2.0
	HMDB0001311	D-Lactic acid	C3H6O3	M+K	128.9949	-2.0
	HMDB0001882	Dihydroxyacetone	C3H6O3	M+K	128.9949	-2.0
129.0308	HMDB0062492	L-lactate	C3H5O3	M+K	128.9943	2.3
	HMDB0171200	2-methylpropane-1,2-diol	C4H10O2	M+K	129.0312	-3.4
	HMDB0171201	2-methylpropane-1,3-diol	C4H10O2	M+K	129.0312	-3.4
	HMDB0240297	1,2-butanediol	C4H10O2	M+K	129.0312	-3.4
	HMDB0033007	(2R,3R)-2,3-Butanediol	C4H10O2	M+K	129.0312	-3.4
	HMDB0031320	1,3-Butanediol	C4H10O2	M+K	129.0312	-3.4
	HMDB0030061	1,1-Dimethoxyethane	C4H10O2	M+K	129.0312	-3.4
	HMDB0003156	2,3-Butanediol	C4H10O2	M+K	129.0312	-3.4
	HMDB0031213	2-Ethoxyethanol	C4H10O2	M+K	129.0312	-3.4
129.0543	HMDB0006115	Benzaldehyde	C7H6O	M+Na	129.0311	-2.2
	HMDB0040732	2,7-Oxepanedione	C6H8O3	M+H	129.0546	-2.5
	HMDB0062047	3,4-dimethylloxolane-2,5-dione	C6H8O3	M+H	129.0546	-2.5
	HMDB0031847	2-Ethyl-3,4-dihydroxyfuran	C6H8O3	M+H	129.0546	-2.5
	HMDB0033517	5,6-Dihydro-4-methoxy-2H-pyran-2-one	C6H8O3	M+H	129.0546	-2.5
	HMDB0031306	3-Hydroxy-4,5-dimethyl-2(5H)-furanone	C6H8O3	M+H	129.0546	-2.5
	HMDB0040594	Furaneol	C6H8O3	M+H	129.0546	-2.5
	HMDB0031303	Osmundalactone	C6H8O3	M+H	129.0546	-2.5
	HMDB0038072	xi-5-Acetyltetrahydro-2(3H)-furanone	C6H8O3	M+H	129.0546	-2.5
	HMDB0033285	L-erythro-5-(1-Hydroxyethyl)-2(5H)-furanone	C6H8O3	M+H	129.0546	-2.5
	HMDB0179349	(2Z)-3-(3-methyloxiran-2-yl)prop-2-enoic acid	C6H8O3	M+H	129.0546	-2.5
	HMDB0179348	3-[(1E)-prop-1-en-1-yl]oxirane-2-carboxylic acid	C6H8O3	M+H	129.0546	-2.5
	HMDB0179347	(2Z)-6-hydroxyhexa-2,4-dienoic acid	C6H8O3	M+H	129.0546	-2.5
	HMDB0163704	SCHEMBL144397	C6H8O3	M+H	129.0546	-2.5
	HMDB0173548	2,5-furandimethanol	C6H8O3	M+H	129.0546	-2.5
129.0655	HMDB0038175	2-Acetyloxazole	C5H5NO2	M+NH4	129.0659	-2.7
	HMDB0004230	Pyrrole-2-carboxylic acid	C5H5NO2	M+NH4	129.0659	-2.7
	HMDB0062558	2,6-Piperidinedione, 3-amino-, (3S)-	C5H8N2O2	M+H	129.0659	-2.7
	HMDB0031547	L-Cyclo(alanylglycyl)	C5H8N2O2	M+H	129.0659	-2.7
	HMDB0029874	Squamolone	C5H8N2O2	M+H	129.0659	-2.7
	HMDB0000079	(5s)-dihydrothymine	C5H8N2O2	M+H	129.0659	-2.7
	HMDB0059876	Pantolactone	C7H12O2	M+H	129.0910	-3.1

129.0906	HMDB0166738	3-butyloxirane-2-carbaldehyde	C7H12O2	M+H	129.0910	-3.1
	HMDB0180322	3-(3-ethyloxiran-2-yl)propanal	C7H12O2	M+H	129.0910	-3.1
	HMDB0180323	(2E)-3-(3-ethyloxiran-2-yl)prop-2-en-1-ol	C7H12O2	M+H	129.0910	-3.1
	HMDB0173763	1-methyl-7-oxabicyclo[4.1]heptan-3-ol	C7H12O2	M+H	129.0910	-3.1
	HMDB0173761	3-methylcyclohex-3-ene-1,2-diol	C7H12O2	M+H	129.0910	-3.1
	HMDB0173762	5-methylcyclohex-4-ene-1,3-diol	C7H12O2	M+H	129.0910	-3.1
	HMDB0173760	SCHEMBL14734478	C7H12O2	M+H	129.0910	-3.1
	HMDB0166737	6-Hydroxy-2-heptenal	C7H12O2	M+H	129.0910	-3.1
	HMDB0166736	4-Hydroxyheptenal	C7H12O2	M+H	129.0910	-3.1
	HMDB0166739	(2E)-7-hydroxyhept-2-enal	C7H12O2	M+H	129.0910	-3.1
	HMDB0165097	SCHEMBL132855	C7H12O2	M+H	129.0910	-3.1
	HMDB0165094	3-(Hydroxymethyl)cyclohexanone	C7H12O2	M+H	129.0910	-3.1
	HMDB0165095	3-Hydroxy-3-methylcyclohexan-1-one	C7H12O2	M+H	129.0910	-3.1
	HMDB0165096	SCHEMBL443446	C7H12O2	M+H	129.0910	-3.1
	HMDB0164724	4-Hydroxy-4-methylcyclohexanone	C7H12O2	M+H	129.0910	-3.1
	HMDB0039819	2,4-Dimethyl-2-pentenoic acid	C7H12O2	M+H	129.0910	-3.1
	HMDB0031593	5-Methyl-2,3-hexanedione	C7H12O2	M+H	129.0910	-3.1
	HMDB0033793	4-Heptenoic acid	C7H12O2	M+H	129.0910	-3.1
	HMDB0038962	Ethyl tiglate	C7H12O2	M+H	129.0910	-3.1
	HMDB0031500	Methyl 2E-hexenoate	C7H12O2	M+H	129.0910	-3.1
	HMDB0031484	2-Heptenoic acid	C7H12O2	M+H	129.0910	-3.1
	HMDB0029314	Isopentenyl acetate	C7H12O2	M+H	129.0910	-3.1
	HMDB0031477	3,4-Heptanedione	C7H12O2	M+H	129.0910	-3.1
	HMDB0031476	2,3-Heptanedione	C7H12O2	M+H	129.0910	-3.1
	HMDB0031504	Methyl (Z)-3-hexenoate	C7H12O2	M+H	129.0910	-3.1
	HMDB0031603	Ethyl 4-pentenoate	C7H12O2	M+H	129.0910	-3.1
	HMDB0040214	cis-3-Hexenyl formate	C7H12O2	M+H	129.0910	-3.1
	HMDB0031342	Cyclohexanecarboxylic acid	C7H12O2	M+H	129.0910	-3.1
	HMDB0038271	2-Hexenyl formate	C7H12O2	M+H	129.0910	-3.1
	HMDB0031174	4-Methyl-5-hexanolide	C7H12O2	M+H	129.0910	-3.1
	HMDB0030330	1-Methoxy-3-methylene-2-pentanone	C7H12O2	M+H	129.0910	-3.1
	HMDB0031351	Cyclohexyl formate	C7H12O2	M+H	129.0910	-3.1
	HMDB0040591	Allyl butyrate	C7H12O2	M+H	129.0910	-3.1
	HMDB0029165	1,3-Diacetylpropane	C7H12O2	M+H	129.0910	-3.1
	HMDB0032391	3-Methyl-3-butenyl acetate	C7H12O2	M+H	129.0910	-3.1
	HMDB0032460	4-Pentenyl acetate	C7H12O2	M+H	129.0910	-3.1
	HMDB0031681	Dihydro-5-propyl-2(3H)-furanone	C7H12O2	M+H	129.0910	-3.1
129.1019	HMDB0037837	2-Ethyl-4-methyloxazole	C6H9NO	M+NH4	129.1022	-2.6
	HMDB0040148	Trimethyloxazole	C6H9NO	M+NH4	129.1022	-2.6
	HMDB0039584	5-Imino-2-methyl-1-cyclopenten-1-ol	C6H9NO	M+NH4	129.1022	-2.6
	HMDB0031308	5-Acetyl-3,4-dihydro-2H-pyrrole	C6H9NO	M+NH4	129.1022	-2.6
	HMDB0037863	5-Ethyl-4-methyloxazole	C6H9NO	M+NH4	129.1022	-2.6
	HMDB0031163	N-Acetyl-2,3-dihydro-1H-pyrrole	C6H9NO	M+NH4	129.1022	-2.6
	HMDB0037858	2-Ethyl-5-methyloxazole	C6H9NO	M+NH4	129.1022	-2.6
	HMDB0037838	4-Ethyl-2-methyloxazole	C6H9NO	M+NH4	129.1022	-2.6
129.1270	HMDB0037859	5-Ethyl-2-methyloxazole	C6H9NO	M+NH4	129.1022	-2.6
	HMDB0062076	6-Methylheptan-2-one	C8H16O	M+H	129.1274	-3.0
	HMDB0062072	5-methylheptan-2-one	C8H16O	M+H	129.1274	-3.0
	HMDB0013821	2-Methyl-4-heptanone	C8H16O	M+H	129.1274	-3.0
	HMDB0172314	1-OCTEN-2-OL	C8H16O	M+H	129.1274	-3.0
	HMDB0170962	7-Octen-1-ol	C8H16O	M+H	129.1274	-3.0
	HMDB0061986	2-ethylhexanal	C8H16O	M+H	129.1274	-3.0
	HMDB0061913	3,5-Dimethylcyclohexanol	C8H16O	M+H	129.1274	-3.0
	HMDB0031298	(Z)-5-Octen-1-ol	C8H16O	M+H	129.1274	-3.0
	HMDB0031295	Ethyl pentyl ketone	C8H16O	M+H	129.1274	-3.0
	HMDB0032450	trans-3-Octen-2-ol	C8H16O	M+H	129.1274	-3.0
	HMDB0030030	(R)-Sulcatol	C8H16O	M+H	129.1274	-3.0
	HMDB0031299	(R)-1-Octen-3-ol	C8H16O	M+H	129.1274	-3.0
	HMDB0037181	xi-7-Octen-2-ol	C8H16O	M+H	129.1274	-3.0
	HMDB0029574	2,5-Diethyltetrahydrofuran	C8H16O	M+H	129.1274	-3.0
	HMDB0001140	Octanal	C8H16O	M+H	129.1274	-3.0
	HMDB0035768	(E)-3-Octen-1-ol	C8H16O	M+H	129.1274	-3.0
	HMDB0035231	(Z)-3-Octen-1-ol	C8H16O	M+H	129.1274	-3.0
	HMDB0031296	(E)-2-Octen-1-ol	C8H16O	M+H	129.1274	-3.0
	HMDB0061912	3,4-Dimethylcyclohexanol	C8H16O	M+H	129.1274	-3.0

	HMDB0032402	2-Methyl-3-heptanone	C8H16O	M+H	129.1274	-3.0
	HMDB0031294	2-Octanone	C8H16O	M+H	129.1274	-3.0
	HMDB0031300	(E)-2-Octen-4-ol	C8H16O	M+H	129.1274	-3.0
130.0495	HMDB0032994	3-Hydroxy-2H-pyran-2-one	C5H4O3	M+NH4	130.0499	-2.8
	HMDB0039437	2,3-Dihydroxy-2,4-cyclopentadien-1-one	C5H4O3	M+NH4	130.0499	-2.8
	HMDB0000617	2-Furoic acid	C5H4O3	M+NH4	130.0499	-2.8
	HMDB0000444	3-Furoic acid	C5H4O3	M+NH4	130.0499	-2.8
	HMDB0062585	(3R,5S)-1-pyrroline-3-hydroxy-5-carboxylic acid	C5H7NO3	M+H	130.0499	-2.8
	HMDB0000267	Pyroglutamic acid	C5H7NO3	M+H	130.0499	-2.8
	HMDB0000805	Pyrrolidonecarboxylic acid	C5H7NO3	M+H	130.0499	-2.8
	HMDB0060262	Pyrrolidonecarboxylic acid	C5H7NO3	M+H	130.0499	-2.8
	HMDB0001369	Pyrroline hydroxycarboxylic acid	C5H7NO3	M+H	130.0499	-2.8
	HMDB0001843	N-Acryloylglycine	C5H7NO3	M+H	130.0499	-2.8
	HMDB0002234	1-Pyrroline-4-hydroxy-2-carboxylate	C5H7NO3	M+H	130.0499	-2.8
	HMDB0061093	dimethadione	C5H7NO3	M+H	130.0499	-2.8
130.0648	HMDB0034244	Isoquinoline	C9H7N	M+H	130.0651	-2.5
	HMDB0011664	3-Methylene-indolenine	C9H7N	M+H	130.0651	-2.5
	HMDB0033731	Quinoline	C9H7N	M+H	130.0651	-2.5
130.0859	HMDB0187593	1,4-Cyclohexanedione	C6H8O2	M+NH4	130.0863	-2.7
	HMDB0179339	3-[(1E)-prop-1-en-1-yl]oxirane-2-carbaldehyde	C6H8O2	M+NH4	130.0863	-2.7
	HMDB0179337	(2Z,4E)-hexa-2,4-dienoic acid	C6H8O2	M+NH4	130.0863	-2.7
	HMDB0179340	(2Z)-3-(3-methyloxiran-2-yl)prop-2-enal	C6H8O2	M+NH4	130.0863	-2.7
	HMDB0179338	(2Z,4E)-6-hydroxyhexa-2,4-dienal	C6H8O2	M+NH4	130.0863	-2.7
	HMDB0001164	trans-1,2-Dihydrobenzene-1,2-diol	C6H8O2	M+NH4	130.0863	-2.7
	HMDB0039778	xi-3,5-Dimethyl-2(5H)-furanone	C6H8O2	M+NH4	130.0863	-2.7
	HMDB0033569	Soyualdehyde	C6H8O2	M+NH4	130.0863	-2.7
	HMDB0031344	1,2-Cyclohexanedione	C6H8O2	M+NH4	130.0863	-2.7
	HMDB0034247	2-(Methoxymethyl)furan	C6H8O2	M+NH4	130.0863	-2.7
	HMDB0032233	2,5-Dimethyl-3(2H)-furanone	C6H8O2	M+NH4	130.0863	-2.7
	HMDB0029581	(2E,4E)-2,4-Hexadienoic acid	C6H8O2	M+NH4	130.0863	-2.7
	HMDB0031543	3-Methyl-1,2-cyclopentanedione	C6H8O2	M+NH4	130.0863	-2.7
	HMDB0031759	(E)-4-Oxo-2-hexen-1-al	C6H8O2	M+NH4	130.0863	-2.7
	HMDB0040260	5,5-Dimethyl-2(5H)-furanone	C6H8O2	M+NH4	130.0863	-2.7
	HMDB0029444	56633-75-1	C6H11NO2	M+H	130.0863	-2.7
	HMDB0094697	piperidine-1-carboxylic acid	C6H11NO2	M+H	130.0863	-2.7
	HMDB0059649	3-Acetamidobutanal	C6H11NO2	M+H	130.0863	-2.7
	HMDB0015212	Vigabatrin	C6H11NO2	M+H	130.0863	-2.7
	HMDB0029435	L-trans-4-Methyl-2-pyrrolidinecarboxylic acid	C6H11NO2	M+H	130.0863	-2.7
	HMDB0005960	D-Pipecolic acid	C6H11NO2	M+H	130.0863	-2.7
	HMDB0004226	N4-Acetylaminobutanal	C6H11NO2	M+H	130.0863	-2.7
	HMDB0000716	L-Pipecolic acid	C6H11NO2	M+H	130.0863	-2.7
	HMDB0000070	Pipecolic acid	C6H11NO2	M+H	130.0863	-2.7
	HMDB0062767	Pipecolic acid	C6H11NO2	M+H	130.0863	-2.7
	HMDB0062225	(2E)-Decenoyl-ACP	C6H11NO2	M+H	130.0863	-2.7
	HMDB0094696	N-Methyl-L-proline	C6H11NO2	M+H	130.0863	-2.7
130.1223	HMDB0062028	3-Ethylcyclopentanone	C7H12O	M+NH4	130.1226	-2.6
	HMDB0061957	(Z)-2-Heptenal	C7H12O	M+NH4	130.1226	-2.6
	HMDB0031486	3-Hepten-2-one	C7H12O	M+NH4	130.1226	-2.6
	HMDB0031540	4-Methylcyclohexanone	C7H12O	M+NH4	130.1226	-2.6
	HMDB0033667	(R)-3-Methylcyclohexanone	C7H12O	M+NH4	130.1226	-2.6
	HMDB0033827	(2E)-2-Heptenal	C7H12O	M+NH4	130.1226	-2.6
	HMDB0031539	2-Methylcyclohexanone	C7H12O	M+NH4	130.1226	-2.6
	HMDB0031487	(E)-4-Hepten-2-one	C7H12O	M+NH4	130.1226	-2.6
	HMDB0034372	xi-3-Methyl-3-cyclohexen-1-ol	C7H12O	M+NH4	130.1226	-2.6
	HMDB0040339	2,5-Heptadien-1-ol	C7H12O	M+NH4	130.1226	-2.6
	HMDB0031550	5-Methyl-3-hexen-2-one	C7H12O	M+NH4	130.1226	-2.6
	HMDB0031483	(Z)-4-Heptenal	C7H12O	M+NH4	130.1226	-2.6
	HMDB0061994	2-methyl-2-hexenal	C7H12O	M+NH4	130.1226	-2.6
	HMDB0061985	2-ethylcyclopentan-1-one	C7H12O	M+NH4	130.1226	-2.6
	HMDB0032301	trans-2-trans-4-Heptadien-1-ol	C7H12O	M+NH4	130.1226	-2.6
	HMDB0031551	5-Methyl-5-hexen-2-one	C7H12O	M+NH4	130.1226	-2.6
	HMDB0031488	2-Hepten-4-one	C7H12O	M+NH4	130.1226	-2.6
	HMDB0145092	2-(piperidin-1-yl)ethanol	C7H15NO	M+H	130.1226	-2.6
	HMDB0094705	6-methylhept-1-ene	C8H16	M+NH4	130.1590	-2.5
	HMDB0032449	1-Octene	C8H16	M+NH4	130.1590	-2.5

130.1587	HMDB0061904	(E)-2-Octene	C8H16	M+NH4	130.1590	-2.5
	HMDB0061903	(Z)-2-Octene	C8H16	M+NH4	130.1590	-2.5
	HMDB0061906	(E)-3-Octene	C8H16	M+NH4	130.1590	-2.5
	HMDB0061905	(Z)-3-Octene	C8H16	M+NH4	130.1590	-2.5
	HMDB0061907	3-Methylenheptane	C8H16	M+NH4	130.1590	-2.5
	HMDB0061909	3-Methyl-3-heptene	C8H16	M+NH4	130.1590	-2.5
	HMDB0061910	(E)-4-Methyl-2-heptene	C8H16	M+NH4	130.1590	-2.5
	HMDB0061908	3-Methyl-1-heptene	C8H16	M+NH4	130.1590	-2.5
	HMDB0061911	4-Methyl-3-heptene	C8H16	M+NH4	130.1590	-2.5
131.0101	HMDB0000131	Glycerol	C3H8O3	M+K	131.0105	-3.1
	HMDB0003364	Quinone	C6H4O2	M+Na	131.0103	-1.9
	HMDB0012133	1,2-Benzoquinone	C6H4O2	M+Na	131.0103	-1.9
131.0529	HMDB0037493	S-2-Propenyl propanethioate	C6H10OS	M+H	131.0525	3.0
	HMDB0031370	2-[(Methylthio)methyl]-2-butenal	C6H10OS	M+H	131.0525	3.0
	HMDB0040238	2-Ethylidihydro-3(2H)-thiophenone	C6H10OS	M+H	131.0525	3.0
	HMDB0041306	Methyl 2-(methylthio)butyrate	C6H12O2S	M+H-H2O	131.0531	-1.5
	HMDB0032271	Ethyl 3-mercaptoputyrate	C6H12O2S	M+H-H2O	131.0531	-1.5
	HMDB0032495	Propyl 2-mercaptopropionate	C6H12O2S	M+H-H2O	131.0531	-1.5
	HMDB0032410	Methyl 3-(methylthio)butanoate	C6H12O2S	M+H-H2O	131.0531	-1.5
	HMDB0036193	3-Mercapto-3-methylbutyl formate	C6H12O2S	M+H-H2O	131.0531	-1.5
	HMDB0040413	Ethyl 3-(methylthio)propanoate	C6H12O2S	M+H-H2O	131.0531	-1.5
	HMDB0031717	3-(Methylthio)propyl acetate	C6H12O2S	M+H-H2O	131.0531	-1.5
	HMDB0038299	Methylthiomethyl butyrate	C6H12O2S	M+H-H2O	131.0531	-1.5
	HMDB0039653	2,4,6-Trimethyl-1,3,5-dioxathiane	C6H12O2S	M+H-H2O	131.0531	-1.5
	HMDB0037619	Methyl 4-(methylthio)butyrate	C6H12O2S	M+H-H2O	131.0531	-1.5
	HMDB0167024	acetyl(2-hydroxypropyl)methylsulfanium	C6H13O2S	M+H-H2O	131.0531	-1.5
	HMDB0167027	acetyl(3-hydroxypropyl)methylsulfanium	C6H13O2S	M+H-H2O	131.0531	-1.5
	HMDB0167030	(2-hydroxyacetyl)(methyl)propylsulfanium	C6H13O2S	M+H-H2O	131.0531	-1.5
	HMDB0173817	SCHEMBL12997424	C6H13O2S	M+H-H2O	131.0531	-1.5
131.0699	HMDB0162571	SCHEMBL13481223	C6H10O3	M+H	131.0703	-2.8
	HMDB0163359	(4Z)-6-hydroxyhex-4-enoic acid	C6H10O3	M+H	131.0703	-2.8
	HMDB0163361	3-(3-methyloxiran-2-yl)propanoic acid	C6H10O3	M+H	131.0703	-2.8
	HMDB0163360	SCHEMBL667341	C6H10O3	M+H	131.0703	-2.8
	HMDB0163362	AKO06375916	C6H10O3	M+H	131.0703	-2.8
	HMDB0163706	(3Z)-5-hydroxy-3-(hydroxymethyl)pent-3-en-2-one	C6H10O3	M+H	131.0703	-2.8
	HMDB0169698	SCHEMBL6488	C6H10O3	M+H	131.0703	-2.8
	HMDB0169697	(2E)-3-(hydroxymethyl)pent-2-enoic acid	C6H10O3	M+H	131.0703	-2.8
	HMDB0169696	(2Z)-4-hydroxy-3-methylpent-2-enoic acid	C6H10O3	M+H	131.0703	-2.8
	HMDB0169669	3-ethyl-3-methyl-oxiranecarboxylic acid	C6H10O3	M+H	131.0703	-2.8
	HMDB0169670	SCHEMBL1645858	C6H10O3	M+H	131.0703	-2.8
	HMDB0169668	AKO238761	C6H10O3	M+H	131.0703	-2.8
	HMDB0169667	SCHEMBL159549	C6H10O3	M+H	131.0703	-2.8
	HMDB0165593	(2Z)-5-hydroxy-2-methylpent-2-enoic acid	C6H10O3	M+H	131.0703	-2.8
	HMDB0165590	(2Z)-2-(hydroxymethyl)pent-2-enoic acid	C6H10O3	M+H	131.0703	-2.8
	HMDB0165591	(2Z)-4-hydroxy-2-methylpent-2-enoic acid	C6H10O3	M+H	131.0703	-2.8
	HMDB0165592	SCHEMBL2684392	C6H10O3	M+H	131.0703	-2.8
	HMDB0163708	(3Z)-1,5-dihydroxy-3-methylpent-3-en-2-one	C6H10O3	M+H	131.0703	-2.8
	HMDB0163705	3-(hydroxymethyl)-4-oxopentanal	C6H10O3	M+H	131.0703	-2.8
	HMDB0163707	1-[3-(hydroxymethyl)-2-methyloxiran-2-yl]ethan-1-one	C6H10O3	M+H	131.0703	-2.8
	HMDB0041602	Methyl levulinate	C6H10O3	M+H	131.0703	-2.8
	HMDB0012882	Adipate semialdehyde	C6H10O3	M+H	131.0703	-2.8

	HMDB0000491	(S)-3-methyl-2-oxopentanoate	C6H10O3	M+H	131.0703	-2.8
	HMDB0031214	5-Ethoxy-4,5-dihydro-2(3H)furanone	C6H10O3	M+H	131.0703	-2.8
	HMDB0033698	Acetoin acetate	C6H10O3	M+H	131.0703	-2.8
	HMDB0031216	Ethyl acetoacetate	C6H10O3	M+H	131.0703	-2.8
	HMDB0031218	Ethyl acetoacetate	C6H10O3	M+H	131.0703	-2.8
	HMDB0033286	Sherry lactone	C6H10O3	M+H	131.0703	-2.8
	HMDB0033302	(4S,6S)-3,4,5,6-Tetrahydro-4-hydroxy-6-methyl-2H-pyran-2-one	C6H10O3	M+H	131.0703	-2.8
	HMDB0010717	3-Oxohexanoic acid	C6H10O3	M+H	131.0703	-2.8
	HMDB0006024	Mevalonolactone	C6H10O3	M+H	131.0703	-2.8
	HMDB0001864	2-Ketohexanoic acid	C6H10O3	M+H	131.0703	-2.8
	HMDB0000408	2-Methyl-3-ketovaleric acid	C6H10O3	M+H	131.0703	-2.8
	HMDB0061881	4-Acetylbutyrate	C6H10O3	M+H	131.0703	-2.8
	HMDB0163716	3-Methyl-4-oxopentanoic acid	C6H10O3	M+H	131.0703	-2.8
	HMDB0000695	Ketoleucine	C6H10O3	M+H	131.0703	-2.8
131.0835	HMDB0061897	(Z)-1,3-Octadiene	C8H12	M+Na	131.0831	2.9
131.0888	HMDB0031537	3-Methylcyclohexanethiol	C7H14S	M+H	131.0889	-0.7
131.1063	HMDB0166741	(2E)-hept-2-ene-1,6-diol	C7H14O2	M+H	131.1067	-2.7
	HMDB0166742	3-Butyloxirane-2-methanol	C7H14O2	M+H	131.1067	-2.7
	HMDB0166743	(2E)-hept-2-ene-1,7-diol	C7H14O2	M+H	131.1067	-2.7
	HMDB0166740	SCHEMBL32814	C7H14O2	M+H	131.1067	-2.7
	HMDB0039618	Propyl butyrate	C7H14O2	M+H	131.1067	-2.7
	HMDB0035238	Methyl hexanoate	C7H14O2	M+H	131.1067	-2.7
	HMDB0036237	Methyl 2-methylpentanoate	C7H14O2	M+H	131.1067	-2.7
	HMDB0030052	Butyl propionate	C7H14O2	M+H	131.1067	-2.7
	HMDB0031600	2-Pentanol acetate	C7H14O2	M+H	131.1067	-2.7
	HMDB0036238	Methyl 4-methylpentanoate	C7H14O2	M+H	131.1067	-2.7
	HMDB0031594	2-Methylhexanoic acid	C7H14O2	M+H	131.1067	-2.7
	HMDB0031528	Isopentyl acetate	C7H14O2	M+H	131.1067	-2.7
	HMDB0033745	Ethyl 2-methylbutyrate	C7H14O2	M+H	131.1067	-2.7
	HMDB0030028	Ethyl isovalerate	C7H14O2	M+H	131.1067	-2.7
	HMDB0038227	Isopropyl 2-methylpropanoate	C7H14O2	M+H	131.1067	-2.7
	HMDB0034239	2-Methylpropyl propanoate	C7H14O2	M+H	131.1067	-2.7
	HMDB0032204	cis- and trans-2-Isopropyl-4-methyl-1,3-dioxolane	C7H14O2	M+H	131.1067	-2.7
	HMDB0032874	Hexyl formate	C7H14O2	M+H	131.1067	-2.7
	HMDB0040297	Ethyl pentanoate	C7H14O2	M+H	131.1067	-2.7
	HMDB0039619	Isopropyl butyrate	C7H14O2	M+H	131.1067	-2.7
	HMDB0036209	Propyl 2-methylpropanoate	C7H14O2	M+H	131.1067	-2.7
	HMDB0039095	Pentyl acetate	C7H14O2	M+H	131.1067	-2.7
	HMDB0031595	5-Methylhexanoic acid	C7H14O2	M+H	131.1067	-2.7
	HMDB0034166	2-Methylbutyl acetate	C7H14O2	M+H	131.1067	-2.7
	HMDB0000666	Heptanoic acid	C7H14O2	M+H	131.1067	-2.7
131.1177	HMDB0031702	1-Piperidinecarboxaldehyde	C6H11NO	M+NH4	131.1179	-1.4
	HMDB0031199	2,5-Dihydro-2,4,5-trimethyloxazole	C6H11NO	M+NH4	131.1179	-1.4
	HMDB0037293	2-Acetylpyrrolidine	C6H11NO	M+NH4	131.1179	-1.4
	HMDB0062769	Epsilon-caprolactam	C6H11NO	M+NH4	131.1179	-1.4
	HMDB0002064	N-Acetylputrescine	C6H14N2O	M+H	131.1179	-1.4
	HMDB0060268	N-Acetylputrescine	C6H14N2O	M+H	131.1179	-1.4
132.0652	HMDB0031859	Norfuraneol	C5H6O3	M+NH4	132.0655	-2.4
	HMDB0060461	cis-Acetylacrylate	C5H6O3	M+NH4	132.0655	-2.4
	HMDB0000783	Propionylglycine	C5H9NO3	M+H	132.0655	-2.4
	HMDB0061880	N-Acetyl-beta-alanine	C5H9NO3	M+H	132.0655	-2.4
	HMDB0006272	5-Amino-2-oxopentanoic acid	C5H9NO3	M+H	132.0655	-2.4
	HMDB0006055	4-Hydroxy-L-proline	C5H9NO3	M+H	132.0655	-2.4
	HMDB0002113	3-Hydroxy-L-proline	C5H9NO3	M+H	132.0655	-2.4
	HMDB0000766	N-Acetyl-L-alanine	C5H9NO3	M+H	132.0655	-2.4
	HMDB0000725	4-Hydroxyproline	C5H9NO3	M+H	132.0655	-2.4
	HMDB0036576	4-Hydroxyproline	C5H9NO3	M+H	132.0655	-2.4
	HMDB0002104	L-Glutamic gamma-semialdehyde	C5H9NO3	M+H	132.0655	-2.4
	HMDB0059659	Trans-3-hydroxy-L-proline	C5H9NO3	M+H	132.0655	-2.4
	HMDB0240251	cis-4-Hydroxyproline	C5H9NO3	M+H	132.0655	-2.4
	HMDB0060460	cis-4-Hydroxy-D-proline	C5H9NO3	M+H	132.0655	-2.4
	HMDB0001149	5-Aminolevulinic acid	C5H9NO3	M+H	132.0655	-2.4
	HMDB0000076	Dihydrouracil	C4H6N2O2	M+NH4	132.0768	-2.6
	HMDB0003646	N-Methylhydantoin	C4H6N2O2	M+NH4	132.0768	-2.6

132.0764	HMDB0060245	L-3-Cyanoalanine	C4H6N2O2	M+NH4	132.0768	-2.6
	HMDB0013222	Beta-Guanidinopropionic acid	C4H9N3O2	M+H	132.0768	-2.7
	HMDB0000064	Creatine	C4H9N3O2	M+H	132.0768	-2.7
132.1015	HMDB0169664	(E)-3-Methyl-2-pentenoic acid	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0169695	(Z)-3-methyl-2-pentenoic acid	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0179342	(4E)-3-hydroxyhex-4-enal	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0179343	(4E)-2-hydroxyhex-4-enal	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0179341	(4E)-6-hydroxyhex-4-enal	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0179344	cis-2,4-hexadien-1,6-diol	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0179345	{3-[(1E)-prop-1-en-1-yl]oxiran-2-yl}methanol	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0179346	(2Z)-3-(3-methyloxiran-2-yl)prop-2-en-1-ol	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0179351	4-Hexenoic acid	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0165582	(2Z)-4-hydroxy-2-methylpent-2-enal	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0165583	2-Methyl-3-ethyloxirane-2-carbaldehyde	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0163350	(Z)-hex-4-enoic acid	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0163351	(4Z)-6-hydroxyhex-4-enal	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0163354	(4Z)-2-hydroxyhex-4-enal	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0163352	(4Z)-3-hydroxyhex-4-enal	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0163353	3-(3-methyloxiran-2-yl)propanal	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0163703	(3Z)-5-hydroxy-3-methylpent-3-en-2-one	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0163702	Pentanal, 3-methyl-4-oxo-	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0165584	(2Z)-5-hydroxy-2-methylpent-2-enal	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0039581	Ethyl crotonate	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0010719	Isohydrosorbic acid	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0031561	4-Methyl-2-pentenoic acid	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0031492	3,4-Hexanedione	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0165581	(2Z)-2-(hydroxymethyl)pent-2-enal	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0033568	5-Oxohexanal	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0060476	epsilon-Caprolactone	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0032490	Prenyl formate	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0031501	3-Hexenoic acid	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0031560	2-Methyl-2-pentenoic acid	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0031491	2,3-Hexanedione	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0031559	4-Methyl-2,3-pentanedione	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0031562	2-Methyl-3-pentenoic acid	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0031158	2-Methyl-4-pentenoic acid	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0003843	Gamma-Caprolactone	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0029487	Allyl propionate	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0240384	4-Hydroxyhexanal	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0000453	delta-Hexanolactone	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0061929	Dihydro-4,4-dimethyl-2(3H)-furanone	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0040328	Methyl 4-pentenoate	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0062135	methyl (2E)-2-methylbut-2-enoate	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0061965	1-methyl-2,3-dioxabicyclo[2.2.1]heptane	C6H10O2	M+NH4	132.1019	-3.1
	HMDB0036382	6-Deoxyfagomine	C6H13NO2	M+H	132.1019	-3.1
	HMDB0003640	Beta-Leucine	C6H13NO2	M+H	132.1019	-3.1
	HMDB0029168	3-Aminocaproic acid	C6H13NO2	M+H	132.1019	-3.1
	HMDB0013773	D-Leucine	C6H13NO2	M+H	132.1019	-3.1
	HMDB0001645	L-Norleucine	C6H13NO2	M+H	132.1019	-3.1
	HMDB0240479	Alanine betaine	C6H13NO2	M+H	132.1019	-3.1
	HMDB0033923	erythro-Isoleucine	C6H13NO2	M+H	132.1019	-3.1
	HMDB0000687	L-Leucine	C6H13NO2	M+H	132.1019	-3.1
	HMDB0062203	L-Leucine	C6H13NO2	M+H	132.1019	-3.1
	HMDB0000557	L-Alloisoleucine	C6H13NO2	M+H	132.1019	-3.1
	HMDB0001901	Aminocaproic acid	C6H13NO2	M+H	132.1019	-3.1
	HMDB0000172	L-Isoleucine	C6H13NO2	M+H	132.1019	-3.1
	HMDB0171681	SCHEMBL1266	C6H13NO2	M+H	132.1019	-3.1
	HMDB0171682	N-(2-methylpropyl)glycolamide	C6H13NO2	M+H	132.1019	-3.1
	HMDB0061716	N-methylvaline	C6H13NO2	M+H	132.1019	-3.1
	HMDB0171680	SCHEMBL311743	C6H13NO2	M+H	132.1019	-3.1
	HMDB0168722	N,N-diethyl-2-oxoethanamine oxide	C6H13NO2	M+H	132.1019	-3.1
	HMDB0168719	SCHEMBL63485	C6H13NO2	M+H	132.1019	-3.1
	HMDB0168720	2-[ethyl(1-hydroxyethyl)amino]acetaldehyde	C6H13NO2	M+H	132.1019	-3.1
	HMDB0168721	SCHEMBL124646	C6H13NO2	M+H	132.1019	-3.1
	HMDB0145163	2-hydroxy-3-(propylamino)propanal	C6H13NO2	M+H	132.1019	-3.1

	HMDB0144645	N,N-Diethylglycine	C6H13NO2	M+H	132.1019	-3.1
	HMDB0060650	N-(2-Hydroxyethyl)-morpholine	C6H13NO2	M+H	132.1019	-3.1
	HMDB0062052	4-(dimethylamino)butanoic acid	C6H13NO2	M+H	132.1019	-3.1
132.1499	HMDB0011634	Norspermidine	C6H17N3	M+H	132.1495	2.8
133.0314	HMDB0059667	3-Methyl sulfolene	C5H8O2S	M+H	133.0318	-2.8
	HMDB0182893	[(1E)-2-carboxyeth-1-en-1-yl]dimethylsulfonium	C5H9O2S	M+H	133.0318	-2.8
133.0492	HMDB0154760	alpha-keto-beta-methyl-gamma-hydroxy-butyric acid	C5H8O4	M+H	133.0495	-2.5
	HMDB0006855	(S)-2-Acetolactate	C5H8O4	M+H	133.0495	-2.5
	HMDB0001844	(S)-methylsuccinic acid	C5H8O4	M+H	133.0495	-2.5
	HMDB0145654	SCHEMBL17123851	C5H8O4	M+H	133.0495	-2.5
	HMDB0040531	2-Hydroxy-4-oxopentanoic acid	C5H8O4	M+H	133.0495	-2.5
	HMDB0033958	2-Deoxy-L-ribono-1,4-lactone	C5H8O4	M+H	133.0495	-2.5
	HMDB0029884	2-C-Methyl-1,4-erythrano-D-lactone	C5H8O4	M+H	133.0495	-2.5
	HMDB0154759	3-Hydroxy-3-methyl-2-oxobutanoic acid	C5H8O4	M+H	133.0495	-2.5
	HMDB0006833	2-Acetolactate	C5H8O4	M+H	133.0495	-2.5
	HMDB0002001	Dimethylmalonic acid	C5H8O4	M+H	133.0495	-2.5
	HMDB0000622	Ethylmalonic acid	C5H8O4	M+H	133.0495	-2.5
	HMDB0000576	Monoethyl malonic acid	C5H8O4	M+H	133.0495	-2.5
	HMDB0000661	Glutaric acid	C5H8O4	M+H	133.0495	-2.5
133.0604	HMDB0240339	maleamate	C4H4NO3	M+NH4	133.0608	-2.8
	HMDB0012265	N-Carbamoylsarcosine	C4H8N2O3	M+H	133.0608	-2.8
	HMDB0011733	Glycyl-glycine	C4H8N2O3	M+H	133.0608	-2.8
	HMDB0062812	Ureidopropionic acid	C4H8N2O3	M+H	133.0608	-2.8
	HMDB0000026	Ureidopropionic acid	C4H8N2O3	M+H	133.0608	-2.8
	HMDB0033780	D-Asparagine	C4H8N2O3	M+H	133.0608	-2.8
	HMDB0000168	L-Asparagine	C4H8N2O3	M+H	133.0608	-2.8
133.0644	HMDB0003441	Cinnamaldehyde	C9H8O	M+H	133.0648	-2.9
	HMDB0060671	Atropaldehyde	C9H8O	M+H	133.0648	-2.9
	HMDB0059847	2-Methylcumarone	C9H8O	M+H	133.0648	-2.9
	HMDB0059602	Indanone	C9H8O	M+H	133.0648	-2.9
	HMDB0032072	(Z)-Cinnamaldehyde	C9H8O	M+H	133.0648	-2.9
133.0855	HMDB0061652	(S)-3-hydroxyhexanoic acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0171222	4-hydroxy-3-methylbutyl formate	C6H12O3	M+H	133.0859	-3.2
	HMDB0165043	5-hydroxy-3-methylpentanoic acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0165041	4-hydroxy-3-methyl-valeric acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0165042	3-hydroxymethyl-valeric acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0163681	3,6-dihydroxyhexan-2-one	C6H12O3	M+H	133.0859	-3.2
	HMDB0163682	1,6-dihydroxy-2-hexanone	C6H12O3	M+H	133.0859	-3.2
	HMDB0163680	SCHEMBL5464	C6H12O3	M+H	133.0859	-3.2
	HMDB0163679	5,6-dihydroxyhexan-2-one	C6H12O3	M+H	133.0859	-3.2
	HMDB0161115	4-hydroxy-4-methylpentanoic acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0161116	5-hydroxy-4-methylpentanoic acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0040409	Ethyl 3-hydroxybutyrate	C6H12O3	M+H	133.0859	-3.2
	HMDB0033851	4,4-Dimethoxy-2-butanone	C6H12O3	M+H	133.0859	-3.2
	HMDB0010718	(R)-3-Hydroxyhexanoic acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0001975	2-Ethyl-2-Hydroxybutyric acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0001624	2-Hydroxycaproic acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0000746	Hydroxyisocaproic acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0000665	Leucinic acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0000624	D-Leucic acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0000525	5-Hydroxyhexanoic acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0000409	(5R)-5-Hydroxyhexanoic acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0000317	2-Hydroxy-3-methylpentanoic acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0032456	Paraldehyde	C6H12O3	M+H	133.0859	-3.2
	HMDB0032158	(+/-)-1-Acetoxy-1-ethoxyethane	C6H12O3	M+H	133.0859	-3.2
	HMDB0059770	Threo-3-Hydroxy-2-methylbutyric acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0041844	Butoxyacetic acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0029166	2-Methyl-3-hydroxyvaleric acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0165040	3-hydroxy-3-methylpentanoic acid	C6H12O3	M+H	133.0859	-3.2
	HMDB0012843	6-Hydroxyhexanoic acid	C6H12O3	M+H	133.0859	-3.2
133.1008	HMDB0029641	p-Mentha-1,3,5,8-tetraene	C10H12	M+H	133.1012	-2.8
	HMDB0061996	(2-methylprop-2-en-1-yl)benzene	C10H12	M+H	133.1012	-2.8
	HMDB0062046	4-ethenyl-1,2-dimethylbenzene	C10H12	M+H	133.1012	-2.8
	HMDB0062142	1-methyl-2-(prop-1-en-2-yl)benzene	C10H12	M+H	133.1012	-2.8
133.1040	HMDB0032303	2-Heptanethiol	C7H16S	M+H	133.1045	2.7

133.1047	HMDB0032304	Heptane-1-thiol	C7H16S	M+H	133.1045	2.7
134.0267	HMDB0062164	Thioproline	C4H7NO2S	M+H	134.0270	-2.4
134.0444	HMDB0000176	Maleic acid	C4H4O4	M+NH4	134.0448	-2.8
	HMDB0187641	SCHEMBL127359	C4H4O4	M+NH4	134.0448	-2.8
	HMDB0000134	Fumaric acid	C4H4O4	M+NH4	134.0448	-2.8
	HMDB0161155	AC1N37K4	C4H6NO4	M+H	134.0448	-2.9
	HMDB0159995	SCHEMBL51875	C4H7NO4	M+H	134.0448	-2.9
	HMDB0006483	D-Aspartic acid	C4H7NO4	M+H	134.0448	-2.9
	HMDB0011753	Iminodiacetic acid	C4H7NO4	M+H	134.0448	-2.9
	HMDB0000191	L-Aspartic acid	C4H7NO4	M+H	134.0448	-2.9
134.0808	HMDB0129097	4-hydroxy-2-methylbut-2-enoic acid	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0003771	2-Methylacetoacetic acid	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0132477	2-(hydroxymethyl)but-2-enoic acid	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0168839	2-HYDROXYETHYL ACRYLATE	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0177210	4-hydroxytiglic acid	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0177209	2-Hydroxymethyl-trans-crotonsaure	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0169666	SCHEMBL4558754	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0168838	Ethyl 2,3-epoxypropanoate	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0129098	2,3-dimethyloxirane-2-carboxylic acid	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0129096	(2Z)-2-(hydroxymethyl)but-2-enoic acid	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0128943	(2E)-4-hydroxy-3-methylbut-2-enoic acid	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0128917	dimethyloxirane-2-carboxylic acid	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0128916	4-hydroxy-3-methylbut-2-enoic acid	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0012233	Glutarate semialdehyde	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0031643	Ethyl pyruvate	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0034466	Acetoxyacetone	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0029172	2-Methylacetoacetic acid	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0001865	2-Oxovaleric acid	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0000310	Methylacetoacetic acid	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0000019	alpha-Ketoisovaleric acid	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0000720	Levulinic acid	C5H8O3	M+NH4	134.0812	-2.7
	HMDB0032356	N-Lactoyl ethanolamine	C5H11NO3	M+H	134.0812	-2.8
	HMDB0039499	1,4-Dideoxy-1,4-imino-D-ribitol	C5H11NO3	M+H	134.0812	-2.8
	HMDB0171727	4-amino-4-methoxybutanoic acid	C5H11NO3	M+H	134.0812	-2.8
	HMDB0031658	L-2-Amino-5-hydroxypentanoic acid	C5H11NO3	M+H	134.0812	-2.8
134.1172	HMDB0163678	6-hydroxyhexan-2-one	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0165585	(2Z)-2-methylpent-2-ene-1,4-diol	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0163355	(4Z)-hex-4-ene-1,2-diol	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0185846	4-(hydroxymethyl)-2-pentanone	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0176891	(E)-2-Hexene-1,6-diol	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0176889	SCHEMBL58684	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0176888	2-Hexene-1,4-diol	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0176890	(3-propyloxiran-2-yl)methanol	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0165589	SCHEMBL63629	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0165588	2-propylidene-1,3-propanediol	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0165586	(2Z)-2-methylpent-2-ene-1,5-diol	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0163715	1567-93-7	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0163356	(2Z)-hex-2-ene-1,6-diol	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0163357	(4Z)-hex-4-ene-1,3-diol	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0163358	3-(3-methyloxiranyl)propan-1-ol	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0000689	Isocaproic acid	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0031246	2-Methylpropyl acetate	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0031325	n-Butyl acetate	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0031248	Ethyl 2-methylpropanoate	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0033889	Ethyl butyrate	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0031207	Methyl pentanoate	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0030059	Propyl propionate	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0040279	2,4,5-Trimethyl-1,3-dioxolane	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0033774	3-Methylpentanoic acid	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0034163	3-Methylbutyl formate	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0031511	Diacetone alcohol	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0031580	2-Methylpentanoic acid	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0030027	Methyl 3-methylbutanoate	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0037266	2,2,4-Trimethyl-1,3-dioxolane	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0029762	Methyl (S)-2-Methylbutanoate	C6H12O2	M+NH4	134.1176	-2.6

	HMDB0062131	Methyl (S)-2-Methylbutanoate	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0000535	Caproic acid	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0061883	Caproic acid	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0030056	Isopropyl propionate	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0031221	2-Ethylbutanoic acid	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0040327	Pentyl formate	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0176566	3,3-dimethylbutyric acid	C6H12O2	M+NH4	134.1176	-2.6
	HMDB0168717	N-ethyl-diethanolamine	C6H15NO2	M+H	134.1176	-2.6
	HMDB0168716	SCHEMBL596841	C6H15NO2	M+H	134.1176	-2.6
	HMDB0168715	SCHEMBL2193	C6H15NO2	M+H	134.1176	-2.6
	HMDB0168718	Diethylaminoethanol-N-oxide	C6H15NO2	M+H	134.1176	-2.6
135.0437	HMDB0129378	1-benzofuran-4-ol	C8H6O2	M+H	135.0441	-2.6
	HMDB0062159	TEREPHTHALALDEHYDE	C8H6O2	M+H	135.0441	-2.6
	HMDB0032469	Phthalide	C8H6O2	M+H	135.0441	-2.6
	HMDB0061916	Phenylglyoxal	C8H6O2	M+H	135.0441	-2.6
135.0648	HMDB0167973	2-deoxypentose	C5H10O4	M+H	135.0652	-2.9
	HMDB0127615	3-hydroxy-2-(hydroxymethyl)-2-methylpropanoic acid	C5H10O4	M+H	135.0652	-2.9
	HMDB0158453	SCHEMBL8384843	C5H10O4	M+H	135.0652	-2.9
	HMDB0158454	SCHEMBL36647	C5H10O4	M+H	135.0652	-2.9
	HMDB0158455	ethyl glycerol ether	C5H10O4	M+H	135.0652	-2.9
	HMDB0001292	1-Deoxy-D-xylulose	C5H10O4	M+H	135.0652	-2.9
	HMDB0003224	Deoxyribose	C5H10O4	M+H	135.0652	-2.9
	HMDB0012141	(R)-2,3-Dihydroxy-isovalerate	C5H10O4	M+H	135.0652	-2.9
	HMDB0029576	2,3-Dihydroxy-2-methylbutanoic acid	C5H10O4	M+H	135.0652	-2.9
	HMDB0012485	(R)-glycerol 1-acetate	C5H10O4	M+H	135.0652	-2.9
	HMDB0000421	2,3-Dihydroxyvaleric acid	C5H10O4	M+H	135.0652	-2.9
135.0801	HMDB0061984	2-ethylbenzaldehyde	C9H10O	M+H	135.0804	-2.5
	HMDB0062048	3,5-Dimethylbenzaldehyde	C9H10O	M+H	135.0804	-2.5
	HMDB0032386	1-(2-methylphenyl)ethan-1-one	C9H10O	M+H	135.0804	-2.5
	HMDB0173827	Benzenemethanol,4-methyl-a-methylene-	C9H10O	M+H	135.0804	-2.5
	HMDB0175242	beta-Methylenephenethyl alcohol	C9H10O	M+H	135.0804	-2.5
	HMDB0061970	phenylacetone	C9H10O	M+H	135.0804	-2.5
	HMDB0061961	1-ethenyl-3-methoxybenzene	C9H10O	M+H	135.0804	-2.5
	HMDB0030839	(Z)-4-(1-Propenyl)phenol	C9H10O	M+H	135.0804	-2.5
	HMDB0034563	7-Nonene-3,5-diyn-1-ol	C9H10O	M+H	135.0804	-2.5
	HMDB0033716	3-Phenylpropanal	C9H10O	M+H	135.0804	-2.5
	HMDB0034107	Chavicol	C9H10O	M+H	135.0804	-2.5
	HMDB0029639	(4-Methylphenyl)acetaldehyde	C9H10O	M+H	135.0804	-2.5
	HMDB0029697	Cinnamyl alcohol	C9H10O	M+H	135.0804	-2.5
	HMDB0036441	o-Vinylanisole	C9H10O	M+H	135.0804	-2.5
	HMDB0032024	4-Ethylbenzaldehyde	C9H10O	M+H	135.0804	-2.5
	HMDB0031626	2-Phenylpropanal	C9H10O	M+H	135.0804	-2.5
	HMDB0029698	trans-Cinnamyl alcohol	C9H10O	M+H	135.0804	-2.5
	HMDB0032142	2,4-Dimethylbenzaldehyde	C9H10O	M+H	135.0804	-2.5
	HMDB0032608	4'-Methylacetophenone	C9H10O	M+H	135.0804	-2.5
	HMDB0032623	1-Phenyl-1-propanone	C9H10O	M+H	135.0804	-2.5
	HMDB0059601	Indan-1-ol	C9H10O	M+H	135.0804	-2.5
	HMDB0059895	m-Methylacetophenone	C9H10O	M+H	135.0804	-2.5
135.1012	HMDB0062104	diethylene glycol monoethyl ether	C6H14O3	M+H	135.1016	-2.7
	HMDB0032478	Polypropylene glycol (m w 1,0-3)	C6H14O3	M+H	135.1016	-2.7
135.1165	HMDB0059812	Butylbenzene	C10H14	M+H	135.1168	-2.4
	HMDB0005805	p-Cymene	C10H14	M+H	135.1168	-2.4
	HMDB0037013	p-Mentha-1,3,8-triene	C10H14	M+H	135.1168	-2.4
	HMDB0037050	1-Isopropyl-2-methylbenzene	C10H14	M+H	135.1168	-2.4
	HMDB0037051	1-Isopropyl-3-methylbenzene	C10H14	M+H	135.1168	-2.4
	HMDB0032627	1-Methyl-2-propylbenzene	C10H14	M+H	135.1168	-2.4
	HMDB0059832	4-Ethyl-o-xylene	C10H14	M+H	135.1168	-2.4
	HMDB0059821	m-Propyltoluene	C10H14	M+H	135.1168	-2.4
	HMDB0059823	Prehnitene	C10H14	M+H	135.1168	-2.4
	HMDB0059890	2-Ethyl-p-xylene	C10H14	M+H	135.1168	-2.4
	HMDB0061787	(3E,5E)-2,6-Dimethyl-1,3,5,7-octatetraene	C10H14	M+H	135.1168	-2.4
136.0211	HMDB0032930	Benzothiazole	C7H5NS	M+H	136.0215	-3.3
136.0614	HMDB0000034	Adenine	C5H5N5	M+H	136.0618	-2.7
	HMDB0030968	2,4,6-Octatriyn-1-ol	C8H6O	M+NH4	136.0757	-2.9
	HMDB0038998	3,5,7-Octatriyn-1-ol	C8H6O	M+NH4	136.0757	-2.9

136.0753	HMDB0032929	Benzofuran	C8H6O	M+NH4	136.0757	-2.9
	HMDB0040549	xi-2,3-Octadiene-5,7-diyn-1-ol	C8H6O	M+NH4	136.0757	-2.9
	HMDB0170598	p-hydroxystyrylamine	C8H9NO	M+H	136.0757	-2.9
	HMDB0032628	2-Aminoacetophenone	C8H9NO	M+H	136.0757	-2.9
	HMDB0037072	2-Acetyl-6-methylpyridine	C8H9NO	M+H	136.0757	-2.9
	HMDB0040224	4-Acetyl-3-methylpyridine	C8H9NO	M+H	136.0757	-2.9
	HMDB0040222	2-Acetyl-5-methylpyridine	C8H9NO	M+H	136.0757	-2.9
	HMDB0040223	4-Acetyl-2-methylpyridine	C8H9NO	M+H	136.0757	-2.9
	HMDB0037071	2-Acetyl-4-methylpyridine	C8H9NO	M+H	136.0757	-2.9
	HMDB0010715	2-Phenylacetamide	C8H9NO	M+H	136.0757	-2.9
	HMDB0032630	2'-Aminoacetophenone	C8H9NO	M+H	136.0757	-2.9
	HMDB0040013	5-(2-Furanyl)-3,4-dihydro-2H-pyrrole	C8H9NO	M+H	136.0757	-2.9
	HMDB0062068	5-Acetyl-2-methylpyridine	C8H9NO	M+H	136.0757	-2.9
	HMDB0040008	2,3-Dihydro-1H-pyrrolizine-5-carboxaldehyde	C8H9NO	M+H	136.0757	-2.9
136.0964	HMDB0001250	N-Acetylarlylamine	C8H9NO	M+H	136.0757	-2.9
	HMDB0041603	Methyl-beta-hydroxybutyrate	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0062584	2-Hydroxy-3-methylbutyric acid	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0130836	4-hydroxy-2-methylbutanoic acid	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0161205	4-hydroxy-3-methylbutanoate	C5H9O3	M+NH4	136.0968	-3.1
	HMDB0161204	3-Hydroxy-3-methylbutyrate	C5H9O3	M+NH4	136.0968	-3.1
	HMDB0161206	2-hydroxy-3-methylbutanoate	C5H9O3	M+NH4	136.0968	-3.1
	HMDB0172068	3-hydroxypropyl Acetate	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0172067	2-hydroxypropyl acetate	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0172069	Propyl glycolate	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0062057	4-hydroxy-valeric acid	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0000351	(2S,3R)-3-Hydroxy-2-methylbutanoic acid	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0000354	2-Methyl-3-hydroxybutyric acid	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0000396	2-Ethylhydraacrylic acid	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0000407	2-Hydroxy-3-methylbutyric acid	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0000410	3-Hydroxy-2-methyl-[S-(R,R)]-butanoic acid	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0000531	3-Hydroxyvaleric acid	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0000754	3-Hydroxyisovaleric acid	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0001863	2-Hydroxyvaleric acid	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0001987	2-Hydroxy-2-methylbutyric acid	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0002011	4-Hydroxyisovaleric acid	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0040735	Ethyl lactate	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0000642	Erythronilic acid	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0059844	Diethyl carbonate	C5H10O3	M+NH4	136.0968	-3.1
	HMDB0061927	5-Hydroxypentanoic acid	C5H10O3	M+NH4	136.0968	-3.1
136.1117	HMDB0059899	alpha-Methylstyrene	C9H10	M+NH4	136.1121	-2.7
	HMDB0062099	cyclopropylbenzene	C9H10	M+NH4	136.1121	-2.7
	HMDB0059837	Indane	C9H10	M+NH4	136.1121	-2.7
	HMDB0014328	Amphetamine	C9H13N	M+H	136.1121	-2.8
	HMDB0037291	2-(2-Methylpropyl)pyridine	C9H13N	M+H	136.1121	-2.8
	HMDB0037287	3-(2-Methylpropyl)pyridine	C9H13N	M+H	136.1121	-2.8
	HMDB0032934	3-Butylpyridine	C9H13N	M+H	136.1121	-2.8
	HMDB0012128	(R)-Amphetamine	C9H13N	M+H	136.1121	-2.8
	HMDB0062481	iso-nLc8Cer	C9H13N	M+H	136.1121	-2.8
136.1328	HMDB0015516	Dextroamphetamine	C9H13N	M+H	136.1121	-2.8
	HMDB0164618	Hexane-1,6-Diol	C6H14O2	M+NH4	136.1332	-3.0
	HMDB0165148	3-Methyl-1,5-pentanediol	C6H14O2	M+NH4	136.1332	-3.0
	HMDB0165146	3-methylpentane-1,3-diol	C6H14O2	M+NH4	136.1332	-3.0
	HMDB0165145	3-methyl-1,4-pentanediol	C6H14O2	M+NH4	136.1332	-3.0
	HMDB0031490	1,5-Hexanediol	C6H14O2	M+NH4	136.1332	-3.0
	HMDB0031327	2-Butoxyethanol	C6H14O2	M+NH4	136.1332	-3.0
	HMDB0031644	1,1-Diethoxyethane	C6H14O2	M+NH4	136.1332	-3.0
	HMDB0059740	4-Methyl-1,2-dihydroxypentane	C6H14O2	M+NH4	136.1332	-3.0
136.9397	HMDB0165147	2-ethylbutane-1,4-diol	C6H14O2	M+NH4	136.1332	-3.0
	HMDB0000973	Phosphate	H3O4P	M+K	136.9401	-2.6
	HMDB0001429	Phosphate	H3O4P	M+K	136.9401	-2.6
	HMDB0002105	Phosphate	H3O4P	M+K	136.9401	-2.6
137.0454	HMDB0002142	Phosphate	H3O4P	M+K	136.9401	-2.6
	HMDB0014581	Allopurinol	C5H4N4O	M+H	137.0458	-2.8
	HMDB0000157	Hypoxanthine	C5H4N4O	M+H	137.0458	-2.8
	HMDB0033054	Ethyl isopropyl disulfide	C5H12S2	M+H	137.0453	0.6

	HMDB0033053	Ethyl propyl disulfide	C5H12S2	M+H	137.0453	0.6
	HMDB0031160	1-Pentanesulfenothioic acid	C5H12S2	M+H	137.0453	0.6
137.0594	HMDB0126385	4-ethenylbenzene-1,3-diol	C8H8O2	M+H	137.0597	-2.2
	HMDB0167829	1-(3-hydroxyphenyl)ethan-1-one	C8H8O2	M+H	137.0597	-2.2
	HMDB0183895	phenylacetate	C8H7O2	M+H	137.0597	-2.2
	HMDB0125535	5-ethenylbenzene-1,3-diol	C8H8O2	M+H	137.0597	-2.2
	HMDB0062810	m-toluic acid	C8H8O2	M+H	137.0597	-2.2
	HMDB0124942	4-ethenylbenzene-1,2-diol	C8H8O2	M+H	137.0597	-2.2
	HMDB0038176	alpha-Methyl-2-furanacrolein	C8H8O2	M+H	137.0597	-2.2
	HMDB0167830	4'-Hydroxyacetophenone	C8H8O2	M+H	137.0597	-2.2
	HMDB0033968	Methyl benzoate	C8H8O2	M+H	137.0597	-2.2
	HMDB0040733	Phenyl acetate	C8H8O2	M+H	137.0597	-2.2
	HMDB0003767	4-Hydroxyphenylacetaldehyde	C8H8O2	M+H	137.0597	-2.2
	HMDB0000209	Phenylacetic acid	C8H8O2	M+H	137.0597	-2.2
	HMDB0041485	Benzyl formate	C8H8O2	M+H	137.0597	-2.2
	HMDB0029635	4-Methylbenzoic acid	C8H8O2	M+H	137.0597	-2.2
	HMDB0033128	4-(2-Furanyl)-3-buten-2-one	C8H8O2	M+H	137.0597	-2.2
	HMDB0033766	2-Methoxybenzaldehyde	C8H8O2	M+H	137.0597	-2.2
	HMDB0040638	3-(3-Furanyl)-2-methyl-2-propenal	C8H8O2	M+H	137.0597	-2.2
	HMDB0032568	2'-Hydroxyacetophenone	C8H8O2	M+H	137.0597	-2.2
	HMDB0029686	4-Methoxybenzaldehyde	C8H8O2	M+H	137.0597	-2.2
	HMDB0002340	2-Methylbenzoic acid	C8H8O2	M+H	137.0597	-2.2
	HMDB0032603	2-Hydroxy-4-methylbenzaldehyde	C8H8O2	M+H	137.0597	-2.2
	HMDB0032400	3-(5-Methyl-2-furyl)prop-2-enal	C8H8O2	M+H	137.0597	-2.2
	HMDB0031459	3-Methoxybenzaldehyde	C8H8O2	M+H	137.0597	-2.2
137.0706	HMDB0062270	1,2-Diacylglycerol-LD-PI-pool	C7H5NO	M+NH4	137.0709	-2.5
	HMDB0033947	2-Aminobenzamide	C7H8N2O	M+H	137.0709	-2.5
	HMDB0037819	4-Acetyl-2-methylpyrimidine	C7H8N2O	M+H	137.0709	-2.5
	HMDB0030001	2-Acetyl-3-methylpyrazine	C7H8N2O	M+H	137.0709	-2.5
	HMDB0059711	2-Methylnicotinamide	C7H8N2O	M+H	137.0709	-2.5
	HMDB0062267	1,2-Diacylglycerol-Bile-PC-pool	C7H8N2O	M+H	137.0709	-2.5
	HMDB0062268	1,2-Diacylglycerol-Bile-PC-pool	C7H8N2O	M+H	137.0709	-2.5
137.0807	HMDB0003152	N-Methylnicotinamide	C7H8N2O	M+H	137.0709	-2.5
	HMDB0011659	2-Methylerythritol	C5H12O4	M+H	137.0808	-1.0
	HMDB0062269	Pentaerithritol	C5H12O4	M+H	137.0808	-1.0
	HMDB0062440	Pentaerithritol	C5H12O4	M+H	137.0808	-1.0
	HMDB0041486	1-Deoxy-D-ribitol	C5H12O4	M+H	137.0808	-1.0
	HMDB0031201	3-Deoxy-D-arabinitol	C5H12O4	M+H	137.0808	-1.0
137.0957	HMDB0033919	2-Deoxy-D-ribitol	C5H12O4	M+H	137.0808	-1.0
	HMDB0125105	1-ethyl-3-methoxybenzene	C9H12O	M+H	137.0961	-2.9
	HMDB0169117	alpha, alpha-Dimethylbenzyl alcohol	C9H12O	M+H	137.0961	-2.9
	HMDB0169118	3-(propan-2-yl)phenol	C9H12O	M+H	137.0961	-2.9
	HMDB0038986	3-Ethyl-4-methylphenol	C9H12O	M+H	137.0961	-2.9
	HMDB0032624	2-Propylphenol	C9H12O	M+H	137.0961	-2.9
	HMDB0038988	2-Ethyl-4-methylphenol	C9H12O	M+H	137.0961	-2.9
	HMDB0032621	(2-Methoxyethyl)benzene	C9H12O	M+H	137.0961	-2.9
	HMDB0038985	3-Ethyl-5-methylphenol	C9H12O	M+H	137.0961	-2.9
	HMDB0031312	Benzyl ethyl ether	C9H12O	M+H	137.0961	-2.9
	HMDB0033962	3-Phenyl-1-propanol	C9H12O	M+H	137.0961	-2.9
	HMDB0031627	1-Phenyl-1-propanol	C9H12O	M+H	137.0961	-2.9
	HMDB0034378	1-(4-Methylphenyl)ethanol	C9H12O	M+H	137.0961	-2.9
	HMDB0039782	2-(1-Pentenyl)furan	C9H12O	M+H	137.0961	-2.9
	HMDB0029667	2,3,6-Trimethylphenol	C9H12O	M+H	137.0961	-2.9
	HMDB0032625	4-Propylphenol	C9H12O	M+H	137.0961	-2.9
	HMDB0059896	6-Ethyl-o-cresol	C9H12O	M+H	137.0961	-2.9
	HMDB0032441	Nona-2,4,6-trienal	C9H12O	M+H	137.0961	-2.9
	HMDB0031446	p-Isopropylphenol	C9H12O	M+H	137.0961	-2.9
	HMDB0032544	2,4,6-Trimethylphenol	C9H12O	M+H	137.0961	-2.9
	HMDB0038984	4-Ethyl-2-methylphenol	C9H12O	M+H	137.0961	-2.9
	HMDB0038987	2-Ethyl-5-methylphenol	C9H12O	M+H	137.0961	-2.9
	HMDB0032029	2-Isopropylphenol	C9H12O	M+H	137.0961	-2.9
	HMDB0032149	1-Methoxy-2,4-dimethylbenzene	C9H12O	M+H	137.0961	-2.9
	HMDB0031628	2-Phenyl-1-propanol	C9H12O	M+H	137.0961	-2.9
	HMDB0061790	Santolina triene	C10H16	M+H	137.1325	-2.7
	HMDB0035658	(-)-alpha-Pinene	C10H16	M+H	137.1325	-2.7

137.1321	HMDB0061791	2,7,7-Trimethyl-bicyclo[2.2.1]hept-2-ene	C10H16	M+H	137.1325	-2.7
	HMDB0061793	Isolimonene	C10H16	M+H	137.1325	-2.7
	HMDB0061792	3-Methylene-1,5,5-trimethylcyclohexene	C10H16	M+H	137.1325	-2.7
	HMDB0061978	1,5,5-Trimethyl-6-methylene-cyclohexene	C10H16	M+H	137.1325	-2.7
	HMDB0062083	alpha-Myrcene	C10H16	M+H	137.1325	-2.7
	HMDB0062101	Decatriene	C10H16	M+H	137.1325	-2.7
	HMDB0062126	(3E)-2,6-dimethylocta-1,3,7-triene	C10H16	M+H	137.1325	-2.7
	HMDB0041633	(-)-beta-phellandrene	C10H16	M+H	137.1325	-2.7
	HMDB0041574	Artemisiatriene	C10H16	M+H	137.1325	-2.7
	HMDB0036104	(Z)-3,7-Dimethyl-1,3,7-octatriene	C10H16	M+H	137.1325	-2.7
	HMDB0038150	p-Mentha-2,4-diene	C10H16	M+H	137.1325	-2.7
	HMDB0036559	(-)-beta-Pinene	C10H16	M+H	137.1325	-2.7
	HMDB0036560	(-)-beta-Pinene	C10H16	M+H	137.1325	-2.7
	HMDB0006525	(+)-alpha-Pinene	C10H16	M+H	137.1325	-2.7
	HMDB0032473	Polylimonene	C10H16	M+H	137.1325	-2.7
	HMDB0036081	beta-Phellandrene	C10H16	M+H	137.1325	-2.7
	HMDB0034697	(+)-alpha-Carene	C10H16	M+H	137.1325	-2.7
	HMDB0035087	(+)-alpha-Carene	C10H16	M+H	137.1325	-2.7
	HMDB0037046	Sylveterpinolene	C10H16	M+H	137.1325	-2.7
	HMDB0033200	5-Isosylveterpinolene	C10H16	M+H	137.1325	-2.7
	HMDB0004321	(-)-Limonene	C10H16	M+H	137.1325	-2.7
	HMDB0003375	d-Limonene	C10H16	M+H	137.1325	-2.7
	HMDB0005806	gamma-Terpinene	C10H16	M+H	137.1325	-2.7
	HMDB0038169	7-Methyl-3-methylene-1,6-octadiene	C10H16	M+H	137.1325	-2.7
	HMDB0036116	(-)-3-Thujene	C10H16	M+H	137.1325	-2.7
	HMDB0035625	(-)-7,7-Dimethyl-2-methylenebicyclo[2.2.1]heptane	C10H16	M+H	137.1325	-2.7
	HMDB0030089	trans-Ocimen	C10H16	M+H	137.1325	-2.7
	HMDB0036997	beta-Terpinene	C10H16	M+H	137.1325	-2.7
	HMDB0034928	(-)-4(-)-Thujene	C10H16	M+H	137.1325	-2.7
	HMDB0035851	(R)-alpha-Phellandrene	C10H16	M+H	137.1325	-2.7
	HMDB0059839	Camphene	C10H16	M+H	137.1325	-2.7
	HMDB0041634	(-)-beta-Phellandrene	C10H16	M+H	137.1325	-2.7
	HMDB0059726	(+)-4-Carene	C10H16	M+H	137.1325	-2.7
	HMDB0062124	Sylvestrine	C10H16	M+H	137.1325	-2.7
	HMDB0059884	2-Carene	C10H16	M+H	137.1325	-2.7
	HMDB0030088	cis-Ocimene	C10H16	M+H	137.1325	-2.7
	HMDB0061938	Isoterpinolene	C10H16	M+H	137.1325	-2.7
	HMDB0062128	Isoterpinolene	C10H16	M+H	137.1325	-2.7
	HMDB0061789	2,6-Dimethyl-2,4,6-octatriene	C10H16	M+H	137.1325	-2.7
	HMDB0062156	4(-)-Thujene	C10H16	M+H	137.1325	-2.7
	HMDB0035619	alpha-Carene	C10H16	M+H	137.1325	-2.7
	HMDB0036995	alpha-Terpinene	C10H16	M+H	137.1325	-2.7
	HMDB0038121	1,7,7-Trimethyltricyclo[2.2.12,6]heptane	C10H16	M+H	137.1325	-2.7
	HMDB0035850	alpha-Phellandrene	C10H16	M+H	137.1325	-2.7
	HMDB0036994	Terpinolene	C10H16	M+H	137.1325	-2.7
	HMDB0034970	(S)-alpha-Phellandrene	C10H16	M+H	137.1325	-2.7
	HMDB0036076	(+)-sabinene	C10H16	M+H	137.1325	-2.7
138.0312	HMDB0162803	3-methyl-2,3-dihydro-1H-pyrrol-2-ol	C5H9NO	M+K	138.0316	-2.7
	HMDB0162804	3-methyl-2,3-dihydro-1H-pyrrol-3-ol	C5H9NO	M+K	138.0316	-2.7
	HMDB0162806	(2,3-dihydro-1H-pyrrol-3-yl)methanol	C5H9NO	M+K	138.0316	-2.7
	HMDB0179972	3-Hydroxy-3-methylbutanenitrile	C5H9NO	M+K	138.0316	-2.7
	HMDB0167280	2-hydroxy-2-methylbutanenitrile	C5H9NO	M+K	138.0316	-2.7
	HMDB0034587	1-Pyrrolidinecarboxaldehyde	C5H9NO	M+K	138.0316	-2.7
	HMDB0060309	(2R)-2-Hydroxy-2-methylbutanenitrile	C5H9NO	M+K	138.0316	-2.7
	HMDB0040518	2,5-Dihydro-2,4-dimethyloxazole	C5H9NO	M+K	138.0316	-2.7
	HMDB0011749	2-Piperidinone	C5H9NO	M+K	138.0316	-2.7
138.0524	HMDB0000162	L-Proline	C5H9NO2	M+Na	138.0525	-1.1
	HMDB0167283	2,4-dihydroxy-2-methylbutanenitrile	C5H9NO2	M+Na	138.0525	-1.1
	HMDB0167282	2-hydroxy-2-(hydroxymethyl)butanenitrile	C5H9NO2	M+Na	138.0525	-1.1
	HMDB0167281	2,3-dihydroxy-2-methylbutanenitrile	C5H9NO2	M+Na	138.0525	-1.1
	HMDB0177063	1-formyl-pyrrolidin-2-ol	C5H9NO2	M+Na	138.0525	-1.1
	HMDB0003411	D-Proline	C5H9NO2	M+Na	138.0525	-1.1
	HMDB0030409	4-Amino-2-methylenebutanoic acid	C5H9NO2	M+Na	138.0525	-1.1
	HMDB0034208	Pterolactam	C5H9NO2	M+Na	138.0525	-1.1
	HMDB0012880	Acetamidopropanal	C5H9NO2	M+Na	138.0525	-1.1

	HMDB0179973	SCHEMBL55844	C5H9NO2	M+Na	138.0525	-1.1
138.0580	HMDB0001527	3-Methylthiopropionic acid	C4H8O2S	M+NH4	138.0583	-2.3
	HMDB0035646	Methyl 2-(methylthio)acetate	C4H8O2S	M+NH4	138.0583	-2.3
	HMDB0112255	3-methanesulfonylprop-1-ene	C4H8O2S	M+NH4	138.0583	-2.3
	HMDB0040072	2,5-Dimethyl-4-propylthiazole	C8H13NS	M+H-H2O	138.0742	-1.2
138.0740	HMDB0040064	4-Ethyl-5-propylthiazole	C8H13NS	M+H-H2O	138.0742	-1.2
	HMDB0040063	4-Butyl-5-methylthiazole	C8H13NS	M+H-H2O	138.0742	-1.2
	HMDB0040073	4,5-Dimethyl-2-propylthiazole	C8H13NS	M+H-H2O	138.0742	-1.2
	HMDB0040105	4-Ethyl-2-propylthiazole	C8H13NS	M+H-H2O	138.0742	-1.2
	HMDB0040071	2,4-Dimethyl-5-propylthiazole	C8H13NS	M+H-H2O	138.0742	-1.2
	HMDB0040074	4,5-Dimethyl-2-(1-methylethyl)thiazole	C8H13NS	M+H-H2O	138.0742	-1.2
	HMDB0040102	2-Butyl-4-methylthiazole	C8H13NS	M+H-H2O	138.0742	-1.2
	HMDB0040035	2-Pentylthiazole	C8H13NS	M+H-H2O	138.0742	-1.2
	HMDB0040104	2-Ethyl-4-propylthiazole	C8H13NS	M+H-H2O	138.0742	-1.2
	HMDB0040075	2,5-Diethyl-4-methylthiazole	C8H13NS	M+H-H2O	138.0742	-1.2
	HMDB0038434	7-Isothiocyanto-1-heptene	C8H13NS	M+H-H2O	138.0742	-1.2
	HMDB0040103	4-Butyl-2-methylthiazole	C8H13NS	M+H-H2O	138.0742	-1.2
	HMDB0163714	1-(2-methyloxiran-2-yl)ethan-1-one	C5H8O2	M+K	139.0156	-2.8
	HMDB0163713	73255-29-5	C5H8O2	M+K	139.0156	-2.8
139.0152	HMDB0163712	SCHEMBL69133	C5H8O2	M+K	139.0156	-2.8
	HMDB0149276	SCHEMBL15659879	C5H8O2	M+K	139.0156	-2.8
	HMDB0130837	2-methylbut-3-enoic acid	C5H8O2	M+K	139.0156	-2.8
	HMDB0170858	Isopropenylacetic acid	C5H8O2	M+K	139.0156	-2.8
	HMDB0180166	3-methyl-4-trans-hydroxy-2-butenal	C5H8O2	M+K	139.0156	-2.8
	HMDB0132474	2-methylbut-2-enoic acid	C5H8O2	M+K	139.0156	-2.8
	HMDB0129418	3,3-dimethyloxirane-2-carbaldehyde	C5H8O2	M+K	139.0156	-2.8
	HMDB0031598	2,3-Pentanedione	C5H8O2	M+K	139.0156	-2.8
	HMDB0033978	Ethyl acrylate	C5H8O2	M+K	139.0156	-2.8
	HMDB0002167	3-Methylbutyrolactone	C5H8O2	M+K	139.0156	-2.8
	HMDB0001862	2-Ethylacrylic acid	C5H8O2	M+K	139.0156	-2.8
	HMDB0001470	Tiglic acid	C5H8O2	M+K	139.0156	-2.8
	HMDB0000509	Senecioic acid	C5H8O2	M+K	139.0156	-2.8
	HMDB0031178	2-Methyltetrahydrofuran-3-one	C5H8O2	M+K	139.0156	-2.8
	HMDB0031648	2,4-Pentanedione	C5H8O2	M+K	139.0156	-2.8
	HMDB0029599	Glutaral	C5H8O2	M+K	139.0156	-2.8
	HMDB0032459	2-Pentenoic acid	C5H8O2	M+K	139.0156	-2.8
	HMDB0032385	Methyl methacrylate	C5H8O2	M+K	139.0156	-2.8
	HMDB0032351	Isopropenyl acetate	C5H8O2	M+K	139.0156	-2.8
	HMDB0035143	Dihydro-3-methyl-2(3H)-furanone	C5H8O2	M+K	139.0156	-2.8
	HMDB0029608	Angelic acid	C5H8O2	M+K	139.0156	-2.8
	HMDB0031602	4-Pentenoic acid	C5H8O2	M+K	139.0156	-2.8
	HMDB0033840	Dihydro-5-methyl-2(3H)-furanone	C5H8O2	M+K	139.0156	-2.8
	HMDB0032634	Diammonium sulfite	H8N2O3S	M+Na	139.0148	3.0
	HMDB0014966	Fosfomycin	C3H7O4P	M+H	139.0155	-1.9
139.0498	HMDB0000301	Urocanic acid	C6H6N2O2	M+H	139.0502	-2.9
	HMDB0062562	urocanic acid	C6H6N2O2	M+H	139.0502	-2.9
	HMDB0061680	2-Aminonicotinic acid	C6H6N2O2	M+H	139.0502	-2.9
	HMDB0031338	5-Oxo-2(5H)-isoxazolepropanenitrile	C6H6N2O2	M+H	139.0502	-2.9
	HMDB0034174	(E)-Urocanic acid	C6H6N2O2	M+H	139.0502	-2.9
	HMDB0002730	Nicotinamide N-oxide	C6H6N2O2	M+H	139.0502	-2.9
	HMDB0126388	4-ethylbenzene-1,3-diol	C8H10O2	M+H	139.0754	-2.6
	HMDB0041607	2-Phenoxyethanol	C8H10O2	M+H	139.0754	-2.6

139.0750	HMDB0168418	3-(2-Hydroxyethyl)phenol	C8H10O2	M+H	139.0754	-2.6
	HMDB0166105	2-Methoxybenzyl alcohol	C8H10O2	M+H	139.0754	-2.6
	HMDB0125590	5-ethylbenzene-1,3-diol	C8H10O2	M+H	139.0754	-2.6
	HMDB0168417	1-phenylethane-1,2-diol	C8H10O2	M+H	139.0754	-2.6
	HMDB0029563	3-Acetyl-2,5-dimethylfuran	C8H10O2	M+H	139.0754	-2.6
	HMDB0032136	2-Methoxy-4-methylphenol	C8H10O2	M+H	139.0754	-2.6
	HMDB0034241	4-Methoxybenzyl alcohol	C8H10O2	M+H	139.0754	-2.6
	HMDB0029672	1,3-Dimethoxybenzene	C8H10O2	M+H	139.0754	-2.6
	HMDB0029671	1,4-Dimethoxybenzene	C8H10O2	M+H	139.0754	-2.6
	HMDB0039802	1-(2-Furanyl)-1-butanone	C8H10O2	M+H	139.0754	-2.6
	HMDB0032036	4-Ethoxyphenol	C8H10O2	M+H	139.0754	-2.6
	HMDB0032139	1,2-Dimethoxybenzene	C8H10O2	M+H	139.0754	-2.6
	HMDB0040177	3-Ethyl-1,2-benzenediol	C8H10O2	M+H	139.0754	-2.6
	HMDB0040174	4-Ethyl-1,2-benzenediol	C8H10O2	M+H	139.0754	-2.6
	HMDB0032137	2,6-Dimethyl-1,4-benzenediol	C8H10O2	M+H	139.0754	-2.6
	HMDB0032159	2-Acetyl-3,5-dimethylfuran	C8H10O2	M+H	139.0754	-2.6
	HMDB0032290	1-(2-Furyl)butan-3-one	C8H10O2	M+H	139.0754	-2.6
	HMDB0168448	2-hydroxyphenylethanol	C8H10O2	M+H	139.0754	-2.6
	HMDB0004284	Tyrosol	C8H10O2	M+H	139.0754	-2.6
139.1114	HMDB0036092	exo-2-Methyl-3-methylenebicyclo[2.2.1]heptan-2-ol	C9H14O	M+H	139.1117	-2.5
	HMDB0167046	SCHEMBL19577743	C9H14O	M+H	139.1117	-2.5
	HMDB0036091	exo-5,6-Dimethylbicyclo[2.2.1]hept-5-en-2-ol	C9H14O	M+H	139.1117	-2.5
	HMDB0036069	Pulegone	C9H14O	M+H	139.1117	-2.5
	HMDB0035929	(R)-Cryptone	C9H14O	M+H	139.1117	-2.5
	HMDB0031685	2,4-Nonadienal	C9H14O	M+H	139.1117	-2.5
	HMDB0013824	2-Pentylfuran	C9H14O	M+H	139.1117	-2.5
	HMDB0031084	2-Pentylfuran	C9H14O	M+H	139.1117	-2.5
	HMDB0033434	4-Acetyl-1-methylcyclohexene	C9H14O	M+H	139.1117	-2.5
	HMDB0040338	3,5,5-Trimethyl-3-cyclohexen-1-one	C9H14O	M+H	139.1117	-2.5
	HMDB0031195	3,5,5-Trimethyl-2-cyclohexen-1-one	C9H14O	M+H	139.1117	-2.5
	HMDB0035229	5-Isopropylbicyclo[3.1]hexan-2-one	C9H14O	M+H	139.1117	-2.5
	HMDB0031261	(2E,6E)-2,6-Nonadienal	C9H14O	M+H	139.1117	-2.5
	HMDB0033857	Violet-leaf aldehyde	C9H14O	M+H	139.1117	-2.5
	HMDB0031152	(3Z,6Z)-3,6-Nonadienal	C9H14O	M+H	139.1117	-2.5
140.0469	HMDB0180424	Nona-trans-2-trans-4-dien-1-al	C9H14O	M+H	139.1117	-2.5
	HMDB0172632	2-Piperidinol	C5H11NO	M+K	140.0472	-2.3
	HMDB0012815	5-Aminopentanal	C5H11NO	M+K	140.0472	-2.3
	HMDB0062600	N-butylformamide	C5H11NO	M+K	140.0472	-2.3
	HMDB0062122	INDOLIZINE	C8H7N	M+Na	140.0471	-1.2
	HMDB0000738	Indole	C8H7N	M+Na	140.0471	-1.2
	HMDB0034171	Benzeneacetonitrile	C8H7N	M+Na	140.0471	-1.2
140.0679	HMDB0062169	5H-Cyclopenta[b]pyridine	C8H7N	M+Na	140.0471	-1.2
	HMDB0000883	L-Valine	C5H11NO2	M+Na	140.0682	-2.1
	HMDB0061966	1-nitropentane	C5H11NO2	M+Na	140.0682	-2.1
	HMDB0062141	N,N-Dimethyl-L-Alanine	C5H11NO2	M+Na	140.0682	-2.1
	HMDB0015550	Amyl Nitrite	C5H11NO2	M+Na	140.0682	-2.1
	HMDB0001382	Vaporole	C5H11NO2	M+Na	140.0682	-2.1
	HMDB0002141	N-Methyl-a-aminoisobutyric acid	C5H11NO2	M+Na	140.0682	-2.1
	HMDB0003355	5-Aminopentanoic acid	C5H11NO2	M+Na	140.0682	-2.1
140.0915	HMDB0013716	Norvaline	C5H11NO2	M+Na	140.0682	-2.1
	HMDB0002994	Erythritol	C4H10O4	M+NH4	140.0917	-1.7
	HMDB0004136	D-Threitol	C4H10O4	M+NH4	140.0917	-1.7
141.0543	HMDB0094689	D-Threitol	C4H10O4	M+NH4	140.0917	-1.7
	HMDB0137138	2-methoxybenzene-1,4-diol	C7H8O3	M+H	141.0546	-2.3
	HMDB0181055	1-[3-(hydroxymethyl)furan-2-yl]ethan-1-one	C7H8O3	M+H	141.0546	-2.3
	HMDB0172014	4-methoxy-5-methyl-2-methylidene-2,3-dihydrofuran-3-one	C7H8O3	M+H	141.0546	-2.3
	HMDB0137137	4-methoxybenzene-1,2-diol	C7H8O3	M+H	141.0546	-2.3
	HMDB0169074	Gentisyl alcohol	C7H8O3	M+H	141.0546	-2.3
	HMDB0179995	4-(hydroxymethyl)benzene-1,2-diol	C7H8O3	M+H	141.0546	-2.3
	HMDB0151713	2,4,6-trihydroxytoluene	C7H8O3	M+H	141.0546	-2.3
	HMDB0132905	5-methoxybenzene-1,3-diol	C7H8O3	M+H	141.0546	-2.3
	HMDB0059862	Ethyl furoate	C7H8O3	M+H	141.0546	-2.3
	HMDB0059880	Ethyl 3-furoate	C7H8O3	M+H	141.0546	-2.3
	HMDB0034246	Furfuryl acetate	C7H8O3	M+H	141.0546	-2.3

	HMDB0031735	Ethyl maltol	C7H8O3	M+H	141.0546	-2.3
	HMDB0125538	3-methoxybenzene-1,2-diol	C7H8O3	M+H	141.0546	-2.3
	HMDB0169073	3-(Hydroxymethyl)pyrocatechol	C7H8O3	M+H	141.0546	-2.3
	HMDB0125014	4-methoxybenzene-1,3-diol	C7H8O3	M+H	141.0546	-2.3
	HMDB0133970	2-methoxybenzene-1,3-diol	C7H8O3	M+H	141.0546	-2.3
141.0906	HMDB0040526	3,4,4-Trimethyl-1,2-cyclopentanedione	C8H12O2	M+H	141.0910	-2.9
	HMDB0037625	Allyl tiglate	C8H12O2	M+H	141.0910	-2.9
	HMDB0036176	3-Ethyl-2-hydroxy-4-methyl-2-cyclopenten-1-one	C8H12O2	M+H	141.0910	-2.9
	HMDB0039652	2-Hydroxy-3,4,5-trimethyl-2-cyclopenten-1-one	C8H12O2	M+H	141.0910	-2.9
	HMDB0039680	3,5,5-Trimethyl-1,2-cyclopentanedione	C8H12O2	M+H	141.0910	-2.9
	HMDB0039651	3-Propyl-1,2-cyclopentanedione	C8H12O2	M+H	141.0910	-2.9
	HMDB0039673	4-Ethyl-2-hydroxy-3-methyl-2-cyclopenten-1-one	C8H12O2	M+H	141.0910	-2.9
	HMDB0040463	Ethyl sorbate	C8H12O2	M+H	141.0910	-2.9
	HMDB0037196	Ethyl 2-methyl-3,4-pentadienoate	C8H12O2	M+H	141.0910	-2.9
	HMDB0037167	3-Ethyl-5-methyl-1,2-cyclopentanedione	C8H12O2	M+H	141.0910	-2.9
	HMDB0060682	2-Propyl-2,4-pentadienoic acid	C8H12O2	M+H	141.0910	-2.9
	HMDB0032311	2,4-Hexadienyl acetate	C8H12O2	M+H	141.0910	-2.9
	HMDB0039681	3-Isopropyl-1,2-cyclopentanedione	C8H12O2	M+H	141.0910	-2.9
141.1270	HMDB0062671	(3E)-2,3,4-trimethylhex-3-enal	C9H16O	M+H	141.1274	-2.8
	HMDB0167031	Violet alcohol	C9H16O	M+H	141.1274	-2.8
	HMDB0037170	3-Methylene-2-octanone	C9H16O	M+H	141.1274	-2.8
	HMDB0035927	1-Nonen-4-one	C9H16O	M+H	141.1274	-2.8
	HMDB0030957	(3Z,6Z)-3,6-Nonadien-1-ol	C9H16O	M+H	141.1274	-2.8
	HMDB0035926	8-Nonen-2-one	C9H16O	M+H	141.1274	-2.8
	HMDB0031269	2-Nonenal	C9H16O	M+H	141.1274	-2.8
	HMDB0034764	3-Nonen-2-one	C9H16O	M+H	141.1274	-2.8
	HMDB0034761	5-Nonen-2-one	C9H16O	M+H	141.1274	-2.8
	HMDB0033554	2-Methyl-2-octenal	C9H16O	M+H	141.1274	-2.8
	HMDB0035916	(E)-2-Nonen-4-one	C9H16O	M+H	141.1274	-2.8
	HMDB0038400	(2xi,4xi)-2,4-Nonadien-1-ol	C9H16O	M+H	141.1274	-2.8
	HMDB0031834	2,6-Dimethyl-5-heptenal	C9H16O	M+H	141.1274	-2.8
	HMDB0034758	8-Nonen-3-one	C9H16O	M+H	141.1274	-2.8
	HMDB0031262	2,6-Nonadien-1-ol	C9H16O	M+H	141.1274	-2.8
	HMDB0038067	(3E,6Z)-3,6-Nonadien-1-ol	C9H16O	M+H	141.1274	-2.8
	HMDB0034845	2,4-Nonadien-1-ol	C9H16O	M+H	141.1274	-2.8
	HMDB0059828	3-Nonen-5-one	C9H16O	M+H	141.1274	-2.8
	HMDB0032535	trans-4-Nonenal	C9H16O	M+H	141.1274	-2.8
	HMDB0039461	7-Methyl-3-octen-2-one	C9H16O	M+H	141.1274	-2.8
	HMDB0030958	(Z)-6-Nonenal	C9H16O	M+H	141.1274	-2.8
	HMDB0037001	Santene hydrate	C9H16O	M+H	141.1274	-2.8
	HMDB0037150	2-Ethyl-2-heptenal	C9H16O	M+H	141.1274	-2.8
	HMDB0033794	2,2,6-Trimethylcyclohexanone	C9H16O	M+H	141.1274	-2.8
142.0261	HMDB0240305	N-acetyethanolamine	C4H9NO2	M+K	142.0265	-2.7
	HMDB0167366	4-hydroxybutanamide	C4H9NO2	M+K	142.0265	-2.7
	HMDB0167365	3-hydroxybutanimidic acid	C4H9NO2	M+K	142.0265	-2.7
	HMDB0167367	2-hydroxybutanamide	C4H9NO2	M+K	142.0265	-2.7
	HMDB0000112	gamma-Aminobutyric acid	C4H9NO2	M+K	142.0265	-2.7
	HMDB0000092	Dimethylglycine	C4H9NO2	M+K	142.0265	-2.7
	HMDB0031654	3-Aminobutanoic acid	C4H9NO2	M+K	142.0265	-2.7
	HMDB0094693	3-Aminobutanoic acid	C4H9NO2	M+K	142.0265	-2.7
	HMDB0031329	Butyl nitrite	C4H9NO2	M+K	142.0265	-2.7
	HMDB0038394	O-Acetyethanolamine	C4H9NO2	M+K	142.0265	-2.7
	HMDB0003911	3-Aminoisobutanoic acid	C4H9NO2	M+K	142.0265	-2.7
	HMDB0002299	(R)-beta-Aminoisobutyric acid	C4H9NO2	M+K	142.0265	-2.7
	HMDB0002166	(S)-beta-Aminoisobutyric acid	C4H9NO2	M+K	142.0265	-2.7
	HMDB0000452	L-alpha-Aminobutyric acid	C4H9NO2	M+K	142.0265	-2.7
	HMDB0001906	2-Aminoisobutyric acid	C4H9NO2	M+K	142.0265	-2.7
	HMDB0000650	D-alpha-Aminobutyric acid	C4H9NO2	M+K	142.0265	-2.7
	HMDB0061050	D-alpha-Aminobutyric acid	C4H9NO2	M+K	142.0265	-2.7
	HMDB0094692	N-Methylalanine	C4H9NO2	M+K	142.0265	-2.7
	HMDB0041945	N-Ethylglycine	C4H9NO2	M+K	142.0265	-2.7
	HMDB0172018	(1Z)-3-chloroprop-1-ene-1,2,3-triol	C3H5ClO3	M+NH4	142.0265	-3.1
	HMDB0062270	1,2-Diacylglycerol-LD-PI-pool	C7H5NO	M+Na	142.0263	-1.6
	HMDB0000224	O-Phosphoethanolamine	C2H8NO4P	M+H	142.0264	-1.9
	HMDB0060151	O-Phosphoethanolamine	C2H8NO4P	M+H	142.0264	-1.9

	HMDB0060152	O-Phosphoethanolamine	C2H8NO4P	M+H	142.0264	-1.9
	HMDB0161316	4-aminobutanoate	C4H8NO2	M+K	142.0259	1.1
142.0471	HMDB0000167	L-Threonine	C4H9NO3	M+Na	142.0475	-2.5
	HMDB0155268	N,N-dimethylhydroxyglycine	C4H9NO3	M+Na	142.0475	-2.5
	HMDB0162440	3-amino-4-hydroxybutanoic acid	C4H9NO3	M+Na	142.0475	-2.5
	HMDB0061148	Hydroxyethyl glycine	C4H9NO3	M+Na	142.0475	-2.5
	HMDB0000719	L-Homoserine	C4H9NO3	M+Na	142.0475	-2.5
	HMDB0159152	L-Homoserine	C4H9NO3	M+Na	142.0475	-2.5
	HMDB0004041	L-Allothreonine	C4H9NO3	M+Na	142.0475	-2.5
	HMDB0159151	alpha-Amino-beta-hydroxybutyric acid	C4H9NO3	M+Na	142.0475	-2.5
	HMDB0240310	2-methylserine zwitterion	C4H9NO3	M+Na	142.0475	-2.5
	HMDB0061877	4-Amino-3-hydroxybutyrate	C4H9NO3	M+Na	142.0475	-2.5
	HMDB0060587	Aminoethoxyacetic acid	C4H9NO3	M+Na	142.0475	-2.5
142.1223	HMDB0062073	5-Octen-2-yn-4-ol	C8H12O	M+NH4	142.1226	-2.4
	HMDB0061898	Methyl-1-cyclopenten-1-yl)-ethanone	C8H12O	M+NH4	142.1226	-2.4
	HMDB0040272	2-Butylfuran	C8H12O	M+NH4	142.1226	-2.4
	HMDB0033238	2-Isopropyl-5-methylfuran	C8H12O	M+NH4	142.1226	-2.4
	HMDB0039844	(E,E)-2,6-Octadienal	C8H12O	M+NH4	142.1226	-2.4
	HMDB0031414	2,3-Dimethyl-2-cyclohexen-1-one	C8H12O	M+NH4	142.1226	-2.4
	HMDB0040246	3,5,5-Trimethyl-2-cyclopenten-1-one	C8H12O	M+NH4	142.1226	-2.4
	HMDB0032446	trans, trans-3,5-Octadien-2-one	C8H12O	M+NH4	142.1226	-2.4
	HMDB0031582	6-Methyl-3,5-heptadien-2-one	C8H12O	M+NH4	142.1226	-2.4
	HMDB0032447	1,5-Octadien-3-one	C8H12O	M+NH4	142.1226	-2.4
	HMDB0031686	(E,E)-2,4-Octadienal	C8H12O	M+NH4	142.1226	-2.4
	HMDB0030325	Pelletierine	C8H15NO	M+H	142.1226	-2.4
	HMDB0039839	1-(1-Pyrrolidinyl)-2-butanone	C8H15NO	M+H	142.1226	-2.4
	HMDB0030338	Physoperuvine	C8H15NO	M+H	142.1226	-2.4
	HMDB0033364	Conhydrinone	C8H15NO	M+H	142.1226	-2.4
	HMDB0030324	(R)-Pelletierine	C8H15NO	M+H	142.1226	-2.4
	HMDB0039840	3-(1-Pyrrolidinyl)-2-butanone	C8H15NO	M+H	142.1226	-2.4
143.0011	HMDB0062027	3-pyridinecarbonitrile	C6H4N2	M+K	143.0006	3.5
	HMDB0131295	(2-hydroxyethoxy)sulfonic acid	C2H6O5S	M+H	143.0009	1.6
143.0481	HMDB0000251	Taurine	C2H7NO3S	M+NH4	143.0485	-2.7
143.0699	HMDB0180324	(2E)-3-(3-ethyloxiran-2-yl)prop-2-enoic acid	C7H10O3	M+H	143.0703	-2.6
	HMDB0180325	(2E)-4,5-dihydroxyhepta-2,4-dienal	C7H10O3	M+H	143.0703	-2.6
	HMDB0172015	4-methoxy-5-methyl-2-methylideneoxolan-3-one	C7H10O3	M+H	143.0703	-2.6
	HMDB0165787	2-ethyl-5-methyloxolane-3,4-dione	C7H10O3	M+H	143.0703	-2.6
	HMDB0041427	Erinapyrone B	C7H10O3	M+H	143.0703	-2.6
	HMDB0041426	Erinapyrone A	C7H10O3	M+H	143.0703	-2.6
	HMDB0033736	Homofureanol	C7H10O3	M+H	143.0703	-2.6
	HMDB0034230	Mesifurane	C7H10O3	M+H	143.0703	-2.6
	HMDB0164727	4,6-dihydroxy-4-methylcyclohex-2-en-1-one	C7H10O3	M+H	143.0703	-2.6
	HMDB0164725	4-hydroxy-4-(hydroxymethyl)cyclohex-2-en-1-one	C7H10O3	M+H	143.0703	-2.6
	HMDB0164726	5-hydroxy-5-methyl-7-oxabicyclo[4.1]heptan-2-one	C7H10O3	M+H	143.0703	-2.6
	HMDB0163404	5-ethyl-4-methyloxolane-2,3-dione	C7H10O3	M+H	143.0703	-2.6
	HMDB0033551	5-Ethyl-3-hydroxy-4-methyl-2(5H)-furanone	C7H10O3	M+H	143.0703	-2.6
	HMDB0163318	(E)-8-Hydroxy-3-octene-2-one	C8H14O2	M+H	143.1067	-2.5
	HMDB0163315	SCHEMBL17867	C8H14O2	M+H	143.1067	-2.5
	HMDB0163317	Ethanone, 1-(3-butyloxiranyl)-	C8H14O2	M+H	143.1067	-2.5
	HMDB0163316	(3E)-7-hydroxyoct-3-en-2-one	C8H14O2	M+H	143.1067	-2.5
	HMDB0163319	(3E)-1-hydroxyoct-3-en-2-one	C8H14O2	M+H	143.1067	-2.5
	HMDB0000392	2-Octenoic acid	C8H14O2	M+H	143.1067	-2.5
	HMDB0032266	Ethyl (E)-3-hexenoate	C8H14O2	M+H	143.1067	-2.5
	HMDB0037624	Isopropyl tiglate	C8H14O2	M+H	143.1067	-2.5
	HMDB0031293	2,3-Octanedione	C8H14O2	M+H	143.1067	-2.5
	HMDB0029761	Ethyl 2-methyl-4-pentenoate	C8H14O2	M+H	143.1067	-2.5
	HMDB0031403	Cyclohexanecarboxylic acid	C8H14O2	M+H	143.1067	-2.5
	HMDB0035422	4-Butyl-gamma-butyrolactone	C8H14O2	M+H	143.1067	-2.5
	HMDB0031352	Cyclohexyl acetate	C8H14O2	M+H	143.1067	-2.5
	HMDB0031343	Methyl cyclohexanecarboxylate	C8H14O2	M+H	143.1067	-2.5
	HMDB0036236	2-Methylallyl butyrate	C8H14O2	M+H	143.1067	-2.5
	HMDB0032268	Ethyl 2E-hexenoate	C8H14O2	M+H	143.1067	-2.5
	HMDB0040212	2-Hexenyl acetate	C8H14O2	M+H	143.1067	-2.5
	HMDB0001568	trans-2-Octenoic acid	C8H14O2	M+H	143.1067	-2.5
	HMDB0038036	2-Propenyl 3-methylbutanoate	C8H14O2	M+H	143.1067	-2.5

143.1063	HMDB0039793	(E)-4-Octenoic acid	C8H14O2	M+H	143.1067	-2.5
	HMDB0037630	xi-Tetrahydro-3-propyl-2H-pyran-2-one	C8H14O2	M+H	143.1067	-2.5
	HMDB0038310	xi-Tetrahydro-6-propyl-2H-pyran-2-one	C8H14O2	M+H	143.1067	-2.5
	HMDB0039872	Methyl 2-heptenoate	C8H14O2	M+H	143.1067	-2.5
	HMDB0037622	Ethyl 2-methyl-3-pentenoate	C8H14O2	M+H	143.1067	-2.5
	HMDB0040215	cis-3-Hexenyl acetate	C8H14O2	M+H	143.1067	-2.5
	HMDB0036212	2-Methylpropyl (2E)-butenoate	C8H14O2	M+H	143.1067	-2.5
	HMDB0032533	trans-3-Hexenyl acetate	C8H14O2	M+H	143.1067	-2.5
	HMDB0013902	2-ene-Valproic acid	C8H14O2	M+H	143.1067	-2.5
	HMDB0013904	(3E)-2-Propylpent-3-enoic acid	C8H14O2	M+H	143.1067	-2.5
	HMDB0062077	6-methylheptan-2,4-dione	C8H14O2	M+H	143.1067	-2.5
	HMDB0062166	Vinyl hexanoate	C8H14O2	M+H	143.1067	-2.5
	HMDB0013903	(3Z)-2-Propylpent-3-enoic acid	C8H14O2	M+H	143.1067	-2.5
	HMDB0061342	(3Z)-2-Propylpent-3-enoic acid	C8H14O2	M+H	143.1067	-2.5
	HMDB0013897	4-ene-Valproic acid	C8H14O2	M+H	143.1067	-2.5
	HMDB0240301	3-Octenoic acid	C8H14O2	M+H	143.1067	-2.5
	HMDB0032164	Allyl valerate	C8H14O2	M+H	143.1067	-2.5
	HMDB0032278	Ethyl trans-2-methyl-2-pentenoate	C8H14O2	M+H	143.1067	-2.5
	HMDB0032207	cis-5-Octenoic acid	C8H14O2	M+H	143.1067	-2.5
	HMDB0032267	Ethyl 5-hexenoate	C8H14O2	M+H	143.1067	-2.5
	HMDB0059908	Ethyl-3-hexanoate	C8H14O2	M+H	143.1067	-2.5
144.0053	HMDB0000187	L-Serine	C3H7NO3	M+K	144.0058	-3.1
	HMDB0062263	L-Serine	C3H7NO3	M+K	144.0058	-3.1
	HMDB0003406	D-Serine	C3H7NO3	M+K	144.0058	-3.1
	HMDB0014670	Foscarnet	CH3O5P	M+NH4	144.0056	-2.3
144.0653	HMDB0187592	5-hydroxycyclohex-2-ene-1,4-dione	C6H6O3	M+NH4	144.0655	-1.5
	HMDB0030776	Maltol	C6H6O3	M+NH4	144.0655	-1.5
	HMDB0032651	(Z)-Tamarindial	C6H6O3	M+NH4	144.0655	-1.5
	HMDB0031256	4-Hydroxy-2H-pyran-3-carboxaldehyde	C6H6O3	M+NH4	144.0655	-1.5
	HMDB0029750	Methyl 2-furoate	C6H6O3	M+NH4	144.0655	-1.5
	HMDB0013674	1,2,3-Trihydroxybenzene	C6H6O3	M+NH4	144.0655	-1.5
	HMDB0013675	1,3,5-Trihydroxybenzene	C6H6O3	M+NH4	144.0655	-1.5
	HMDB0034355	5-Hydroxymethyl-2-furancarboxaldehyde	C6H6O3	M+NH4	144.0655	-1.5
	HMDB0124831	benzene-1,2,4-triol	C6H6O3	M+NH4	144.0655	-1.5
	HMDB0059735	5-Methylfuran-2-carboxylic acid	C6H6O3	M+NH4	144.0655	-1.5
	HMDB0187591	7-Oxabicyclo[4.1]heptane-2,5-dione	C6H6O3	M+NH4	144.0655	-1.5
	HMDB0014491	Trimethadione	C6H9NO3	M+H	144.0655	-1.5
	HMDB0000894	Vinylacetylglycine	C6H9NO3	M+H	144.0655	-1.5
	HMDB0032161	Acrylamide-acrylic acid resin	C6H9NO3	M+H	144.0655	-1.5
	HMDB0061705	6-Oxopiperidine-2-carboxylic acid	C6H9NO3	M+H	144.0655	-1.5
	HMDB0061082	5-ethyl-5-methyl-2,4-oxazolidinedione	C6H9NO3	M+H	144.0655	-1.5
144.0805	HMDB0033115	6-Methylquinoline	C10H9N	M+H	144.0808	-1.9
	HMDB0041802	2-Aminonaphthalene	C10H9N	M+H	144.0808	-1.9
	HMDB0042004	Quinaldine	C10H9N	M+H	144.0808	-1.9
144.1015	HMDB0029582	Methyl sorbate	C7H10O2	M+NH4	144.1019	-2.8
	HMDB0037026	3,4-Dimethyl-1,2-cyclopentanedione	C7H10O2	M+NH4	144.1019	-2.8
	HMDB0034835	3-(3-Ethylloxiranyl)-2-propenal	C7H10O2	M+NH4	144.1019	-2.8
	HMDB0031222	3-Ethyl-1,2-cyclopentanedione	C7H10O2	M+NH4	144.1019	-2.8
	HMDB0037027	3,5-Dimethyl-1,2-cyclopentanedione	C7H10O2	M+NH4	144.1019	-2.8
	HMDB0041474	xi-5-Isopropyl-2(5H)-furanone	C7H10O2	M+NH4	144.1019	-2.8
	HMDB0031223	Enol-3-Ethyl-1,2-cyclopentanedione	C7H10O2	M+NH4	144.1019	-2.8
	HMDB0034080	3-Methyl-1,2-cyclohexanedione	C7H10O2	M+NH4	144.1019	-2.8
	HMDB0033629	xi-4-Hydroxy-4-methyl-2-cyclohexen-1-one	C7H10O2	M+NH4	144.1019	-2.8
	HMDB0040445	2-(Ethoxymethyl)furan	C7H10O2	M+NH4	144.1019	-2.8
	HMDB0032067	Allyl crotonate	C7H10O2	M+NH4	144.1019	-2.8
	HMDB0032333	4-Hydroxy-4-methyl-5-hexenoic acid gamma lactone	C7H10O2	M+NH4	144.1019	-2.8
	HMDB0038949	3beta,6beta-Dihydroxynortropane	C7H13NO2	M+H	144.1019	-2.8
	HMDB0004827	Proline betaine	C7H13NO2	M+H	144.1019	-2.8
	HMDB0030410	L-2-Amino-3-methylenehexanoic acid	C7H13NO2	M+H	144.1019	-2.8
	HMDB0181106	7-Octen-3-one	C8H14O	M+NH4	144.1383	-2.7
	HMDB0062529	3,5-Dimethyl-1-hexyn-3-ol	C8H14O	M+NH4	144.1383	-2.7
	HMDB0040146	2,5-Octadien-1-ol	C8H14O	M+NH4	144.1383	-2.7
	HMDB0040151	(2E,4E)-2,4-Octadien-1-ol	C8H14O	M+NH4	144.1383	-2.7
	HMDB0037152	2-Ethylidenehexanal	C8H14O	M+NH4	144.1383	-2.7
	HMDB0033547	3-Octen-2-one	C8H14O	M+NH4	144.1383	-2.7

144.1379	HMDB0031197	2,4,4-Trimethylcyclopentanone	C8H14O	M+NH4	144.1383	-2.7
	HMDB0039769	6-Octenal	C8H14O	M+NH4	144.1383	-2.7
	HMDB0031301	2-Octen-4-one	C8H14O	M+NH4	144.1383	-2.7
	HMDB0031591	5-Methyl-5-hepten-2-one	C8H14O	M+NH4	144.1383	-2.7
	HMDB0030966	(3xi,5Z)-1,5-Octadien-3-ol	C8H14O	M+NH4	144.1383	-2.7
	HMDB0030961	2-Octenal	C8H14O	M+NH4	144.1383	-2.7
	HMDB0035915	Sulcatone	C8H14O	M+NH4	144.1383	-2.7
	HMDB0031309	1-Octen-3-one	C8H14O	M+NH4	144.1383	-2.7
	HMDB0035242	(S,E)-Filbertone	C8H14O	M+NH4	144.1383	-2.7
	HMDB0040149	(3E,5Z)-3,5-Octadien-1-ol	C8H14O	M+NH4	144.1383	-2.7
	HMDB0035390	5-Octen-2-one	C8H14O	M+NH4	144.1383	-2.7
	HMDB0031590	3-Methyl-3-hepten-2-one	C8H14O	M+NH4	144.1383	-2.7
	HMDB0039770	(Z)-5-Octenal	C8H14O	M+NH4	144.1383	-2.7
	HMDB0013809	(E)-2-octenal	C8H14O	M+NH4	144.1383	-2.7
	HMDB0032451	4-Octen-3-one	C8H14O	M+NH4	144.1383	-2.7
	HMDB0032403	6-Methyl-3-hepten-2-one, trans-	C8H14O	M+NH4	144.1383	-2.7
	HMDB0163322	7-octen-2-one	C8H14O	M+NH4	144.1383	-2.7
	HMDB0061945	2-Ethyl-2-hexenal	C8H14O	M+NH4	144.1383	-2.7
144.9261	HMDB0060344	2-Bromoacetaldehyde	C2H3BrO	M+Na	144.9259	1.1
145.0258	HMDB0061944	Trihydroxybutane	C4H10O3	M+K	145.0262	-2.4
	HMDB0240298	1,2,4-butanetriol	C4H10O3	M+K	145.0262	-2.4
	HMDB0034778	(2R*,3R*)-1,2,3-Butanetriol	C4H10O3	M+K	145.0262	-2.4
	HMDB0011718	4-Hydroxybenzaldehyde	C7H6O2	M+Na	145.0260	-1.4
	HMDB0034170	2-Hydroxybenzaldehyde	C7H6O2	M+Na	145.0260	-1.4
	HMDB0032918	3-(2-Furanyl)-2-propenal	C7H6O2	M+Na	145.0260	-1.4
	HMDB0001870	Benzoic acid	C7H6O2	M+Na	145.0260	-1.4
	HMDB0186744	3-hydroxybenzaldehyde	C7H6O2	M+Na	145.0260	-1.4
145.0491	HMDB0038379	1-Piperazinecarbodithioic acid	C5H10N2S2	M+H-H2O	145.0258	-0.3
	HMDB0180627	2,4-Dioxohexanoic acid	C6H8O4	M+H	145.0495	-3.0
	HMDB0163711	(2Z)-5-hydroxy-3-methyl-4-oxopent-2-enoic acid	C6H8O4	M+H	145.0495	-3.0
	HMDB0163710	3-acetyl-3-methyloxirane-2-carboxylic acid	C6H8O4	M+H	145.0495	-3.0
	HMDB0163709	(2Z)-3-(hydroxymethyl)-4-oxopent-2-enoic acid	C6H8O4	M+H	145.0495	-3.0
	HMDB0029171	3-Hydroxyadipic acid 3,6-lactone	C6H8O4	M+H	145.0495	-3.0
	HMDB0013311	trans-2-Hexenedioic acid	C6H8O4	M+H	145.0495	-3.0
	HMDB0036232	Maleic acid homopolymer	C6H8O4	M+H	145.0495	-3.0
	HMDB0040207	Ethyl hydrogen fumarate	C6H8O4	M+H	145.0495	-3.0
	HMDB0031257	Dimethyl fumarate	C6H8O4	M+H	145.0495	-3.0
	HMDB0002266	(E)-2-Methylglutaconic acid	C6H8O4	M+H	145.0495	-3.0
	HMDB0000522	3-Methylglutaconic acid	C6H8O4	M+H	145.0495	-3.0
	HMDB0240300	3-methylpent-2-enedioic acid	C6H8O4	M+H	145.0495	-3.0
145.0855	HMDB0000393	3-Hexenedioic acid	C6H8O4	M+H	145.0495	-3.0
	HMDB0166500	SCHEMBL26282	C7H12O3	M+H	145.0859	-2.9
	HMDB0166499	SCHEMBL7994854	C7H12O3	M+H	145.0859	-2.9
	HMDB0166497	(4Z)-6-hydroxyhept-4-enoic acid	C7H12O3	M+H	145.0859	-2.9
	HMDB0166498	(4Z)-3-hydroxyhept-4-enoic acid	C7H12O3	M+H	145.0859	-2.9
	HMDB0165786	2(5)-ethyl-4-hydroxy-5(2)-methyl-3(2H)-furanone (ethylfuranol)	C7H12O3	M+H	145.0859	-2.9
	HMDB0164728	4-hydroxy-4-(hydroxymethyl)cyclohexan-1-one	C7H12O3	M+H	145.0859	-2.9
	HMDB0164729	2,4-dihydroxy-4-methylcyclohexan-1-one	C7H12O3	M+H	145.0859	-2.9
	HMDB0163403	5-ethyl-3-hydroxy-4-methyloxolan-2-one	C7H12O3	M+H	145.0859	-2.9
	HMDB0166501	(4Z)-2-hydroxyhept-4-enoic acid	C7H12O3	M+H	145.0859	-2.9
	HMDB0180835	pentyl 2-oxoacetate	C7H12O3	M+H	145.0859	-2.9
	HMDB0180326	(2E)-3-[3-(1-hydroxyethyl)oxiran-2-yl]prop-2-en-1-ol	C7H12O3	M+H	145.0859	-2.9
	HMDB0180327	(2E)-3-[3-(2-hydroxyethyl)oxiran-2-yl]prop-2-en-1-ol	C7H12O3	M+H	145.0859	-2.9
	HMDB0172013	4-methoxy-2,5-dimethyloxolan-3-one	C7H12O3	M+H	145.0859	-2.9
	HMDB0166746	ACMC-mulz	C7H12O3	M+H	145.0859	-2.9
	HMDB0166745	(2E)-6-hydroxyhept-2-enoic acid	C7H12O3	M+H	145.0859	-2.9
	HMDB0166744	(2E)-4-hydroxyhept-2-enoic acid	C7H12O3	M+H	145.0859	-2.9
	HMDB0166747	SCHEMBL088	C7H12O3	M+H	145.0859	-2.9
	HMDB0061990	2-hydroxycyclohexanecarboxylic acid	C7H12O3	M+H	145.0859	-2.9
	HMDB0031176	Tetrahydrofurfuryl acetate	C7H12O3	M+H	145.0859	-2.9
	HMDB0040433	Ethyl levulinate	C7H12O3	M+H	145.0859	-2.9
	HMDB0036594	Botryodiplodin	C7H12O3	M+H	145.0859	-2.9
	HMDB0037114	Methyl (R)-3-methyl-2-oxopentanoate	C7H12O3	M+H	145.0859	-2.9

145.1219	HMDB0001988	4-Hydroxycyclohexylcarboxylic acid	C7H12O3	M+H	145.0859	-2.9
	HMDB0181107	4-Hydroxyoctane-3-one	C8H16O2	M+H	145.1223	-2.8
	HMDB0062151	Propyl 2-methylbutanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0061998	2-methylbutyl propanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0061931	Tetrahydro-2,5-dimethyl-2H-pyranmethanol	C8H16O2	M+H	145.1223	-2.8
	HMDB0032272	Ethyl 4-methylpentanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0032225	1,1-Dimethoxy-trans-2-hexene	C8H16O2	M+H	145.1223	-2.8
	HMDB0032335	3-Hydroxy-2-octanone	C8H16O2	M+H	145.1223	-2.8
	HMDB0032203	cis- and trans-2-Isobutyl-4-methyl-1,3-dioxolane	C8H16O2	M+H	145.1223	-2.8
	HMDB0032551	Valeraldehyde propyleneglycol acetal	C8H16O2	M+H	145.1223	-2.8
	HMDB0181105	8-hydroxyoctan-3-one	C8H16O2	M+H	145.1223	-2.8
	HMDB0181104	7-hydroxyoctan-3-one	C8H16O2	M+H	145.1223	-2.8
	HMDB0163321	8-Hydroxy-2-octanone	C8H16O2	M+H	145.1223	-2.8
	HMDB0163320	7-hydroxyoctan-2-one	C8H16O2	M+H	145.1223	-2.8
	HMDB0163323	1-hydroxy-2-octanone	C8H16O2	M+H	145.1223	-2.8
	HMDB0181103	2-hydroxyoctan-3-one	C8H16O2	M+H	145.1223	-2.8
	HMDB0031579	Ethyl 2-methylpentanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0034234	Ethyl 3-methylpentanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0034161	2-Methylpropyl butanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0031478	Methyl heptanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0040209	Ethyl hexanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0034164	3-Methylbutyl propanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0034459	Heptyl formate	C8H16O2	M+H	145.1223	-2.8
	HMDB0029980	Hexyl acetate	C8H16O2	M+H	145.1223	-2.8
	HMDB0036165	3-(Hydroxymethyl)-2-heptanone	C8H16O2	M+H	145.1223	-2.8
	HMDB0030368	(3R,5Z)-5-Octene-1,3-diol	C8H16O2	M+H	145.1223	-2.8
	HMDB0035457	5-Hydroxy-4-octanone	C8H16O2	M+H	145.1223	-2.8
	HMDB0031290	1-Hydroxy-3-octanone	C8H16O2	M+H	145.1223	-2.8
	HMDB0000482	Caprylic acid	C8H16O2	M+H	145.1223	-2.8
	HMDB0062511	Caprylic acid	C8H16O2	M+H	145.1223	-2.8
	HMDB0031703	2-Ethylbutyl acetate	C8H16O2	M+H	145.1223	-2.8
	HMDB0031587	2-Methylheptanoic acid	C8H16O2	M+H	145.1223	-2.8
	HMDB0031588	6-Methylheptanoic acid	C8H16O2	M+H	145.1223	-2.8
	HMDB0039217	Isopropyl 2-methylbutanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0039620	Butyl butyrate	C8H16O2	M+H	145.1223	-2.8
	HMDB0040298	Ethyl 2-ethylbutanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0040252	Isobutyl isobutyrate	C8H16O2	M+H	145.1223	-2.8
	HMDB0040251	Butyl isobutyrate	C8H16O2	M+H	145.1223	-2.8
	HMDB0032047	Propyl 3-methylbutanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0031638	Pentyl propanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0032046	Isopropyl 3-methylbutanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0040296	Propyl pentanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0031230	2-Ethylhexanoic acid	C8H16O2	M+H	145.1223	-2.8
	HMDB0062546	2-Ethylhexanoic acid	C8H16O2	M+H	145.1223	-2.8
	HMDB0031596	Methyl 5-methylhexanoate	C8H16O2	M+H	145.1223	-2.8
	HMDB0001877	Valproic acid	C8H16O2	M+H	145.1223	-2.8
146.0808	HMDB0062047	3,4-dimethyloxolane-2,5-dione	C6H8O3	M+NH4	146.0812	-2.5
	HMDB0173548	2,5-furandimethanol	C6H8O3	M+NH4	146.0812	-2.5
	HMDB0040732	2,7-Oxepanedione	C6H8O3	M+NH4	146.0812	-2.5
	HMDB0179349	(2Z)-3-(3-methyloxiran-2-yl)prop-2-enoic acid	C6H8O3	M+NH4	146.0812	-2.5
	HMDB0179347	(2Z)-6-hydroxyhexa-2,4-dienoic acid	C6H8O3	M+NH4	146.0812	-2.5
	HMDB0179348	3-[(1E)-prop-1-en-1-yl]oxirane-2-carboxylic acid	C6H8O3	M+NH4	146.0812	-2.5
	HMDB0163704	SCHEMBL144397	C6H8O3	M+NH4	146.0812	-2.5
	HMDB0033285	L-erythro-5-(1-Hydroxyethyl)-2(5H)-furanone	C6H8O3	M+NH4	146.0812	-2.5
	HMDB0038072	xi-5-Acetyltetrahydro-2(3H)-furanone	C6H8O3	M+NH4	146.0812	-2.5
	HMDB0031306	3-Hydroxy-4,5-dimethyl-2(5H)-furanone	C6H8O3	M+NH4	146.0812	-2.5
	HMDB0031303	Osmundalactone	C6H8O3	M+NH4	146.0812	-2.5
	HMDB0031847	2-Ethyl-3,4-dihydroxyfuran	C6H8O3	M+NH4	146.0812	-2.5
	HMDB0040594	Furaneol	C6H8O3	M+NH4	146.0812	-2.5
	HMDB0033517	5,6-Dihydro-4-methoxy-2H-pyran-2-one	C6H8O3	M+NH4	146.0812	-2.5
	HMDB0240326	N-(1-carboxypropyl)ethanecarboximidate	C6H10NO3	M+H	146.0812	-2.5
	HMDB0094698	N-PROPIONYLALANINE	C6H11NO3	M+H	146.0812	-2.5
	HMDB0061156	N-(2-Carboxymethyl)-morpholine	C6H11NO3	M+H	146.0812	-2.5
	HMDB0015127	Methyl aminolevulinate	C6H11NO3	M+H	146.0812	-2.5
	HMDB0029426	L-trans-5-Hydroxy-2-piperidinecarboxylic acid	C6H11NO3	M+H	146.0812	-2.5

	HMDB0029425	L-cis-4-(Hydroxymethyl)-2-pyrrolidinecarboxylic acid	C6H11NO3	M+H	146.0812	-2.5
	HMDB0012151	2-Keto-6-aminocaproate	C6H11NO3	M+H	146.0812	-2.5
	HMDB0012131	(S)-5-Amino-3-oxohexanoate	C6H11NO3	M+H	146.0812	-2.5
	HMDB0003681	4-Acetamidobutanoic acid	C6H11NO3	M+H	146.0812	-2.5
	HMDB0060265	4-Acetamidobutanoic acid	C6H11NO3	M+H	146.0812	-2.5
	HMDB0000808	N-Butyrylglycine	C6H11NO3	M+H	146.0812	-2.5
	HMDB0000730	Isobutyrylglycine	C6H11NO3	M+H	146.0812	-2.5
	HMDB0001263	(S)-2-amino-6-oxohexanoate	C6H11NO3	M+H	146.0812	-2.5
	HMDB0059595	(S)-2-amino-6-oxohexanoate	C6H11NO3	M+H	146.0812	-2.5
146.1172	HMDB0166738	3-butyloxirane-2-carbaldehyde	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0164724	4-Hydroxy-4-methylcyclohexanone	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0165094	3-(Hydroxymethyl)cyclohexanone	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0165095	3-Hydroxy-3-methylcyclohexan-1-one	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0165096	SCHEMBL443446	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0165097	SCHEMBL132855	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0031484	2-Heptenoic acid	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0031593	5-Methyl-2,3-hexanedione	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0033793	4-Heptenoic acid	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0038962	Ethyl tiglate	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0031500	Methyl 2E-hexenoate	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0180323	(2E)-3-(3-ethyloxiran-2-yl)prop-2-en-1-ol	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0029314	Isopentenyl acetate	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0031477	3,4-Heptanedione	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0031476	2,3-Heptanedione	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0031504	Methyl (Z)-3-hexenoate	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0031603	Ethyl 4-pentenoate	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0040214	cis-3-Hexenyl formate	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0031342	Cyclohexanecarboxylic acid	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0038271	2-Hexenyl formate	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0031174	4-Methyl-5-hexanolide	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0031681	Dihydro-5-propyl-2(3H)-furanone	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0059876	Pantolactone	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0039819	2,4-Dimethyl-2-pentenoic acid	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0030330	1-Methoxy-3-methylene-2-pentanone	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0166739	(2E)-7-hydroxyhept-2-enal	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0166737	6-Hydroxy-2-heptenal	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0166736	4-Hydroxyheptenal	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0173760	SCHEMBL14734478	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0173761	3-methylcyclohex-3-ene-1,2-diol	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0173762	5-methylcyclohex-4-ene-1,3-diol	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0173763	1-methyl-7-oxabicyclo[4.1]heptan-3-ol	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0032460	4-Pentenyl acetate	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0031351	Cyclohexyl formate	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0180322	3-(3-ethyloxiran-2-yl)propanal	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0029165	1,3-Diacetylpropane	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0032391	3-Methyl-3-butenyl acetate	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0040591	Allyl butyrate	C7H12O2	M+NH4	146.1176	-2.4
	HMDB0145116	SCHEMBL8185	C7H15NO2	M+H	146.1176	-2.4
	HMDB0145125	1-(2-hydroxyethyl)piperidin-3-ol	C7H15NO2	M+H	146.1176	-2.4
	HMDB0145113	SCHEMBL34937	C7H15NO2	M+H	146.1176	-2.4
	HMDB0145115	5-[(2-hydroxyethyl)amino]pentanal	C7H15NO2	M+H	146.1176	-2.4
	HMDB0145114	1-(piperidin-1-yl)ethane-1,2-diol	C7H15NO2	M+H	146.1176	-2.4
	HMDB0094649	L-2-aminoheptanoic acid	C7H15NO2	M+H	146.1176	-2.4
	HMDB0001161	4-Trimethylammoniobutanoic acid	C7H15NO2	M+H	146.1176	-2.4
	HMDB0006831	4-Trimethylammoniobutanoic acid	C7H15NO2	M+H	146.1176	-2.4
146.1648	HMDB0001257	Spermidine	C7H19N3	M+H	146.1652	-2.6
	HMDB0240327	2,3-dimethylbutanedioate	C6H8O4	M+H	147.0652	-2.6
	HMDB0161125	3-hydroxy-4-methyl-2-oxopentanoic acid	C6H10O4	M+H	147.0652	-2.6
	HMDB0155922	Mevaldic acid	C6H10O4	M+H	147.0652	-2.6
	HMDB0158746	SCHEMBL1268	C6H10O4	M+H	147.0652	-2.6
	HMDB0158745	SCHEMBL143458	C6H10O4	M+H	147.0652	-2.6
	HMDB0158748	SCHEMBL2592393	C6H10O4	M+H	147.0652	-2.6
	HMDB0158747	2-(hydroxymethyl)-3-oxopentanoic acid	C6H10O4	M+H	147.0652	-2.6
	HMDB0159477	3-Hydroxy-3-methyl-2-oxopentanoate	C6H10O4	M+H	147.0652	-2.6
	HMDB0159478	SCHEMBL3185864	C6H10O4	M+H	147.0652	-2.6

147.0648	HMDB0159480	SCHEMBL85244	C6H10O4	M+H	147.0652	-2.6
	HMDB0159479	3-(hydroxymethyl)-2-oxopentanoic acid	C6H10O4	M+H	147.0652	-2.6
	HMDB0161124	5-hydroxy-4-methyl-2-oxopentanoic acid	C6H10O4	M+H	147.0652	-2.6
	HMDB0161123	SCHEMBL193563	C6H10O4	M+H	147.0652	-2.6
	HMDB0061930	4-Ethoxy-4-oxobutanoic acid	C6H10O4	M+H	147.0652	-2.6
	HMDB0033837	Dimethyl succinate	C6H10O4	M+H	147.0652	-2.6
	HMDB0006900	(S)-2-Aceto-2-hydroxybutanoic acid	C6H10O4	M+H	147.0652	-2.6
	HMDB0002173	Solerol	C6H10O4	M+H	147.0652	-2.6
	HMDB0002074	2,2-Dimethylsuccinic acid	C6H10O4	M+H	147.0652	-2.6
	HMDB0000858	Monomethyl glutaric acid	C6H10O4	M+H	147.0652	-2.6
	HMDB0000752	Methylglutaric acid	C6H10O4	M+H	147.0652	-2.6
	HMDB0000448	Adipic acid	C6H10O4	M+H	147.0652	-2.6
	HMDB0000422	2-Methylglutaric acid	C6H10O4	M+H	147.0652	-2.6
147.0760	HMDB0001369	Pyrroline hydroxycarboxylic acid	C5H7NO3	M+NH4	147.0764	-2.8
	HMDB0061093	dimethadione	C5H7NO3	M+NH4	147.0764	-2.8
	HMDB0062585	(3R,5S)-1-pyrroline-3-hydroxy-5-carboxylic acid	C5H7NO3	M+NH4	147.0764	-2.8
	HMDB0002234	1-Pyrroline-4-hydroxy-2-carboxylate	C5H7NO3	M+NH4	147.0764	-2.8
	HMDB0000267	Pyroglutamic acid	C5H7NO3	M+NH4	147.0764	-2.8
	HMDB0001843	N-Acryloylglycine	C5H7NO3	M+NH4	147.0764	-2.8
	HMDB0000805	Pyrrolidonecarboxylic acid	C5H7NO3	M+NH4	147.0764	-2.8
	HMDB0060262	Pyrrolidonecarboxylic acid	C5H7NO3	M+NH4	147.0764	-2.8
	HMDB0006899	Alanylglycine	C5H10N2O3	M+H	147.0764	-2.8
	HMDB0240333	4-[(C-hydroxycarbonimidoyl)amino]butanoate	C5H9N2O3	M+H	147.0764	-2.8
	HMDB0000641	L-Glutamine	C5H10N2O3	M+H	147.0764	-2.8
	HMDB0003423	D-Glutamine	C5H10N2O3	M+H	147.0764	-2.8
	HMDB0028687	Alanylglycine	C5H10N2O3	M+H	147.0764	-2.8
147.1012	HMDB0002031	Ureidoisobutyric acid	C5H10N2O3	M+H	147.0764	-2.8
	HMDB0161032	6-hydroxyheptanoic acid	C7H14O3	M+H	147.1016	-2.5
	HMDB0161033	7-Hydroxyheptanoic acid	C7H14O3	M+H	147.1016	-2.5
	HMDB0165833	Ethyl 3-hydroxy-2-methylbutyrate	C7H14O3	M+H	147.1016	-2.5
	HMDB0165834	SCHEMBL934322	C7H14O3	M+H	147.1016	-2.5
	HMDB0165836	SCHEMBL7861	C7H14O3	M+H	147.1016	-2.5
	HMDB0165835	Ethyl 2-(hydroxymethyl)butanoate	C7H14O3	M+H	147.1016	-2.5
	HMDB0036231	Methyl DL-Leucate	C7H14O3	M+H	147.1016	-2.5
	HMDB0039407	Methyl 3-hydroxyhexanoate	C7H14O3	M+H	147.1016	-2.5
	HMDB0040254	Butyl lactate	C7H14O3	M+H	147.1016	-2.5
	HMDB0032269	(+/-)-Ethyl 2-hydroxy-2-methylbutyrate	C7H14O3	M+H	147.1016	-2.5
	HMDB0059842	Ethyl 2-hydroxyisovalerate	C7H14O3	M+H	147.1016	-2.5
	HMDB0061653	3-hydroxyheptanoic acid	C7H14O3	M+H	147.1016	-2.5
147.1124	HMDB0161034	2-hydroxyheptanoic acid	C7H14O3	M+H	147.1016	-2.5
	HMDB0002207	3-Hydroxyisooheptanoic acid	C7H14O3	M+H	147.1016	-2.5
	HMDB0029444	56633-75-1	C6H11NO2	M+NH4	147.1128	-2.7
	HMDB0094696	N-Methyl-L-proline	C6H11NO2	M+NH4	147.1128	-2.7
	HMDB0094697	piperidine-1-carboxylic acid	C6H11NO2	M+NH4	147.1128	-2.7
	HMDB0059649	3-Acetamidobutanal	C6H11NO2	M+NH4	147.1128	-2.7
	HMDB0000070	Pipecolic acid	C6H11NO2	M+NH4	147.1128	-2.7
	HMDB0062767	Pipecolic acid	C6H11NO2	M+NH4	147.1128	-2.7
	HMDB0000716	L-Pipecolic acid	C6H11NO2	M+NH4	147.1128	-2.7
	HMDB0004226	N4-Acetylaminobutanal	C6H11NO2	M+NH4	147.1128	-2.7
	HMDB0029435	L-trans-4-Methyl-2-pyrrolidinecarboxylic acid	C6H11NO2	M+NH4	147.1128	-2.7
	HMDB0005960	D-Pipecolic acid	C6H11NO2	M+NH4	147.1128	-2.7
	HMDB0062225	(2E)-Decenoyl-ACP	C6H11NO2	M+NH4	147.1128	-2.7
147.1375	HMDB0015212	Vigabatrin	C6H11NO2	M+NH4	147.1128	-2.7
	HMDB0142894	2,6-diaminohexanoic acid	C6H14N2O2	M+H	147.1128	-2.7
	HMDB0012115	(3S,5S)-3,5-Diaminohexanoate	C6H14N2O2	M+H	147.1128	-2.7
	HMDB0000182	L-Lysine	C6H14N2O2	M+H	147.1128	-2.7
	HMDB0003405	D-Lysine	C6H14N2O2	M+H	147.1128	-2.7
	HMDB0012114	(3S)-3,6-Diaminohexanoate	C6H14N2O2	M+H	147.1128	-2.7
	HMDB0029359	(R)-1,3-Octanediol	C8H18O2	M+H	147.1380	-3.1
	HMDB0170960	1,7-Octanediol	C8H18O2	M+H	147.1380	-3.1
	HMDB0172313	octane-1,2-diol	C8H18O2	M+H	147.1380	-3.1
	HMDB0170961	octane-1,8-diol	C8H18O2	M+H	147.1380	-3.1
	HMDB0038679	1-Methoxy-1-pentyloxyethane	C8H18O2	M+H	147.1380	-3.1
	HMDB0037635	xi-1-Ethoxy-1-butoxyethane	C8H18O2	M+H	147.1380	-3.1
	HMDB0172312	19686-96-5	C8H18O2	M+H	147.1380	-3.1

148.0600	HMDB0013233	Gamma-delta-Dioxovaleric acid	C5H6O4	M+NH4	148.0604	-2.9
	HMDB0059743	2-Hydroxyglutaric acid lactone	C5H6O4	M+NH4	148.0604	-2.9
	HMDB0033809	Methyl hydrogen fumarate	C5H6O4	M+NH4	148.0604	-2.9
	HMDB0000620	Glutaconic acid	C5H6O4	M+NH4	148.0604	-2.9
	HMDB0061185	Glutaconic acid	C5H6O4	M+NH4	148.0604	-2.9
	HMDB0002092	Itaconic acid	C5H6O4	M+NH4	148.0604	-2.9
	HMDB0000749	Mesaconic acid	C5H6O4	M+NH4	148.0604	-2.9
	HMDB0000634	Citraconic acid	C5H6O4	M+NH4	148.0604	-2.9
	HMDB0060365	2,5-Dioxopentanoate	C5H6O4	M+NH4	148.0604	-2.9
	HMDB0156263	glutamate(1-)	C5H8NO4	M+H	148.0604	-2.9
	HMDB0062183	N-lactoyl-glycine	C5H9NO4	M+H	148.0604	-2.9
	HMDB0000148	L-Glutamic acid	C5H9NO4	M+H	148.0604	-2.9
	HMDB0002931	N-Acetylserine	C5H9NO4	M+H	148.0604	-2.9
	HMDB0002393	N-Methyl-D-aspartic acid	C5H9NO4	M+H	148.0604	-2.9
	HMDB0003011	O-Acetylserine	C5H9NO4	M+H	148.0604	-2.9
	HMDB0003339	D-Glutamic acid	C5H9NO4	M+H	148.0604	-2.9
	HMDB0006556	L-4-Hydroxyglutamate semialdehyde	C5H9NO4	M+H	148.0604	-2.9
	HMDB0060475	DL-Glutamate	C5H9NO4	M+H	148.0604	-2.9
	HMDB0033550	3-(Carboxymethylamino)propanoic acid	C5H9NO4	M+H	148.0604	-2.9
148.0794	HMDB0040238	2-Ethylidihydro-3(2H)-thiophenone	C6H10OS	M+NH4	148.0791	2.3
	HMDB0031370	2-[(Methylthio)methyl]-2-butenal	C6H10OS	M+NH4	148.0791	2.3
	HMDB0037493	S-2-Propenyl propanethioate	C6H10OS	M+NH4	148.0791	2.3
148.0964	HMDB0041602	Methyl levulinate	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0163716	3-Methyl-4-oxopentanoic acid	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0165590	(2Z)-2-(hydroxymethyl)pent-2-enoic acid	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0165593	(2Z)-5-hydroxy-2-methylpent-2-enoic acid	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0169668	AKO238761	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0169667	SCHEMBL159549	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0169670	SCHEMBL1645858	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0169669	3-ethyl-3-methyl-oxiranecarboxylic acid	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0169696	(2Z)-4-hydroxy-3-methylpent-2-enoic acid	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0169698	SCHEMBL6488	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0165591	(2Z)-4-hydroxy-2-methylpent-2-enoic acid	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0163708	(3Z)-1,5-dihydroxy-3-methylpent-3-en-2-one	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0162571	SCHEMBL13481223	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0163359	(4Z)-6-hydroxyhex-4-enoic acid	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0163360	SCHEMBL667341	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0163362	AKO6375916	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0163361	3-(3-methyloxiran-2-yl)propanoic acid	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0163707	1-[3-(hydroxymethyl)-2-methyloxiran-2-yl]ethan-1-one	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0163705	3-(hydroxymethyl)-4-oxopentanal	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0163706	(3Z)-5-hydroxy-3-(hydroxymethyl)pent-3-en-2-one	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0169697	(2E)-3-(hydroxymethyl)pent-2-enoic acid	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0033286	Sherry lactone	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0165592	SCHEMBL2684392	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0033698	Acetoin acetate	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0031214	5-Ethoxy-4,5-dihydro-2(3H)furanone	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0000491	(S)-3-methyl-2-oxopentanoate	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0012882	Adipate semialdehyde	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0061881	4-Acetylbutyrate	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0033302	(4S,6S)-3,4,5,6-Tetrahydro-4-hydroxy-6-methyl-2H-pyran-2-one	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0010717	3-Oxohexanoic acid	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0006024	Mevalonolactone	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0031216	Ethyl acetoacetate	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0031218	Ethyl acetoacetate	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0000695	Ketoleucine	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0000408	2-Methyl-3-ketovaleric acid	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0001864	2-Ketohexanoic acid	C6H10O3	M+NH4	148.0968	-2.8
	HMDB0029449	(2R,3R,4R)-2-Amino-4-hydroxy-3-methylpentanoic acid	C6H13NO3	M+H	148.0968	-2.8
	HMDB0061157	N-(2-Hydroxyethyl)-morpholine N-oxide	C6H13NO3	M+H	148.0968	-2.8
	HMDB0168723	SCHEMBL8751245	C6H13NO3	M+H	148.0968	-2.8
	HMDB0168724	SCHEMBL5934	C6H13NO3	M+H	148.0968	-2.8
	HMDB0142963	2-amino-6-hydroxyhexanoic acid	C6H13NO3	M+H	148.0968	-2.8

	HMDB0033453	Fagomine	C6H13NO3	M+H	148.0968	-2.8
148.1158	HMDB0031537	3-Methylcyclohexanethiol	C7H14S	M+NH4	148.1154	2.4
	HMDB0166743	(2E)-hept-2-ene-1,7-diol	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0166741	(2E)-hept-2-ene-1,6-diol	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0166740	SCHEMBL32814	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0166742	3-Butyloxirane-2-methanol	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0030028	Ethyl isovalerate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0039618	Propyl butyrate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0035238	Methyl hexanoate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0036237	Methyl 2-methylpentanoate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0030052	Butyl propionate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0031600	2-Pentanol acetate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0036238	Methyl 4-methylpentanoate	C7H14O2	M+NH4	148.1332	-0.7
148.1331	HMDB0031594	2-Methylhexanoic acid	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0031528	Isopentyl acetate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0033745	Ethyl 2-methylbutyrate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0038227	Isopropyl 2-methylpropanoate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0034239	2-Methylpropyl propanoate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0032204	cis- and trans-2-Isopropyl-4-methyl-1,3-dioxolane	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0032874	Hexyl formate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0040297	Ethyl pentanoate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0039619	Isopropyl butyrate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0036209	Propyl 2-methylpropanoate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0039095	Pentyl acetate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0031595	5-Methylhexanoic acid	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0034166	2-Methylbutyl acetate	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0000666	Heptanoic acid	C7H14O2	M+NH4	148.1332	-0.7
	HMDB0161319	Itamalic acid	C5H8O5	M+H	149.0444	-1.0
	HMDB0061190	3-methylmalate(2-)	C5H8O5	M+H	149.0444	-1.0
	HMDB0062739	3-methylmalate(2-)	C5H8O5	M+H	149.0444	-1.0
	HMDB0000694	L-2-Hydroxyglutaric acid	C5H8O5	M+H	149.0444	-1.0
	HMDB0160406	SCHEMBL41920	C5H8O5	M+H	149.0444	-1.0
	HMDB0000428	3-Hydroxyglutaric acid	C5H8O5	M+H	149.0444	-1.0
	HMDB0000426	Citramalic acid	C5H8O5	M+H	149.0444	-1.0
149.0443	HMDB0000606	D-2-Hydroxyglutaric acid	C5H8O5	M+H	149.0444	-1.0
	HMDB0001900	Ribonolactone	C5H8O5	M+H	149.0444	-1.0
	HMDB0011676	D-Xylono-1,5-lactone	C5H8O5	M+H	149.0444	-1.0
	HMDB0160668	Aethyltartronsaure	C5H8O5	M+H	149.0444	-1.0
	HMDB0059655	2-Hydroxyglutarate	C5H8O5	M+H	149.0444	-1.0
	HMDB0160666	SCHEMBL1124153	C5H8O5	M+H	149.0444	-1.0
	HMDB0160667	SCHEMBL6374585	C5H8O5	M+H	149.0444	-1.0
	HMDB0160407	3-ethoxy-2-hydroxy-3-oxopropanoic acid	C5H8O5	M+H	149.0444	-1.0
	HMDB0128078	3-phenylprop-2-enoic acid	C9H8O2	M+H	149.0597	-2.7
	HMDB0135273	(2Z)-2-hydroxy-3-phenylprop-2-enal	C9H8O2	M+H	149.0597	-2.7
	HMDB0135274	(2E)-3-(3-hydroxyphenyl)prop-2-enal	C9H8O2	M+H	149.0597	-2.7
	HMDB0135275	3-phenyloxirane-2-carbaldehyde	C9H8O2	M+H	149.0597	-2.7
	HMDB0135648	3-(4-hydroxyphenyl)prop-2-enal	C9H8O2	M+H	149.0597	-2.7
	HMDB0134039	3-(2-hydroxyphenyl)prop-2-enal	C9H8O2	M+H	149.0597	-2.7
149.0593	HMDB0000930	trans-Cinnamic acid	C9H8O2	M+H	149.0597	-2.7
	HMDB0040986	(E)-3-(4-Hydroxyphenyl)-2-propenal	C9H8O2	M+H	149.0597	-2.7
	HMDB0031725	(E)-3-(2-Hydroxyphenyl)-2-propenal	C9H8O2	M+H	149.0597	-2.7
	HMDB0035243	1-Phenyl-1,2-propanedione	C9H8O2	M+H	149.0597	-2.7
	HMDB0032947	Di-2-furanylmethane	C9H8O2	M+H	149.0597	-2.7
	HMDB0036626	3,4-Dihydro-2H-1-benzopyran-2-one	C9H8O2	M+H	149.0597	-2.7
	HMDB0000567	Cinnamic acid	C9H8O2	M+H	149.0597	-2.7
	HMDB0167024	acetyl(2-hydroxypropyl)methylsulfonium	C6H13O2S	M+H	149.0631	2.2
	HMDB0167027	acetyl(3-hydroxypropyl)methylsulfonium	C6H13O2S	M+H	149.0631	2.2
	HMDB0167030	(2-hydroxyacetyl)(methyl)propylsulfonium	C6H13O2S	M+H	149.0631	2.2
	HMDB0173817	SCHEMBL12997424	C6H13O2S	M+H	149.0631	2.2
	HMDB0032271	Ethyl 3-mercaptopbutyrate	C6H12O2S	M+H	149.0631	2.2
	HMDB0039653	2,4,6-Trimethyl-1,3,5-dioxathiane	C6H12O2S	M+H	149.0631	2.2
149.0634	HMDB0038299	Methylthiomethyl butyrate	C6H12O2S	M+H	149.0631	2.2
	HMDB0031717	3-(Methylthio)propyl acetate	C6H12O2S	M+H	149.0631	2.2
	HMDB0040413	Ethyl 3-(methylthio)propanoate	C6H12O2S	M+H	149.0631	2.2
	HMDB0036193	3-Mercapto-3-methylbutyl formate	C6H12O2S	M+H	149.0631	2.2

	HMDB0041306	Methyl 2-(methylthio)butyrate	C6H12O2S	M+H	149.0631	2.2
	HMDB0032410	Methyl 3-(methylthio)butanoate	C6H12O2S	M+H	149.0631	2.2
	HMDB0032495	Propyl 2-mercaptopropionate	C6H12O2S	M+H	149.0631	2.2
	HMDB0037619	Methyl 4-(methylthio)butyrate	C6H12O2S	M+H	149.0631	2.2
149.0925	HMDB0061880	N-Acetyl-beta-alanine	C5H9NO3	M+NH4	149.0921	2.9
	HMDB0240251	cis-4-Hydroxyproline	C5H9NO3	M+NH4	149.0921	2.9
	HMDB0002113	3-Hydroxy-L-proline	C5H9NO3	M+NH4	149.0921	2.9
	HMDB0000783	Propionylglycine	C5H9NO3	M+NH4	149.0921	2.9
	HMDB0000766	N-Acetyl-L-alanine	C5H9NO3	M+NH4	149.0921	2.9
	HMDB0000725	4-Hydroxyproline	C5H9NO3	M+NH4	149.0921	2.9
	HMDB0036576	4-Hydroxyproline	C5H9NO3	M+NH4	149.0921	2.9
	HMDB0002104	L-Glutamic gamma-semialdehyde	C5H9NO3	M+NH4	149.0921	2.9
	HMDB0001149	5-Aminolevulinic acid	C5H9NO3	M+NH4	149.0921	2.9
	HMDB0006055	4-Hydroxy-L-proline	C5H9NO3	M+NH4	149.0921	2.9
	HMDB0006272	5-Amino-2-oxopentanoic acid	C5H9NO3	M+NH4	149.0921	2.9
	HMDB0060460	cis-4-Hydroxy-D-proline	C5H9NO3	M+NH4	149.0921	2.9
149.0957	HMDB0059659	Trans-3-hydroxy-L-proline	C5H9NO3	M+NH4	149.0921	2.9
	HMDB0133746	4-phenylbutan-2-one	C10H12O	M+H	149.0961	-2.6
	HMDB0180475	SCHEMBL295411	C10H12O	M+H	149.0961	-2.6
	HMDB0133593	(2E)-2-methyl-3-phenylprop-2-en-1-ol	C10H12O	M+H	149.0961	-2.6
	HMDB0032015	Duryl aldehyde	C10H12O	M+H	149.0961	-2.6
	HMDB0033382	2-(4-Methylphenyl)propanal	C10H12O	M+H	149.0961	-2.6
	HMDB0032014	2,3,6-Trimethylbenzaldehyde	C10H12O	M+H	149.0961	-2.6
	HMDB0030837	Anethole	C10H12O	M+H	149.0961	-2.6
	HMDB0032016	2,4,6-Trimethylbenzaldehyde	C10H12O	M+H	149.0961	-2.6
	HMDB0032017	3,4,5-Trimethylbenzaldehyde	C10H12O	M+H	149.0961	-2.6
	HMDB0032140	2',4'-Dimethylacetophenone	C10H12O	M+H	149.0961	-2.6
	HMDB0034121	1-Methoxy-4-(2-propenyl)benzene	C10H12O	M+H	149.0961	-2.6
	HMDB0031616	4-Phenyl-3-buten-2-ol	C10H12O	M+H	149.0961	-2.6
	HMDB0002214	Cuminaldehyde	C10H12O	M+H	149.0961	-2.6
149.1322	HMDB0059845	p-Ethylacetophenone	C10H12O	M+H	149.0961	-2.6
	HMDB0061997	2-Methyl-3-phenylpropanal	C10H12O	M+H	149.0961	-2.6
	HMDB0059834	Pentylbenzene	C11H16	M+H	149.1325	-1.9
150.0579	HMDB0061810	2,4-Dimethyl-1-(1-methylethyl)-benzene	C11H16	M+H	149.1325	-1.9
	HMDB0061809	1-Methyl-4-(1-methylpropyl)-benzene	C11H16	M+H	149.1325	-1.9
	HMDB0059667	3-Methyl sulfolene	C5H8O2S	M+NH4	150.0583	-2.8
	HMDB0182893	[(1E)-2-carboxyeth-1-en-1-yl]dimethylsulfonium	C5H9O2S	M+NH4	150.0583	-2.8
	HMDB0033951	Racemethionine	C5H11NO2S	M+H	150.0583	-2.8
150.0757	HMDB0014997	Penicillamine	C5H11NO2S	M+H	150.0583	-2.8
	HMDB0000696	L-Methionine	C5H11NO2S	M+H	150.0583	-2.8
	HMDB0145654	SCHEMBL17123851	C5H8O4	M+NH4	150.0761	-2.5
	HMDB0154760	alpha-keto-beta-methyl-gamma-hydroxy-butyric acid	C5H8O4	M+NH4	150.0761	-2.5
	HMDB0001844	(S)-methylsuccinic acid	C5H8O4	M+NH4	150.0761	-2.5
	HMDB0000661	Glutaric acid	C5H8O4	M+NH4	150.0761	-2.5
	HMDB0006855	(S)-2-Acetolactate	C5H8O4	M+NH4	150.0761	-2.5
	HMDB0029884	2-C-Methyl-1,4-erythrono-D-lactone	C5H8O4	M+NH4	150.0761	-2.5
	HMDB0006833	2-Acetolactate	C5H8O4	M+NH4	150.0761	-2.5
	HMDB0033958	2-Deoxy-L-ribose-1,4-lactone	C5H8O4	M+NH4	150.0761	-2.5
	HMDB0040531	2-Hydroxy-4-oxopentanoic acid	C5H8O4	M+NH4	150.0761	-2.5
	HMDB0002001	Dimethylmalonic acid	C5H8O4	M+NH4	150.0761	-2.5
	HMDB0000576	Monoethyl malonic acid	C5H8O4	M+NH4	150.0761	-2.5
	HMDB0000622	Ethylmalonic acid	C5H8O4	M+NH4	150.0761	-2.5
	HMDB0154759	3-Hydroxy-3-methyl-2-oxobutanoic acid	C5H8O4	M+NH4	150.0761	-2.5
150.0909	HMDB0060671	Atropaldehyde	C9H8O	M+NH4	150.0913	-2.9
	HMDB0059847	2-Methylcumarone	C9H8O	M+NH4	150.0913	-2.9
	HMDB0059602	Indanone	C9H8O	M+NH4	150.0913	-2.9
	HMDB0003441	Cinnamaldehyde	C9H8O	M+NH4	150.0913	-2.9
	HMDB0032072	(Z)-Cinnamaldehyde	C9H8O	M+NH4	150.0913	-2.9
	HMDB0030175	Venoterpene	C9H11NO	M+H	150.0913	-2.9
	HMDB0040029	2,3-Dihydro-5-methyl-1H-pyrrolizine-7-	C9H11NO	M+H	150.0913	-2.9
	HMDB0040016	2-(2-Furanyl)-3,4,5,6-tetrahydropyridine	C9H11NO	M+H	150.0913	-2.9
	HMDB0040043	3-(2-Furanylmethylene)pyrrolidine	C9H11NO	M+H	150.0913	-2.9
	HMDB0040051	5-Acetyl-2,3-dihydro-1H-pyrrolizine	C9H11NO	M+H	150.0913	-2.9
	HMDB0040050	3,4-Dihydro-5-(5-methyl-2-furanyl)-2H-pyrrole	C9H11NO	M+H	150.0913	-2.9
	HMDB0040047	2,3-Dihydro-6-methyl-1H-pyrrolizine-5-	C9H11NO	M+H	150.0913	-2.9

150.1121	HMDB0039662	2,3,6,7-Tetrahydrocyclopent[b]azepin-8(1H)-one	C9H11NO	M+H	150.0913	-2.9
	HMDB0061652	(S)-3-hydroxyhexanoic acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0171222	4-hydroxy-3-methylbutyl formate	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0165042	3-hydroxymethyl-valeric acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0165043	5-hydroxy-3-methylpentanoic acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0165041	4-hydroxy-3-methyl-valeric acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0163682	1,6-dihydroxy-2-hexanone	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0163680	SCHEMBL5464	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0163681	3,6-dihydroxyhexan-2-one	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0163679	5,6-dihydroxyhexan-2-one	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0161116	5-hydroxy-4-methylpentanoic acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0161115	4-hydroxy-4-methylpentanoic acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0040409	Ethyl 3-hydroxybutyrate	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0033851	4,4-Dimethoxy-2-butanone	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0010718	(R)-3-Hydroxyhexanoic acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0001975	2-Ethyl-2-Hydroxybutyric acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0001624	2-Hydroxycaproic acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0000746	Hydroxyisocaproic acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0000665	Leucinic acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0000624	D-Leucic acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0000525	5-Hydroxyhexanoic acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0000409	(5R)-5-Hydroxyhexanoic acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0000317	2-Hydroxy-3-methylpentanoic acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0032456	Paraldehyde	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0032158	(+/-)-1-Acetoxy-1-ethoxyethane	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0059770	Threo-3-Hydroxy-2-methylbutyric acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0041844	Butoxyacetic acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0029166	2-Methyl-3-hydroxyvaleric acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0165040	3-hydroxy-3-methylpentanoic acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0012843	6-Hydroxyhexanoic acid	C6H12O3	M+NH4	150.1125	-2.4
	HMDB0032538	Triethanolamine	C6H15NO3	M+H	150.1125	-2.5
151.0611	HMDB0003162	7-Methylhypoxanthine	C6H6N4O	M+H	151.0614	-2.2
	HMDB0013141	1-Methylhypoxanthine	C6H6N4O	M+H	151.0614	-2.2
	HMDB0032180	Butyl ethyl disulfide	C6H14S2	M+H	151.0610	0.9
	HMDB0040056	xi-1-(Propylthio)-1-propanethiol	C6H14S2	M+H	151.0610	0.9
	HMDB0029578	Diisopropyl disulfide	C6H14S2	M+H	151.0610	0.9
	HMDB0031161	Methyl pentyl disulfide	C6H14S2	M+H	151.0610	0.9
	HMDB0031709	1,6-Hexanedithiol	C6H14S2	M+H	151.0610	0.9
	HMDB0031472	Dipropyl disulfide	C6H14S2	M+H	151.0610	0.9
	HMDB0032408	Methyl isopentyl disulfide	C6H14S2	M+H	151.0610	0.9
151.0749	HMDB0135239	4-(prop-2-en-1-yl)benzene-1,2-diol	C9H10O2	M+H	151.0754	-3.0
	HMDB0062349	4-Chromanol	C9H10O2	M+H	151.0754	-3.0
	HMDB0176418	2-Nonene-4,6-diyne-1,9-diol	C9H10O2	M+H	151.0754	-3.0
	HMDB0170980	4-[(1Z)-prop-1-en-1-yl]benzene-1,2-diol	C9H10O2	M+H	151.0754	-3.0
	HMDB0170763	4-(oxiran-2-ylmethyl)phenol	C9H10O2	M+H	151.0754	-3.0
	HMDB0146657	2-hydroxycinnamyl alcohol	C9H10O2	M+H	151.0754	-3.0
	HMDB0146635	4-vinyl-3-methoxyphenol	C9H10O2	M+H	151.0754	-3.0
	HMDB0135280	3-[(1E)-3-hydroxyprop-1-en-1-yl]phenol	C9H10O2	M+H	151.0754	-3.0
	HMDB0135281	(3-phenyloxiran-2-yl)methanol	C9H10O2	M+H	151.0754	-3.0
	HMDB0135279	3-(4-hydroxyphenyl)propanal	C9H10O2	M+H	151.0754	-3.0
	HMDB0135278	3-(3-hydroxyphenyl)propanal	C9H10O2	M+H	151.0754	-3.0
	HMDB0135276	2-hydroxy-3-phenylpropanal	C9H10O2	M+H	151.0754	-3.0
	HMDB0135277	3-hydroxy-3-phenylpropanal	C9H10O2	M+H	151.0754	-3.0
	HMDB0134027	2-(3-hydroxyprop-1-en-1-yl)phenol	C9H10O2	M+H	151.0754	-3.0
	HMDB0134026	3-(2-hydroxyphenyl)propanal	C9H10O2	M+H	151.0754	-3.0
	HMDB0125532	3-ethenyl-5-methoxyphenol	C9H10O2	M+H	151.0754	-3.0
	HMDB0032592	2'-Hydroxy-5'-methylacetophenone	C9H10O2	M+H	151.0754	-3.0
	HMDB0033967	Ethyl benzoate	C9H10O2	M+H	151.0754	-3.0
	HMDB0032570	4'-Methoxyacetophenone	C9H10O2	M+H	151.0754	-3.0
	HMDB0032075	p-Tolyl acetate	C9H10O2	M+H	151.0754	-3.0
	HMDB0040428	2-Phenylethyl formate	C9H10O2	M+H	151.0754	-3.0
	HMDB0032073	o-Tolyl acetate	C9H10O2	M+H	151.0754	-3.0
	HMDB0032569	2'-Methoxyacetophenone	C9H10O2	M+H	151.0754	-3.0
	HMDB0033970	4-Ethoxybenzaldehyde	C9H10O2	M+H	151.0754	-3.0
	HMDB0031310	Benzyl acetate	C9H10O2	M+H	151.0754	-3.0

	HMDB0011743	2-Phenylpropionate	C9H10O2	M+H	151.0754	-3.0
	HMDB0003654	4-Coumaryl alcohol	C9H10O2	M+H	151.0754	-3.0
	HMDB0002237	3,4-Dimethylbenzoic acid	C9H10O2	M+H	151.0754	-3.0
	HMDB0002222	3-Methylphenylacetic acid	C9H10O2	M+H	151.0754	-3.0
	HMDB0002097	4-Ethylbenzoic acid	C9H10O2	M+H	151.0754	-3.0
	HMDB0013744	2-Methoxy-4-vinylphenol	C9H10O2	M+H	151.0754	-3.0
	HMDB0032617	Methyl phenylacetate	C9H10O2	M+H	151.0754	-3.0
	HMDB0040925	2-(2-Furanyl)-3-methyl-2-butenal	C9H10O2	M+H	151.0754	-3.0
	HMDB0038355	2-Ethyl-4-(2-furanyl)-2-propenal	C9H10O2	M+H	151.0754	-3.0
	HMDB0177508	4-(3-methyloxiran-2-yl)phenol	C9H10O2	M+H	151.0754	-3.0
	HMDB0135644	4-(3-hydroxyprop-1-en-1-yl)phenol	C9H10O2	M+H	151.0754	-3.0
	HMDB0176419	6-(3-methyloxiran-2-yl)hexa-3,5-diyne-1-ol	C9H10O2	M+H	151.0754	-3.0
	HMDB0059824	4-Hydroxy-3-methylacetophenone	C9H10O2	M+H	151.0754	-3.0
	HMDB0037715	1-Phenylethyl formate	C9H10O2	M+H	151.0754	-3.0
	HMDB0000764	Hydrocinnamic acid	C9H10O2	M+H	151.0754	-3.0
151.0961	HMDB0062045	hexane-1,2,5,6-tetrol	C6H14O4	M+H	151.0965	-2.5
	HMDB0062118	hexane-1,2,5,6-tetrol	C6H14O4	M+H	151.0965	-2.5
151.1113	HMDB0133616	2-methyl-3-phenylpropan-1-ol	C10H14O	M+H	151.1117	-2.9
	HMDB0163107	(2E,4Z,7Z)-deca-2,4,7,9-tetraene-1-ol	C10H14O	M+H	151.1117	-2.9
	HMDB0034846	2-(4-Methylphenyl)-1-propanol	C10H14O	M+H	151.1117	-2.9
	HMDB0036061	Safranal	C10H14O	M+H	151.1117	-2.9
	HMDB0035824	Carvone	C10H14O	M+H	151.1117	-2.9
	HMDB0036070	1-Acetyl-4-isopropenylcyclopentene	C10H14O	M+H	151.1117	-2.9
	HMDB0035591	3-Carene-5-one	C10H14O	M+H	151.1117	-2.9
	HMDB0029652	2-(4-Methylphenyl)-2-propanol	C10H14O	M+H	151.1117	-2.9
	HMDB0035770	5-Isopropyl-2-methylphenol	C10H14O	M+H	151.1117	-2.9
	HMDB0033544	(2E,4Z,7Z)-2,4,7-Decatrienal	C10H14O	M+H	151.1117	-2.9
	HMDB0036999	Piperitenone	C10H14O	M+H	151.1117	-2.9
	HMDB0035172	2,6,6-Trimethyl-1,4-cyclohexadiene-1-carboxaldehyde	C10H14O	M+H	151.1117	-2.9
	HMDB0031570	2-Methyl-1-phenyl-2-propanol	C10H14O	M+H	151.1117	-2.9
	HMDB0031817	Cuminyl alcohol	C10H14O	M+H	151.1117	-2.9
	HMDB0037561	Linden ether	C10H14O	M+H	151.1117	-2.9
	HMDB0036089	(R)-Menthofuran	C10H14O	M+H	151.1117	-2.9
	HMDB0001878	Thymol	C10H14O	M+H	151.1117	-2.9
	HMDB0003647	Perillyl aldehyde	C10H14O	M+H	151.1117	-2.9
	HMDB0004487	(S)-Carvone	C10H14O	M+H	151.1117	-2.9
	HMDB0061788	(S)-Carvone	C10H14O	M+H	151.1117	-2.9
	HMDB0038913	4,6-Decadiyne-1-ol	C10H14O	M+H	151.1117	-2.9
	HMDB0031613	4-Phenyl-2-butanol	C10H14O	M+H	151.1117	-2.9
	HMDB0034921	Teresantalal	C10H14O	M+H	151.1117	-2.9
	HMDB0035089	(R)-Carvone	C10H14O	M+H	151.1117	-2.9
	HMDB0035761	(-)-Pinocarvone	C10H14O	M+H	151.1117	-2.9
	HMDB0035250	Myrtenal	C10H14O	M+H	151.1117	-2.9
	HMDB0032626	1-Methoxy-4-propylbenzene	C10H14O	M+H	151.1117	-2.9
	HMDB0032063	4-tert-Butylphenol	C10H14O	M+H	151.1117	-2.9
	HMDB0062147	Perillene	C10H14O	M+H	151.1117	-2.9
	HMDB0032213	2-trans-4-trans-7-cis-Decatrienal	C10H14O	M+H	151.1117	-2.9
152.0229	HMDB0015231	Flucytosine	C4H4FN3O	M+Na	152.0231	-1.0
152.0313	HMDB0062585	(3R,5S)-1-pyrroline-3-hydroxy-5-carboxylic acid	C5H7NO3	M+Na	152.0318	-3.4
	HMDB0061093	dimethadione	C5H7NO3	M+Na	152.0318	-3.4
	HMDB0002234	1-Pyrroline-4-hydroxy-2-carboxylate	C5H7NO3	M+Na	152.0318	-3.4
	HMDB0001843	N-Acryloylglycine	C5H7NO3	M+Na	152.0318	-3.4
	HMDB0001369	Pyrroline hydroxycarboxylic acid	C5H7NO3	M+Na	152.0318	-3.4
	HMDB0000805	Pyrrolidonecarboxylic acid	C5H7NO3	M+Na	152.0318	-3.4
	HMDB0060262	Pyrrolidonecarboxylic acid	C5H7NO3	M+Na	152.0318	-3.4
	HMDB0000267	Pyroglutamic acid	C5H7NO3	M+Na	152.0318	-3.4
152.0467	HMDB0062769	Epsilon-caprolactam	C6H11NO	M+K	152.0472	-3.4
	HMDB0037293	2-Acetylpyrrolidine	C6H11NO	M+K	152.0472	-3.4
	HMDB0031199	2,5-Dihydro-2,4,5-trimethyloxazole	C6H11NO	M+K	152.0472	-3.4
	HMDB0031702	1-Piperidinecarboxaldehyde	C6H11NO	M+K	152.0472	-3.4
	HMDB0033731	Quinoline	C9H7N	M+Na	152.0471	-2.4
	HMDB0011664	3-Methylene-indolenine	C9H7N	M+Na	152.0471	-2.4
	HMDB0034244	Isoquinoline	C9H7N	M+Na	152.0471	-2.4
	HMDB0000542	8-Hydroxyadenine	C5H5N5O	M+H	152.0567	-3.2
	HMDB0000403	2-Hydroxyadenine	C5H5N5O	M+H	152.0567	-3.2

152.0562	HMDB0000132	Guanine	C5H5N5O	M+H	152.0567	-3.2
	HMDB0039789	Tetrahydro-2-methyl-2-thiophenethiol	C5H10S2	M+NH4	152.0562	-0.1
	HMDB0039790	Tetrahydro-2-methyl-3-thiophenethiol	C5H10S2	M+NH4	152.0562	-0.1
	HMDB0038974	3,3-Dimethyl-1,2-dithiolane	C5H10S2	M+NH4	152.0562	-0.1
152.0702	HMDB0062159	TEREPHTHALALDEHYDE	C8H6O2	M+NH4	152.0706	-2.6
	HMDB0129378	1-benzofuran-4-ol	C8H6O2	M+NH4	152.0706	-2.6
	HMDB0032469	Phthalide	C8H6O2	M+NH4	152.0706	-2.6
	HMDB0061916	Phenylglyoxal	C8H6O2	M+NH4	152.0706	-2.6
	HMDB0186197	N-(Acetyloxy)benzenamine	C8H9NO2	M+H	152.0706	-2.7
	HMDB0060680	2-Amino-3-methylbenzoate	C8H9NO2	M+H	152.0706	-2.7
	HMDB0176134	4-(Methylamino)benzoic acid	C8H9NO2	M+H	152.0706	-2.7
	HMDB0012992	Leukoaminochrome	C8H9NO2	M+H	152.0706	-2.7
	HMDB0033903	3alpha,4,7,7alpha-Tetrahydro-1H-isoindole-1,3(2H)-dione	C8H9NO2	M+H	152.0706	-2.7
	HMDB0032609	2-(Methylamino)benzoic acid	C8H9NO2	M+H	152.0706	-2.7
	HMDB0059846	Ethyl nicotinate	C8H9NO2	M+H	152.0706	-2.7
	HMDB0029703	Methyl 2-aminobenzoate	C8H9NO2	M+H	152.0706	-2.7
	HMDB0012219	Dopamine quinone	C8H9NO2	M+H	152.0706	-2.7
	HMDB0002210	2-Phenylglycine	C8H9NO2	M+H	152.0706	-2.7
	HMDB0062129	(Z)-(methyl N-hydroxybenzenecarboximidate)	C8H9NO2	M+H	152.0706	-2.7
	HMDB0061919	2'-Hydroxyacetanilide	C8H9NO2	M+H	152.0706	-2.7
	HMDB0001859	Acetaminophen	C8H9NO2	M+H	152.0706	-2.7
152.0735	HMDB0040410	Ethyl 3-mercaptopropanoic acid	C5H10O2S	M+NH4	152.0740	-3.1
	HMDB0032409	Methyl 3-mercaptobutanoate	C5H10O2S	M+NH4	152.0740	-3.1
	HMDB0040263	Ethyl 2-(methylthio)acetate	C5H10O2S	M+NH4	152.0740	-3.1
	HMDB0031521	Ethyl 2-mercaptopropionate	C5H10O2S	M+NH4	152.0740	-3.1
	HMDB0034377	Methyl 3-(methylthio)propanoate	C5H10O2S	M+NH4	152.0740	-3.1
	HMDB0181361	5-Hydroxy-3-mercaptopentan-2-one	C5H10O2S	M+NH4	152.0740	-3.1
	HMDB0181362	1-hydroxy-3-sulfanylpentan-2-one	C5H10O2S	M+NH4	152.0740	-3.1
	HMDB0181360	4-hydroxy-3-sulfanylpentan-2-one	C5H10O2S	M+NH4	152.0740	-3.1
	HMDB0167019	S-(3-Hydroxypropyl) thioacetate	C5H10O2S	M+NH4	152.0740	-3.1
	HMDB0167020	SCHEMBL8973586	C5H10O2S	M+NH4	152.0740	-3.1
	HMDB0167018	1-[(2-hydroxypropyl)sulfanyl]ethan-1-one	C5H10O2S	M+NH4	152.0740	-3.1
152.0912	HMDB0173819	(2-carboxyethyl)dimethylsulfanium	C5H11O2S	M+NH4	152.0740	-3.1
	HMDB0167973	2-deoxypentose	C5H10O4	M+NH4	152.0917	-3.5
	HMDB0127615	3-hydroxy-2-(hydroxymethyl)-2-methylpropanoic acid	C5H10O4	M+NH4	152.0917	-3.5
	HMDB0158453	SCHEMBL8384843	C5H10O4	M+NH4	152.0917	-3.5
	HMDB0158454	SCHEMBL36647	C5H10O4	M+NH4	152.0917	-3.5
	HMDB0158455	ethyl glycerol ether	C5H10O4	M+NH4	152.0917	-3.5
	HMDB0000421	2,3-Dihydroxyvaleric acid	C5H10O4	M+NH4	152.0917	-3.5
	HMDB0001292	1-Deoxy-D-xylulose	C5H10O4	M+NH4	152.0917	-3.5
	HMDB0003224	Deoxyribose	C5H10O4	M+NH4	152.0917	-3.5
	HMDB0012141	(R)-2,3-Dihydroxy-isovalerate	C5H10O4	M+NH4	152.0917	-3.5
	HMDB0029576	2,3-Dihydroxy-2-methylbutanoic acid	C5H10O4	M+NH4	152.0917	-3.5
	HMDB0012485	(R)-glycerol 1-acetate	C5H10O4	M+NH4	152.0917	-3.5
152.1277	HMDB0062104	diethylene glycol monoethyl ether	C6H14O3	M+NH4	152.1281	-2.7
	HMDB0032478	Polypropylene glycol (m w 1,0-3)	C6H14O3	M+NH4	152.1281	-2.7
	HMDB0163350	(Z)-hex-4-enoic acid	C6H10O2	M+K	153.0312	-1.6
	HMDB0163351	(4Z)-6-hydroxyhex-4-enal	C6H10O2	M+K	153.0312	-1.6
	HMDB0163352	(4Z)-3-hydroxyhex-4-enal	C6H10O2	M+K	153.0312	-1.6
	HMDB0163354	(4Z)-2-hydroxyhex-4-enal	C6H10O2	M+K	153.0312	-1.6
	HMDB0179351	4-Hexenoic acid	C6H10O2	M+K	153.0312	-1.6
	HMDB0179346	(2Z)-3-(3-methyloxiran-2-yl)prop-2-en-1-ol	C6H10O2	M+K	153.0312	-1.6
	HMDB0179345	{3-[(1E)-prop-1-en-1-yl]oxiran-2-yl}methanol	C6H10O2	M+K	153.0312	-1.6
	HMDB0179344	cis-2,4-hexadien-1,6-diol	C6H10O2	M+K	153.0312	-1.6
	HMDB0179341	(4E)-6-hydroxyhex-4-enal	C6H10O2	M+K	153.0312	-1.6
	HMDB0179343	(4E)-2-hydroxyhex-4-enal	C6H10O2	M+K	153.0312	-1.6
	HMDB0179342	(4E)-3-hydroxyhex-4-enal	C6H10O2	M+K	153.0312	-1.6
	HMDB0169695	(Z)-3-methyl-2-pentenoic acid	C6H10O2	M+K	153.0312	-1.6
	HMDB0169664	(E)-3-Methyl-2-pentenoic acid	C6H10O2	M+K	153.0312	-1.6
	HMDB0165582	(2Z)-4-hydroxy-2-methylpent-2-enal	C6H10O2	M+K	153.0312	-1.6
	HMDB0165583	2-Methyl-3-ethyloxirane-2-carbaldehyde	C6H10O2	M+K	153.0312	-1.6
	HMDB0165581	(2Z)-2-(hydroxymethyl)pent-2-enal	C6H10O2	M+K	153.0312	-1.6
	HMDB0165584	(2Z)-5-hydroxy-2-methylpent-2-enal	C6H10O2	M+K	153.0312	-1.6
	HMDB0163703	(3Z)-5-hydroxy-3-methylpent-3-en-2-one	C6H10O2	M+K	153.0312	-1.6

153.0310	HMDB0163702	Pentanal, 3-methyl-4-oxo-	C6H10O2	M+K	153.0312	-1.6
	HMDB0163353	3-(3-methyloxiran-2-yl)propanal	C6H10O2	M+K	153.0312	-1.6
	HMDB0060476	epsilon-Caprolactone	C6H10O2	M+K	153.0312	-1.6
	HMDB0032490	Prenyl formate	C6H10O2	M+K	153.0312	-1.6
	HMDB0039581	Ethyl crotonate	C6H10O2	M+K	153.0312	-1.6
	HMDB0031158	2-Methyl-4-pentenoic acid	C6H10O2	M+K	153.0312	-1.6
	HMDB0031562	2-Methyl-3-pentenoic acid	C6H10O2	M+K	153.0312	-1.6
	HMDB0031559	4-Methyl-2,3-pentanedione	C6H10O2	M+K	153.0312	-1.6
	HMDB0031491	2,3-Hexanedione	C6H10O2	M+K	153.0312	-1.6
	HMDB0031560	2-Methyl-2-pentenoic acid	C6H10O2	M+K	153.0312	-1.6
	HMDB0031501	3-Hexenoic acid	C6H10O2	M+K	153.0312	-1.6
	HMDB0029487	Allyl propionate	C6H10O2	M+K	153.0312	-1.6
	HMDB0033568	5-Oxohexanal	C6H10O2	M+K	153.0312	-1.6
	HMDB0040328	Methyl 4-pentenoate	C6H10O2	M+K	153.0312	-1.6
	HMDB0031492	3,4-Hexanedione	C6H10O2	M+K	153.0312	-1.6
	HMDB0031561	4-Methyl-2-pentenoic acid	C6H10O2	M+K	153.0312	-1.6
	HMDB0010719	Isohydrosorbic acid	C6H10O2	M+K	153.0312	-1.6
	HMDB0003843	Gamma-Caprolactone	C6H10O2	M+K	153.0312	-1.6
	HMDB0240384	4-Hydroxyhexanal	C6H10O2	M+K	153.0312	-1.6
	HMDB0061929	Dihydro-4,4-dimethyl-2(3H)-furanone	C6H10O2	M+K	153.0312	-1.6
	HMDB0061965	1-methyl-2,3-dioxabicyclo[2.2.1]heptane	C6H10O2	M+K	153.0312	-1.6
	HMDB0062135	methyl (2E)-2-methylbut-2-enoate	C6H10O2	M+K	153.0312	-1.6
	HMDB0000453	delta-Hexanolactone	C6H10O2	M+K	153.0312	-1.6
153.0906	HMDB0175244	4-(1-hydroxypropan-2-yl)phenol	C9H12O2	M+H	153.0910	-2.7
	HMDB0175243	SCHEMBL9169343	C9H12O2	M+H	153.0910	-2.7
	HMDB0175240	2-Phenyl-1,2-propanediol	C9H12O2	M+H	153.0910	-2.7
	HMDB0175241	2-PHENYL-1,3-PROPANEDIOL	C9H12O2	M+H	153.0910	-2.7
	HMDB0173826	1-(4-methylphenyl)ethane-1,2-diol	C9H12O2	M+H	153.0910	-2.7
	HMDB0173825	1-[4-(Hydroxymethyl)phenyl]ethanol	C9H12O2	M+H	153.0910	-2.7
	HMDB0150180	2-(3-hydroxypropyl)phenol	C9H12O2	M+H	153.0910	-2.7
	HMDB0150179	3-(3-hydroxypropyl)phenol	C9H12O2	M+H	153.0910	-2.7
	HMDB0150178	1-Phenylpropane-1,3-diol	C9H12O2	M+H	153.0910	-2.7
	HMDB0125537	3-ethyl-5-methoxyphenol	C9H12O2	M+H	153.0910	-2.7
	HMDB0146637	4-ETHYL-3-METHOXYPHENOL	C9H12O2	M+H	153.0910	-2.7
	HMDB0150177	3-phenylpropane-1,2-diol	C9H12O2	M+H	153.0910	-2.7
	HMDB0040175	4-Ethyl-2-methoxyphenol	C9H12O2	M+H	153.0910	-2.7
	HMDB0032132	2-Isopropyl-1,4-benzenediol	C9H12O2	M+H	153.0910	-2.7
	HMDB0032599	3-(4-Hydroxyphenyl)-1-propanol	C9H12O2	M+H	153.0910	-2.7
	HMDB0040216	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	C9H12O2	M+H	153.0910	-2.7
	HMDB0039801	1-(2-Furanyl)-1-pentanone	C9H12O2	M+H	153.0910	-2.7
	HMDB0036227	2-Propenyl 2,4-hexadienoate	C9H12O2	M+H	153.0910	-2.7
	HMDB0039956	4-(Ethoxymethyl)phenol	C9H12O2	M+H	153.0910	-2.7
	HMDB0036169	3-(5-Methyl-2-furanyl)butanal	C9H12O2	M+H	153.0910	-2.7
	HMDB0041326	(Dimethoxymethyl)benzene	C9H12O2	M+H	153.0910	-2.7
	HMDB0040449	2-(Ethoxymethyl)phenol	C9H12O2	M+H	153.0910	-2.7
	HMDB0041804	2-Isopropoxyphenol	C9H12O2	M+H	153.0910	-2.7
	HMDB0059853	3,5-Dimethoxytoluene	C9H12O2	M+H	153.0910	-2.7
	HMDB0168680	(4-ethoxyphenyl)methanol	C9H12O2	M+H	153.0910	-2.7
	HMDB0182523	p-Menth-1(7)-en-2-one	C10H16O	M+H	153.1274	-3.2
	HMDB0187618	isopiperitenol	C10H16O	M+H	153.1274	-3.2
	HMDB0187619	2-methyl-2-(4-methylcyclohex-3-en-1-yl)oxirane	C10H16O	M+H	153.1274	-3.2
	HMDB0182597	SCHEMBL13931696	C10H16O	M+H	153.1274	-3.2
	HMDB0182548	2-[(1R)-4-methylcyclohexa-2,4-dien-1-yl]propan-1-ol	C10H16O	M+H	153.1274	-3.2
	HMDB0182545	(6S)-3-methyl-6-(propan-2-yl)cyclohexa-2,4-dien-1-ol	C10H16O	M+H	153.1274	-3.2
	HMDB0182547	(5S)-2-methyl-5-(propan-2-yl)-7-oxabicyclo[4.1]hept-2-ene	C10H16O	M+H	153.1274	-3.2
	HMDB0182546	(4S)-1-methyl-4-(propan-2-yl)-7-oxabicyclo[4.1]hept-2-ene	C10H16O	M+H	153.1274	-3.2
	HMDB0182544	SCHEMBL4374431	C10H16O	M+H	153.1274	-3.2
	HMDB0182543	(R)-p-Mentha-1,5-diene-8-ol	C10H16O	M+H	153.1274	-3.2
	HMDB0182542	ZINC321828	C10H16O	M+H	153.1274	-3.2
	HMDB0181808	(1S)-4-methylidene-1-(propan-2-yl)bicyclo[3.1]hexan-6-ol	C10H16O	M+H	153.1274	-3.2
	HMDB0181807	(5S)-2-methylidene-5-(propan-2-yl)bicyclo[3.1]hexan-1-ol	C10H16O	M+H	153.1274	-3.2

HMDB0181806	(1R)-4-methylidene-1-(propan-2-yl)bicyclo[3.1]hexan-2-ol	C10H16O	M+H	153.1274	-3.2
HMDB0181809	2-[(1R)-4-methylidenebicyclo[3.1]hexan-1-yl]propan-1-ol	C10H16O	M+H	153.1274	-3.2
HMDB0181804	2-[(1R)-4-methylidenebicyclo[3.1]hexan-1-yl]propan-2-ol	C10H16O	M+H	153.1274	-3.2
HMDB0181805	AC1O5B2Q	C10H16O	M+H	153.1274	-3.2
HMDB0163092	SCHEMBL5863926	C10H16O	M+H	153.1274	-3.2
HMDB0163091	(4Z,7Z)-deca-4,7-dienal	C10H16O	M+H	153.1274	-3.2
HMDB0030893	Isocitral	C10H16O	M+H	153.1274	-3.2
HMDB0036115	(-)-3-Isothujone	C10H16O	M+H	153.1274	-3.2
HMDB0036598	(E,E)-2,4-Decadienal	C10H16O	M+H	153.1274	-3.2
HMDB0035656	3-Pinanone	C10H16O	M+H	153.1274	-3.2
HMDB0035737	(R)-Piperitone	C10H16O	M+H	153.1274	-3.2
HMDB0035738	(R)-Piperitone	C10H16O	M+H	153.1274	-3.2
HMDB0038290	Photocitral A	C10H16O	M+H	153.1274	-3.2
HMDB0035743	Pinocarveol	C10H16O	M+H	153.1274	-3.2
HMDB0037025	Hop ether	C10H16O	M+H	153.1274	-3.2
HMDB0032120	2,6-Dimethyl-1,7-octadien-3-one	C10H16O	M+H	153.1274	-3.2
HMDB0036127	(-)-Pinocamphone	C10H16O	M+H	153.1274	-3.2
HMDB0035744	(-)-Isopinocamphone	C10H16O	M+H	153.1274	-3.2
HMDB0037009	Terpinolene oxide	C10H16O	M+H	153.1274	-3.2
HMDB0037024	4-Acetyl-1,4-dimethyl-1-cyclohexene	C10H16O	M+H	153.1274	-3.2
HMDB0034974	(R)-Carvotanacetone	C10H16O	M+H	153.1274	-3.2
HMDB0040766	Anethofuran	C10H16O	M+H	153.1274	-3.2
HMDB0035092	cis-Citral	C10H16O	M+H	153.1274	-3.2
HMDB0037280	Junionone	C10H16O	M+H	153.1274	-3.2
HMDB0036129	Verbenol	C10H16O	M+H	153.1274	-3.2
HMDB0034973	(R)-Campholenic aldehyde	C10H16O	M+H	153.1274	-3.2
HMDB0034985	(+)-Fenchone	C10H16O	M+H	153.1274	-3.2
HMDB0034975	Piperitone	C10H16O	M+H	153.1274	-3.2
HMDB0036128	(-)-trans-Pinocarveol	C10H16O	M+H	153.1274	-3.2
HMDB0038557	xi-3,6-Dihydro-4-methyl-2-(2-methyl-1-propenyl)-2H-pyran	C10H16O	M+H	153.1274	-3.2
HMDB0035622	(+)-cis-Carveol	C10H16O	M+H	153.1274	-3.2
HMDB0036080	(1S,4S)-Dihydrocarvone	C10H16O	M+H	153.1274	-3.2
HMDB0036114	(-)-3-Thujone	C10H16O	M+H	153.1274	-3.2
HMDB0035054	(1S,4R)-p-Mentha-2,8-dien-1-ol	C10H16O	M+H	153.1274	-3.2
HMDB0035077	(1R,4R)-p-Mentha-2,8-dien-1-ol	C10H16O	M+H	153.1274	-3.2
HMDB0003667	Alpha-Pinene-oxide	C10H16O	M+H	153.1274	-3.2
HMDB0003634	Perillyl alcohol	C10H16O	M+H	153.1274	-3.2
HMDB0003450	(-)-trans-Carveol	C10H16O	M+H	153.1274	-3.2
HMDB0035741	(-)-trans-Isopulegone	C10H16O	M+H	153.1274	-3.2
HMDB0035600	(S)-Phellandral	C10H16O	M+H	153.1274	-3.2
HMDB0034715	p-Mentha-1(6),8-dien-3-ol	C10H16O	M+H	153.1274	-3.2
HMDB0037015	p-Mentha-1,8-dien-4-ol	C10H16O	M+H	153.1274	-3.2
HMDB0037303	xi-p-Mentha-1(7),2-dien-4-ol	C10H16O	M+H	153.1274	-3.2
HMDB0038251	xi-Pinol	C10H16O	M+H	153.1274	-3.2
HMDB0035241	(Z)-2-Methyl-6-methylene-2,7-octadien-1-ol	C10H16O	M+H	153.1274	-3.2
HMDB0037010	(2S,4R)-p-Mentha-1(7),8-dien-2-ol	C10H16O	M+H	153.1274	-3.2
HMDB0035277	(2S,4R)-p-Mentha-1(7),5-dien-2-ol	C10H16O	M+H	153.1274	-3.2
HMDB0036044	Marmelo oxide A	C10H16O	M+H	153.1274	-3.2
HMDB0035203	(S)-9,-Cyclo-p-menth-1-en-4-ol	C10H16O	M+H	153.1274	-3.2
HMDB0037302	xi-p-Mentha-3,8-dien-1-ol	C10H16O	M+H	153.1274	-3.2
HMDB0035120	Dehydrolinalool	C10H16O	M+H	153.1274	-3.2
HMDB0039008	3,4-Epoxy-p-menth-1(7)-ene	C10H16O	M+H	153.1274	-3.2
HMDB0059838	Camphor	C10H16O	M+H	153.1274	-3.2
HMDB0059827	3-Cyclohexene-1-carboxaldehyde, 1,3,4-trimethyl-	C10H16O	M+H	153.1274	-3.2
HMDB0059761	4-(1-Methylethyl)-1-cyclohexene-4-carboxaldehyde	C10H16O	M+H	153.1274	-3.2
HMDB0041631	3-Thujanone	C10H16O	M+H	153.1274	-3.2
HMDB0059608	(+)-trans-Carveol	C10H16O	M+H	153.1274	-3.2
HMDB0032242	(E)-3,7-Dimethyl-1,5,7-octatrien-3-ol	C10H16O	M+H	153.1274	-3.2
HMDB0059875	Carvotanacetone	C10H16O	M+H	153.1274	-3.2
HMDB0035604	Pulegone	C10H16O	M+H	153.1274	-3.2
HMDB0061794	Pulegone	C10H16O	M+H	153.1274	-3.2

	HMDB0061292	SCHEMBL6943113	C10H16O	M+H	153.1274	-3.2
	HMDB0032536	2-(trans-2-Pentenyl)cyclopentanone	C10H16O	M+H	153.1274	-3.2
	HMDB0059885	p-Menth-1-en-9-al	C10H16O	M+H	153.1274	-3.2
	HMDB0031854	3-Methyl-5-propyl-2-cyclohexen-1-one	C10H16O	M+H	153.1274	-3.2
	HMDB0041013	Isocyclocitral	C10H16O	M+H	153.1274	-3.2
	HMDB0035100	2-Pinen--ol	C10H16O	M+H	153.1274	-3.2
	HMDB0035125	Darwinol	C10H16O	M+H	153.1274	-3.2
	HMDB0035280	Teresantalol	C10H16O	M+H	153.1274	-3.2
	HMDB0036083	Carveol	C10H16O	M+H	153.1274	-3.2
	HMDB0035078	Geranial	C10H16O	M+H	153.1274	-3.2
	HMDB0037008	6,8-Epoxy-p-menth-2-ene	C10H16O	M+H	153.1274	-3.2
	HMDB0036082	(-)-cis-Carveol	C10H16O	M+H	153.1274	-3.2
	HMDB0035158	1,2-Epoxy-p-menth-8-ene	C10H16O	M+H	153.1274	-3.2
	HMDB0036085	Dehydro-1,8-cineole	C10H16O	M+H	153.1274	-3.2
	HMDB0037017	(R)-p-Mentha-1,8-dien--ol	C10H16O	M+H	153.1274	-3.2
	HMDB0036079	Dihydrocarvone	C10H16O	M+H	153.1274	-3.2
	HMDB0035706	alpha-Cyclocitral	C10H16O	M+H	153.1274	-3.2
	HMDB0036113	(+)-3-Thujone	C10H16O	M+H	153.1274	-3.2
	HMDB0039816	2-Hexylfuran	C10H16O	M+H	153.1274	-3.2
	HMDB0041011	beta-Cyclocitral	C10H16O	M+H	153.1274	-3.2
	HMDB0034916	cis-2-Thujen-4-ol	C10H16O	M+H	153.1274	-3.2
	HMDB0037172	Tetrahydro-5-isopropenyl-2-methyl-2-vinylfuran	C10H16O	M+H	153.1274	-3.2
	HMDB0030892	p-Menth-3-en-9-al	C10H16O	M+H	153.1274	-3.2
	HMDB0036087	(R)-p-Mentha-1,8-dien-7-ol	C10H16O	M+H	153.1274	-3.2
	HMDB0036088	(R)-p-Mentha-1,8-dien-7-ol	C10H16O	M+H	153.1274	-3.2
154.0260	HMDB0167282	2-hydroxy-2-(hydroxymethyl)butanenitrile	C5H9NO2	M+K	154.0265	-3.2
	HMDB0167283	2,4-dihydroxy-2-methylbutanenitrile	C5H9NO2	M+K	154.0265	-3.2
	HMDB0167281	2,3-dihydroxy-2-methylbutanenitrile	C5H9NO2	M+K	154.0265	-3.2
	HMDB0177063	1-formyl-pyrrolidin-2-ol	C5H9NO2	M+K	154.0265	-3.2
	HMDB0179973	SCHEMBL55844	C5H9NO2	M+K	154.0265	-3.2
	HMDB0012880	Acetamidopropanal	C5H9NO2	M+K	154.0265	-3.2
	HMDB0034208	Pterolactam	C5H9NO2	M+K	154.0265	-3.2
	HMDB0030409	4-Amino-2-methylenebutanoic acid	C5H9NO2	M+K	154.0265	-3.2
	HMDB0003411	D-Proline	C5H9NO2	M+K	154.0265	-3.2
	HMDB0000162	L-Proline	C5H9NO2	M+K	154.0265	-3.2
154.0719	HMDB0014581	Allopurinol	C5H4N4O	M+NH4	154.0723	-2.8
	HMDB0000157	Hypoxanthine	C5H4N4O	M+NH4	154.0723	-2.8
	HMDB0004816	FAPy-adenine	C5H7N5O	M+H	154.0723	-2.8
	HMDB0033054	Ethyl isopropyl disulfide	C5H12S2	M+NH4	154.0719	0.2
	HMDB0033053	Ethyl propyl disulfide	C5H12S2	M+NH4	154.0719	0.2
	HMDB0031160	1-Pentanesulfenothioic acid	C5H12S2	M+NH4	154.0719	0.2
154.0835	HMDB0240479	Alanine betaine	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0171680	SCHEMBL311743	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0171681	SCHEMBL1266	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0171682	N-(2-methylpropyl)glycolamide	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0168722	N,N-diethyl-2-oxoethanamine oxide	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0168721	SCHEMBL124646	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0168720	2-[ethyl(1-hydroxyethyl)amino]acetaldehyde	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0168719	SCHEMBL63485	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0145163	2-hydroxy-3-(propylamino)propanal	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0144645	N,N-Diethylglycine	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0036382	6-Deoxyfagomine	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0033923	erythro-Isoleucine	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0003640	Beta-Leucine	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0001645	L-Norleucine	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0000557	L-Alloisoleucine	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0001901	Aminocaproic acid	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0000172	L-Isoleucine	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0013773	D-Leucine	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0062052	4-(dimethylamino)butanoic acid	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0061716	N-methylvaline	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0060650	N-(2-Hydroxyethyl)-morpholine	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0029168	3-Aminocaproic acid	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0000687	L-Leucine	C6H13NO2	M+Na	154.0838	-2.3
	HMDB0062203	L-Leucine	C6H13NO2	M+Na	154.0838	-2.3

155.0462	HMDB0160104	bis(hydroxymethyl)pyrimidine-2,4-diol	C6H8N2O4	M+H-H2O	155.0457	3.2
	HMDB0001212	Hydantoin-5-propionic acid	C6H8N2O4	M+H-H2O	155.0457	3.2
	HMDB0034322	L-alpha-Amino-5-oxo-2(5H)-isoxazolepropanoic acid	C6H8N2O4	M+H-H2O	155.0457	3.2
	HMDB0059602	Indanone	C9H8O	M+Na	155.0467	-3.4
	HMDB0059847	2-Methylcumarone	C9H8O	M+Na	155.0467	-3.4
	HMDB0060671	Atropaldehyde	C9H8O	M+Na	155.0467	-3.4
	HMDB0032072	(Z)-Cinnamaldehyde	C9H8O	M+Na	155.0467	-3.4
	HMDB0003441	Cinnamaldehyde	C9H8O	M+Na	155.0467	-3.4
155.0699	HMDB0125534	5-ethylbenzene-1,2,3-triol	C8H10O3	M+H	155.0703	-2.4
	HMDB0146874	SCHEMBL093	C8H10O3	M+H	155.0703	-2.4
	HMDB0146894	4-Ethylpyrogallol	C8H10O3	M+H	155.0703	-2.4
	HMDB0169080	2-Hydroxy-3-methoxybenzyl alcohol	C8H10O3	M+H	155.0703	-2.4
	HMDB0131231	5-methoxy-4-methylbenzene-1,3-diol	C8H10O3	M+H	155.0703	-2.4
	HMDB0135785	1-(4-hydroxyphenyl)ethane-1,2-diol	C8H10O3	M+H	155.0703	-2.4
	HMDB0131479	2,3-dimethoxyphenol	C8H10O3	M+H	155.0703	-2.4
	HMDB0059966	3,5-Dimethoxyphenol	C8H10O3	M+H	155.0703	-2.4
	HMDB0037724	Propyl 2-furoate	C8H10O3	M+H	155.0703	-2.4
	HMDB0034158	2,6-Dimethoxyphenol	C8H10O3	M+H	155.0703	-2.4
	HMDB0037728	2-Furanylmethyl propanoate	C8H10O3	M+H	155.0703	-2.4
	HMDB0032012	4-Hydroxy-3-methoxybenzenemethanol	C8H10O3	M+H	155.0703	-2.4
	HMDB0030570	Sylvopinol	C8H10O3	M+H	155.0703	-2.4
	HMDB0005784	Hydroxytyrosol	C8H10O3	M+H	155.0703	-2.4
	HMDB0131232	5-methoxy-2-methylbenzene-1,3-diol	C8H10O3	M+H	155.0703	-2.4
	HMDB0126617	2,4-dimethylbenzene-1,3,5-triol	C8H10O3	M+H	155.0703	-2.4
155.1062	HMDB0163467	(2Z)-2-methylocta-2,7-dienoic acid	C9H14O2	M+H	155.1067	-2.9
	HMDB0180434	(2E,4E)-9-hydroxynona-2,4-dienal	C9H14O2	M+H	155.1067	-2.9
	HMDB0180433	trans-4,5-Epoxy-(E)-nonenal	C9H14O2	M+H	155.1067	-2.9
	HMDB0180430	(2E,4E)-6-hydroxynona-2,4-dienal	C9H14O2	M+H	155.1067	-2.9
	HMDB0180431	SCHEMBL179742	C9H14O2	M+H	155.1067	-2.9
	HMDB0180432	3-[(1E)-hex-1-en-1-yl]oxirane-2-carbaldehyde	C9H14O2	M+H	155.1067	-2.9
	HMDB0167038	(2E,6Z)-9-hydroxynona-2,6-dienal	C9H14O2	M+H	155.1067	-2.9
	HMDB0167037	(2E)-5-(3-ethyloxiran-2-yl)pent-2-enal	C9H14O2	M+H	155.1067	-2.9
	HMDB0167034	(2E,6Z)-8-hydroxynona-2,6-dienal	C9H14O2	M+H	155.1067	-2.9
	HMDB0167035	(2E,6Z)-5-hydroxynona-2,6-dienal	C9H14O2	M+H	155.1067	-2.9
	HMDB0167036	3-[(3Z)-hex-3-en-1-yl]oxirane-2-carbaldehyde	C9H14O2	M+H	155.1067	-2.9
	HMDB0167032	2E,6Z-nonadienoic acid	C9H14O2	M+H	155.1067	-2.9
	HMDB0167033	(2E,6Z)-4-hydroxynona-2,6-dienal	C9H14O2	M+H	155.1067	-2.9
	HMDB0164921	1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O2	M+H	155.1067	-2.9
	HMDB0060285	4-Oxo-2-nonenal	C9H14O2	M+H	155.1067	-2.9
	HMDB0032442	2-Nonenoic acid gamma-lactone	C9H14O2	M+H	155.1067	-2.9
	HMDB0032314	2,4-Hexadienyl propionate	C9H14O2	M+H	155.1067	-2.9
	HMDB0040285	Anapear	C9H14O2	M+H	155.1067	-2.9
	HMDB0036177	3,5,5-Trimethyl-1,2-cyclohexanedione	C9H14O2	M+H	155.1067	-2.9
	HMDB0036239	3,5,5-Trimethyl-1,2-cyclohexanedione	C9H14O2	M+H	155.1067	-2.9
	HMDB0037276	Octahydro-2H-1-benzopyran-2-one	C9H14O2	M+H	155.1067	-2.9
	HMDB0031302	Methyl 2-octynoate	C9H14O2	M+H	155.1067	-2.9
	HMDB0038268	Allyl hexenoate	C9H14O2	M+H	155.1067	-2.9
	HMDB0038697	xi-2,2,6-Trimethyl-1,4-cyclohexanedione	C9H14O2	M+H	155.1067	-2.9
	HMDB0035135	(E)-2,6-Dimethyl-2,5-heptadienoic acid	C9H14O2	M+H	155.1067	-2.9
	HMDB0061802	5-Methyl-2-(1-methylethyl)-cyclohexanone	C10H18O	M+H	155.1430	-2.8
	HMDB0187564	CTK8I1689	C10H18O	M+H	155.1430	-2.8
	HMDB0163116	(4Z,7Z)-deca-4,7-dien-1-ol	C10H18O	M+H	155.1430	-2.8
	HMDB0035815	(+)-Isoborneol	C10H18O	M+H	155.1430	-2.8
	HMDB0032530	(+)-thujan-3-ol	C10H18O	M+H	155.1430	-2.8
	HMDB0036100	3,7-Dimethyl-1,6-octadien-3-ol	C10H18O	M+H	155.1430	-2.8
	HMDB0035825	(-)-Dihydrocarveol	C10H18O	M+H	155.1430	-2.8
	HMDB0035783	(+)-Menthone	C10H18O	M+H	155.1430	-2.8
	HMDB0037016	p-Menth-1-en-5-ol	C10H18O	M+H	155.1430	-2.8
	HMDB0035954	(1R*,3R*,6S*)-3-Caranol	C10H18O	M+H	155.1430	-2.8
	HMDB0035820	(R)-Citronellal	C10H18O	M+H	155.1430	-2.8
	HMDB0035842	(R)-Citronellal	C10H18O	M+H	155.1430	-2.8
	HMDB0034848	9-Decenal	C10H18O	M+H	155.1430	-2.8

HMDB0037019	6,8-Epoxy-p-menthane	C10H18O	M+H	155.1430	-2.8
HMDB0036077	p-Menth-8-en-3-ol	C10H18O	M+H	155.1430	-2.8
HMDB0034976	(-)-Borneol	C10H18O	M+H	155.1430	-2.8
HMDB0035818	(-)-Borneol	C10H18O	M+H	155.1430	-2.8
HMDB0037048	m-Menth-1-en-8-ol	C10H18O	M+H	155.1430	-2.8
HMDB0032118	2,6-Dimethyl-7-octen-3-one	C10H18O	M+H	155.1430	-2.8
HMDB0035841	Citronellal	C10H18O	M+H	155.1430	-2.8
HMDB0037007	p-Menth-1-en-9-ol	C10H18O	M+H	155.1430	-2.8
HMDB0036991	delta-Terpineol	C10H18O	M+H	155.1430	-2.8
HMDB0036993	gamma-Terpineol	C10H18O	M+H	155.1430	-2.8
HMDB0036097	Rose oxide	C10H18O	M+H	155.1430	-2.8
HMDB0037133	Linaloyl oxide	C10H18O	M+H	155.1430	-2.8
HMDB0036096	1,4-Cineole	C10H18O	M+H	155.1430	-2.8
HMDB0035819	(-)-Isoborneol	C10H18O	M+H	155.1430	-2.8
HMDB0041034	(4Z,7Z)-4,7-Decadien-1-ol	C10H18O	M+H	155.1430	-2.8
HMDB0031410	3-Decen-2-one	C10H18O	M+H	155.1430	-2.8
HMDB0037049	(R)-m-Menth-1(6)-en-8-ol	C10H18O	M+H	155.1430	-2.8
HMDB0038025	xi-p-Menth-3-en-1-ol	C10H18O	M+H	155.1430	-2.8
HMDB0035861	trans-(-)-p-Menth-1-en-3-ol	C10H18O	M+H	155.1430	-2.8
HMDB0005812	Geraniol	C10H18O	M+H	155.1430	-2.8
HMDB0004043	alpha-Terpineol	C10H18O	M+H	155.1430	-2.8
HMDB0036126	(-)-Pinocampheol	C10H18O	M+H	155.1430	-2.8
HMDB0036112	(1R,4S,5R)-4-Thujanol	C10H18O	M+H	155.1430	-2.8
HMDB0036068	Campholenic alcohol	C10H18O	M+H	155.1430	-2.8
HMDB0035955	(1R*,2S*,3S*,6S*)-2-Caranol	C10H18O	M+H	155.1430	-2.8
HMDB0036196	(2E,4E)-2,4-Decadien-1-ol	C10H18O	M+H	155.1430	-2.8
HMDB0037047	(-)-trans-m-Menth-8-en-1-ol	C10H18O	M+H	155.1430	-2.8
HMDB0004472	Eucalyptol	C10H18O	M+H	155.1430	-2.8
HMDB0059869	p-tert-Butylcyclohexanone	C10H18O	M+H	155.1430	-2.8
HMDB0059881	Ocimenol	C10H18O	M+H	155.1430	-2.8
HMDB0036086	(S)-alpha-Terpineol	C10H18O	M+H	155.1430	-2.8
HMDB0035833	p-Menth-1-en-4-ol	C10H18O	M+H	155.1430	-2.8
HMDB0035272	p-Menthan-2-one	C10H18O	M+H	155.1430	-2.8
HMDB0036107	Myrcenol	C10H18O	M+H	155.1430	-2.8
HMDB0036101	(R)-3,7-Dimethyl-1,6-octadien-3-ol	C10H18O	M+H	155.1430	-2.8
HMDB0036102	(R)-3,7-Dimethyl-1,6-octadien-3-ol	C10H18O	M+H	155.1430	-2.8
HMDB0030999	2-Decenal	C10H18O	M+H	155.1430	-2.8
HMDB0035155	beta-Geraniol	C10H18O	M+H	155.1430	-2.8
HMDB0041014	4-Decenal	C10H18O	M+H	155.1430	-2.8
HMDB0037215	trans-beta-Terpineol	C10H18O	M+H	155.1430	-2.8
HMDB0037161	2-Isopropyl-5-methyl-2-hexenal	C10H18O	M+H	155.1430	-2.8
HMDB0035823	(S)-p-Menth-1-en-4-ol	C10H18O	M+H	155.1430	-2.8
HMDB0036041	(R)-Lavandulol	C10H18O	M+H	155.1430	-2.8
HMDB0034972	Isomenthone	C10H18O	M+H	155.1430	-2.8
HMDB0040448	2-(1-Methylpropyl)cyclohexanone	C10H18O	M+H	155.1430	-2.8
HMDB0034932	Fenchol	C10H18O	M+H	155.1430	-2.8
HMDB0035162	(-)-Menthone	C10H18O	M+H	155.1430	-2.8
HMDB0059864	(-)-Menthone	C10H18O	M+H	155.1430	-2.8
HMDB0035838	Piperitol	C10H18O	M+H	155.1430	-2.8
HMDB0038185	Ocimen quintoxide	C10H18O	M+H	155.1430	-2.8
HMDB0037006	cis-Isopulegone	C10H18O	M+H	155.1430	-2.8
HMDB0036078	(-)-Isopulegol	C10H18O	M+H	155.1430	-2.8
HMDB0034969	(-)-Carvomenthone	C10H18O	M+H	155.1430	-2.8
HMDB0036996	cis-beta-Terpineol	C10H18O	M+H	155.1430	-2.8
HMDB0037214	cis-beta-Terpineol	C10H18O	M+H	155.1430	-2.8
HMDB0061966	1-nitropentane	C5H11NO2	M+K	156.0421	-2.8
HMDB0002141	N-Methyl-a-aminoisobutyric acid	C5H11NO2	M+K	156.0421	-2.8
HMDB0000883	L-Valine	C5H11NO2	M+K	156.0421	-2.8
HMDB0013716	Norvaline	C5H11NO2	M+K	156.0421	-2.8
HMDB0003355	5-Aminopentanoic acid	C5H11NO2	M+K	156.0421	-2.8
HMDB0001382	Vaporole	C5H11NO2	M+K	156.0421	-2.8
HMDB0015550	Amyl Nitrite	C5H11NO2	M+K	156.0421	-2.8
HMDB0062141	N,N-Dimethyl-L-Alanine	C5H11NO2	M+K	156.0421	-2.8
HMDB0029757	4-Hydroxybenzeneacetone nitrile	C8H7NO	M+Na	156.0420	-1.8
HMDB0032390	2-Methyl-4,5-benzoxazole	C8H7NO	M+Na	156.0420	-1.8

156.0417	HMDB0161291	6-Hydroxyindole	C8H7NO	M+Na	156.0420	-1.8
	HMDB0059805	5-Hydroxyindole	C8H7NO	M+Na	156.0420	-1.8
	HMDB0060486	Mandelonitrile	C8H7NO	M+Na	156.0420	-1.8
	HMDB0171305	(2-hydroxyphenyl)acetonitrile	C8H7NO	M+Na	156.0420	-1.8
	HMDB0161293	4-hydroxyindole	C8H7NO	M+Na	156.0420	-1.8
	HMDB0061918	1,3-Dihydro-(2H)-indol-2-one	C8H7NO	M+Na	156.0420	-1.8
	HMDB0171306	25263-44-9	C8H7NO	M+Na	156.0420	-1.8
	HMDB0161292	7-hydroxyindole	C8H7NO	M+Na	156.0420	-1.8
	HMDB0034666	2-Hydroxy-2-phenylacetonitrile	C8H7NO	M+Na	156.0420	-1.8
	HMDB0004094	Indoxyl	C8H7NO	M+Na	156.0420	-1.8
	HMDB0014966	Fosfomycin	C3H7O4P	M+NH4	156.0420	-2.0
156.0763	HMDB0060173	N-Methylethanolaminium phosphate	C3H10NO4P	M+H	156.0420	-2.1
	HMDB0062562	urocanic acid	C6H6N2O2	M+NH4	156.0768	-2.9
	HMDB0061680	2-Aminonicotinic acid	C6H6N2O2	M+NH4	156.0768	-2.9
	HMDB0034174	(E)-Urocanic acid	C6H6N2O2	M+NH4	156.0768	-2.9
	HMDB0031338	5-Oxo-2(5H)-isoxazolepropanenitrile	C6H6N2O2	M+NH4	156.0768	-2.9
	HMDB0002730	Nicotinamide N-oxide	C6H6N2O2	M+NH4	156.0768	-2.9
	HMDB0000301	Urocanic acid	C6H6N2O2	M+NH4	156.0768	-2.9
	HMDB0034267	L-2-Amino-3-(1-pyrazolyl)propanoic acid	C6H9N3O2	M+H	156.0768	-2.9
156.1015	HMDB0000177	L-Histidine	C6H9N3O2	M+H	156.0768	-2.9
	HMDB0154888	L-Histidine	C6H9N3O2	M+H	156.0768	-2.9
	HMDB0168417	1-phenylethane-1,2-diol	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0126388	4-ethylbenzene-1,3-diol	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0041607	2-Phenoxyethanol	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0125590	5-ethylbenzene-1,3-diol	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0166105	2-Methoxybenzyl alcohol	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0032136	2-Methoxy-4-methylphenol	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0034241	4-Methoxybenzyl alcohol	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0029671	1,4-Dimethoxybenzene	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0039802	1-(2-Furanyl)-1-butanone	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0032036	4-Ethoxyphenol	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0032139	1,2-Dimethoxybenzene	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0040177	3-Ethyl-1,2-benzenediol	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0040174	4-Ethyl-1,2-benzenediol	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0032137	2,6-Dimethyl-1,4-benzenediol	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0004284	Tyrosol	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0029672	1,3-Dimethoxybenzene	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0029563	3-Acetyl-2,5-dimethylfuran	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0032159	2-Acetyl-3,5-dimethylfuran	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0032290	1-(2-Furyl)butan-3-one	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0168418	3-(2-Hydroxyethyl)phenol	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0168448	2-hydroxyphenylethanol	C8H10O2	M+NH4	156.1019	-2.6
	HMDB0181161	2-hydroxy-1-(1,4,5,6-tetrahydropyridin-2-yl)propan-1-one	C8H13NO2	M+H	156.1019	-2.6
	HMDB0181162	3-hydroxy-1-(1,4,5,6-tetrahydropyridin-2-yl)propan-1-one	C8H13NO2	M+H	156.1019	-2.6
	HMDB0062098	4-cyclopropanecarbonylmorpholine	C8H13NO2	M+H	156.1019	-2.6
	HMDB0030353	Arecoline	C8H13NO2	M+H	156.1019	-2.6
156.1379	HMDB0167046	SCHEMBL19577743	C9H14O	M+NH4	156.1383	-2.5
	HMDB0180424	Nona-trans-2-trans-4-dien-1-al	C9H14O	M+NH4	156.1383	-2.5
	HMDB0031685	2,4-Nonadienal	C9H14O	M+NH4	156.1383	-2.5
	HMDB0035929	(R)-Cryptone	C9H14O	M+NH4	156.1383	-2.5
	HMDB0040338	3,5,5-Trimethyl-3-cyclohexen-1-one	C9H14O	M+NH4	156.1383	-2.5
	HMDB0036069	Pulegone	C9H14O	M+NH4	156.1383	-2.5
	HMDB0036091	exo-5,6-Dimethylbicyclo[2.2.1]hept-5-en-2-ol	C9H14O	M+NH4	156.1383	-2.5
	HMDB0013824	2-Pentylfuran	C9H14O	M+NH4	156.1383	-2.5
	HMDB0031084	2-Pentylfuran	C9H14O	M+NH4	156.1383	-2.5
	HMDB0035229	5-Isopropylbicyclo[3.1]hexan-2-one	C9H14O	M+NH4	156.1383	-2.5
	HMDB0036092	exo-2-Methyl-3-methylenebicyclo[2.2.1]heptan-2-ol	C9H14O	M+NH4	156.1383	-2.5
	HMDB0031261	(2E,6E)-2,6-Nonadienal	C9H14O	M+NH4	156.1383	-2.5
	HMDB0033857	Violet-leaf aldehyde	C9H14O	M+NH4	156.1383	-2.5
	HMDB0031152	(3Z,6Z)-3,6-Nonadienal	C9H14O	M+NH4	156.1383	-2.5
	HMDB0031195	3,5,5-Trimethyl-2-cyclohexen-1-one	C9H14O	M+NH4	156.1383	-2.5
	HMDB0033434	4-Acetyl-1-methylcyclohexene	C9H14O	M+NH4	156.1383	-2.5

	HMDB0030326	Methylisopelletierine	C9H17NO	M+H	156.1383	-2.5
	HMDB0031179	2,2,6,6-Tetramethyl-4-piperidinone	C9H17NO	M+H	156.1383	-2.5
	HMDB0039834	2-(1-Pyrrolidinyl)-3-pentanone	C9H17NO	M+H	156.1383	-2.5
	HMDB0039833	3-(1-Pyrrolidinyl)-2-pentanone	C9H17NO	M+H	156.1383	-2.5
157.0622	HMDB0165145	3-methyl-1,4-pentanediol	C6H14O2	M+K	157.0625	-2.2
	HMDB0165147	2-ethylbutane-1,4-diol	C6H14O2	M+K	157.0625	-2.2
	HMDB0165146	3-methylpentane-1,3-diol	C6H14O2	M+K	157.0625	-2.2
	HMDB0165148	3-Methyl-1,5-pentanediol	C6H14O2	M+K	157.0625	-2.2
	HMDB0031490	1,5-Hexanediol	C6H14O2	M+K	157.0625	-2.2
	HMDB0031327	2-Butoxyethanol	C6H14O2	M+K	157.0625	-2.2
	HMDB0031644	1,1-Diethoxyethane	C6H14O2	M+K	157.0625	-2.2
	HMDB0059740	4-Methyl-1,2-dihydroxypentane	C6H14O2	M+K	157.0625	-2.2
	HMDB0164618	Hexane-1,6-Diol	C6H14O2	M+K	157.0625	-2.2
	HMDB0059895	m-Methylacetophenone	C9H10O	M+Na	157.0624	-1.2
	HMDB0061970	phenylacetone	C9H10O	M+Na	157.0624	-1.2
	HMDB0061961	1-ethenyl-3-methoxybenzene	C9H10O	M+Na	157.0624	-1.2
	HMDB0062048	3,5-Dimethylbenzaldehyde	C9H10O	M+Na	157.0624	-1.2
	HMDB0032386	1-(2-methylphenyl)ethan-1-one	C9H10O	M+Na	157.0624	-1.2
	HMDB0059601	Indan-1-ol	C9H10O	M+Na	157.0624	-1.2
	HMDB0032623	1-Phenyl-1-propanone	C9H10O	M+Na	157.0624	-1.2
	HMDB0032608	4'-Methylacetophenone	C9H10O	M+Na	157.0624	-1.2
	HMDB0029697	Cinnamyl alcohol	C9H10O	M+Na	157.0624	-1.2
	HMDB0029639	(4-Methylphenyl)acetaldehyde	C9H10O	M+Na	157.0624	-1.2
	HMDB0061984	2-ethylbenzaldehyde	C9H10O	M+Na	157.0624	-1.2
	HMDB0033716	3-Phenylpropanal	C9H10O	M+Na	157.0624	-1.2
	HMDB0175242	beta-Methylenephenethyl alcohol	C9H10O	M+Na	157.0624	-1.2
	HMDB0034563	7-Nonene-3,5-diyn-1-ol	C9H10O	M+Na	157.0624	-1.2
	HMDB0030839	(Z)-4-(1-Propenyl)phenol	C9H10O	M+Na	157.0624	-1.2
	HMDB0036441	o-Vinylanisole	C9H10O	M+Na	157.0624	-1.2
	HMDB0032024	4-Ethylbenzaldehyde	C9H10O	M+Na	157.0624	-1.2
	HMDB0034107	Chavicol	C9H10O	M+Na	157.0624	-1.2
	HMDB0032142	2,4-Dimethylbenzaldehyde	C9H10O	M+Na	157.0624	-1.2
	HMDB0173827	Benzenemethanol,4-methyl-a-methylene-	C9H10O	M+Na	157.0624	-1.2
	HMDB0029698	trans-Cinnamyl alcohol	C9H10O	M+Na	157.0624	-1.2
	HMDB0031626	2-Phenylpropanal	C9H10O	M+Na	157.0624	-1.2
157.0798	HMDB0037285	2,4-Dimethyl-5-vinylthiazole	C7H9NS	M+NH4	157.0794	2.6
157.0854	HMDB0159132	2-(4-oxocyclohexyl)acetic Acid	C8H12O3	M+H	157.0859	-3.3
	HMDB0032232	2,5-Dimethyl-4-ethoxy-3(2H)-furanone	C8H12O3	M+H	157.0859	-3.3
	HMDB0031101	8-Hydroxy-5,6-octadienoic acid	C8H12O3	M+H	157.0859	-3.3
	HMDB0163456	(2Z)-4-hydroxy-2-methyloct-2-enal	C9H16O2	M+H	157.1223	-3.2
	HMDB0163457	(2Z)-7-hydroxy-2-methyloct-2-enal	C9H16O2	M+H	157.1223	-3.2
	HMDB0163459	(2Z)-8-hydroxy-2-methyloct-2-enal	C9H16O2	M+H	157.1223	-3.2
	HMDB0163458	2-methyl-3-pentyloxirane-2-carbaldehyde	C9H16O2	M+H	157.1223	-3.2
	HMDB0166519	6-(hydroxymethyl)-2,2-dimethylcyclohexan-1-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0166518	2-(hydroxymethyl)-2,6-dimethylcyclohexan-1-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0167039	(6Z)-8-hydroxynon-6-enal	C9H16O2	M+H	157.1223	-3.2
	HMDB0167040	(6Z)-5-hydroxynon-6-enal	C9H16O2	M+H	157.1223	-3.2
	HMDB0167041	5-(3-ethyloxiran-2-yl)pentanal	C9H16O2	M+H	157.1223	-3.2
	HMDB0167044	(2E,6Z)-nona-2,6-diene-1,8-diol	C9H16O2	M+H	157.1223	-3.2
	HMDB0167042	(6Z)-9-hydroxynon-6-enal	C9H16O2	M+H	157.1223	-3.2
	HMDB0167045	(2E,6Z)-nona-2,6-diene-1,9-diol	C9H16O2	M+H	157.1223	-3.2
	HMDB0163455	(2Z)-2-(hydroxymethyl)oct-2-enal	C9H16O2	M+H	157.1223	-3.2
	HMDB0163454	SCHEMBL11263	C9H16O2	M+H	157.1223	-3.2
	HMDB0167043	(6Z)-2-hydroxynon-6-enal	C9H16O2	M+H	157.1223	-3.2
	HMDB0167049	{3-[(3Z)-hex-3-en-1-yl]oxiran-2-yl}methanol	C9H16O2	M+H	157.1223	-3.2
	HMDB0167048	(2E,6Z)-nona-2,6-diene-1,5-diol	C9H16O2	M+H	157.1223	-3.2
	HMDB0179788	(5E)-3-hydroxynon-5-en-2-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0179806	(3Z)-9-hydroxynon-3-en-2-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0179803	(3Z)-5-hydroxynon-3-en-2-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0179804	(3Z)-8-hydroxynon-3-en-2-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0179805	Ethanone, 1-(3-pentyloxiranyl)-	C9H16O2	M+H	157.1223	-3.2
	HMDB0179807	(3Z)-1-hydroxynon-3-en-2-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0180000	7-METHYL-7-OCTENOIC ACID	C9H16O2	M+H	157.1223	-3.2
	HMDB0180425	(2E,4E)-nona-2,4-diene-1,6-diol	C9H16O2	M+H	157.1223	-3.2
	HMDB0180426	(2E,4E)-nona-2,4-diene-1,8-diol	C9H16O2	M+H	157.1223	-3.2

157.1218	HMDB0180427	{3-[(1E)-hex-1-en-1-yl]oxiran-2-yl}methanol	C9H16O2	M+H	157.1223	-3.2
	HMDB0180428	(2E)-3-(3-butyloxiran-2-yl)prop-2-en-1-ol	C9H16O2	M+H	157.1223	-3.2
	HMDB0180429	(2E,4E)-nona-2,4-diene-1,9-diol	C9H16O2	M+H	157.1223	-3.2
	HMDB0179787	(5E)-1-hydroxynon-5-en-2-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0179784	(5E)-8-hydroxynon-5-en-2-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0167047	(2E,6Z)-nona-2,6-diene-1,4-diol	C9H16O2	M+H	157.1223	-3.2
	HMDB0167050	(2E)-5-(3-ethyloxiran-2-yl)pent-2-en-1-ol	C9H16O2	M+H	157.1223	-3.2
	HMDB0167057	6Z-Nonenoic acid	C9H16O2	M+H	157.1223	-3.2
	HMDB0179750	7-hydroxynon-8-en-3-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0179751	2-hydroxynon-8-en-3-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0179752	7-(oxiran-2-yl)heptan-3-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0179753	SCHEMBL18838844	C9H16O2	M+H	157.1223	-3.2
	HMDB0179754	4-hydroxynon-8-en-3-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0179782	(5E)-7-hydroxynon-5-en-2-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0179785	4-(3-propyloxiran-2-yl)butan-2-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0179786	(5E)-9-hydroxynon-5-en-2-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0179783	4-Hydroxynon-5-en-2-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0039794	Methyl 4Z-octenoate	C9H16O2	M+H	157.1223	-3.2
	HMDB0038275	cis-3-Hexenyl propanoate	C9H16O2	M+H	157.1223	-3.2
	HMDB0031271	2-Nonenoic acid	C9H16O2	M+H	157.1223	-3.2
	HMDB0038272	trans-2-Hexenyl propanoate	C9H16O2	M+H	157.1223	-3.2
	HMDB0036208	2-Propenyl 2-ethylbutanoate	C9H16O2	M+H	157.1223	-3.2
	HMDB0032413	Methyl 2-octenoate	C9H16O2	M+H	157.1223	-3.2
	HMDB0032491	Prenyl isobutyrate	C9H16O2	M+H	157.1223	-3.2
	HMDB0032265	cis-Ethyl 4-heptenoate	C9H16O2	M+H	157.1223	-3.2
	HMDB0032307	Hept-trans-2-en-1-yl acetate	C9H16O2	M+H	157.1223	-3.2
	HMDB0059728	Methyl 3-Octenoate	C9H16O2	M+H	157.1223	-3.2
	HMDB0059817	(Z)-Oak lactone	C9H16O2	M+H	157.1223	-3.2
	HMDB0059894	(Z)-Oak lactone	C9H16O2	M+H	157.1223	-3.2
	HMDB0037629	Isobutyl angelate	C9H16O2	M+H	157.1223	-3.2
	HMDB0031514	6-Butyltetrahydro-2H-pyran-2-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0004362	4-Hydroxynonanal	C9H16O2	M+H	157.1223	-3.2
	HMDB0035307	Quercuslactone a	C9H16O2	M+H	157.1223	-3.2
	HMDB0037618	(E)-3-Heptenyl acetate	C9H16O2	M+H	157.1223	-3.2
	HMDB0037023	2-Hydroxy-2,6,6-trimethylcyclohexanone	C9H16O2	M+H	157.1223	-3.2
	HMDB0031531	Dihydro-5-pentyl-2(3H)-furanone	C9H16O2	M+H	157.1223	-3.2
	HMDB0036222	Cyclohexyl propionate	C9H16O2	M+H	157.1223	-3.2
	HMDB0039736	6-Hydroxy-4,6-dimethyl-3-hepten-2-one	C9H16O2	M+H	157.1223	-3.2
	HMDB0031263	2,4-Nonanedione	C9H16O2	M+H	157.1223	-3.2
	HMDB0034716	4-Oxononanal	C9H16O2	M+H	157.1223	-3.2
	HMDB0033167	Ethyl cyclohexanecarboxylate	C9H16O2	M+H	157.1223	-3.2
	HMDB0040210	2-Propenyl hexanoate	C9H16O2	M+H	157.1223	-3.2
	HMDB0037496	Methyl (E)-2-octenoate	C9H16O2	M+H	157.1223	-3.2
	HMDB0059840	(E)-2-Ethyl heptenoate	C9H16O2	M+H	157.1223	-3.2
	HMDB0060286	3,4-Epoxyonanal	C9H16O2	M+H	157.1223	-3.2
	HMDB0170941	8-nonylenic acid	C9H16O2	M+H	157.1223	-3.2
158.0120	HMDB0142001	(2-oxoethoxy)sulfonic acid	C2H4O5S	M+NH4	158.0118	1.5
158.0210	HMDB0032931	2-Benzoxazolol	C7H5NO2	M+Na	158.0212	-1.6
	HMDB0004110	Phosphonoacetate	C2H5O5P	M+NH4	158.0213	-1.8
	HMDB0001494	Acetylphosphate	C2H5O5P	M+NH4	158.0213	-1.8
158.1171	HMDB0040526	3,4,4-Trimethyl-1,2-cyclopentanedione	C8H12O2	M+NH4	158.1176	-2.9
	HMDB0037625	Allyl tiglate	C8H12O2	M+NH4	158.1176	-2.9
	HMDB0039652	2-Hydroxy-3,4,5-trimethyl-2-cyclopenten-1-one	C8H12O2	M+NH4	158.1176	-2.9
	HMDB0039680	3,5,5-Trimethyl-1,2-cyclopentanedione	C8H12O2	M+NH4	158.1176	-2.9
	HMDB0039651	3-Propyl-1,2-cyclopentanedione	C8H12O2	M+NH4	158.1176	-2.9
	HMDB0039673	4-Ethyl-2-hydroxy-3-methyl-2-cyclopenten-1-one	C8H12O2	M+NH4	158.1176	-2.9
	HMDB0040463	Ethyl sorbate	C8H12O2	M+NH4	158.1176	-2.9
	HMDB0039681	3-Isopropyl-1,2-cyclopentanedione	C8H12O2	M+NH4	158.1176	-2.9
	HMDB0036176	3-Ethyl-2-hydroxy-4-methyl-2-cyclopenten-1-one	C8H12O2	M+NH4	158.1176	-2.9
	HMDB0037196	Ethyl 2-methyl-3,4-pentadienoate	C8H12O2	M+NH4	158.1176	-2.9
	HMDB0060682	2-Propyl-2,4-pentadienoic acid	C8H12O2	M+NH4	158.1176	-2.9
	HMDB0032311	2,4-Hexadienyl acetate	C8H12O2	M+NH4	158.1176	-2.9
	HMDB0037167	3-Ethyl-5-methyl-1,2-cyclopentanedione	C8H12O2	M+NH4	158.1176	-2.9
	HMDB0014447	Tranexamic Acid	C8H15NO2	M+H	158.1176	-2.9
	HMDB0033433	(S)-Homostachydrine	C8H15NO2	M+H	158.1176	-2.9

158.1535	HMDB0062671	(3E)-2,3,4-trimethylhex-3-enal	C9H16O	M+NH4	158.1539	-2.8
	HMDB0167031	Violet alcohol	C9H16O	M+NH4	158.1539	-2.8
	HMDB0037150	2-Ethyl-2-heptenal	C9H16O	M+NH4	158.1539	-2.8
	HMDB0037001	Santene hydrate	C9H16O	M+NH4	158.1539	-2.8
	HMDB0034845	2,4-Nonadien-1-ol	C9H16O	M+NH4	158.1539	-2.8
	HMDB0038067	(3E,6Z)-3,6-Nonadien-1-ol	C9H16O	M+NH4	158.1539	-2.8
	HMDB0037170	3-Methylene-2-octanone	C9H16O	M+NH4	158.1539	-2.8
	HMDB0035927	1-Nonen-4-one	C9H16O	M+NH4	158.1539	-2.8
	HMDB0035926	8-Nonen-2-one	C9H16O	M+NH4	158.1539	-2.8
	HMDB0031269	2-Nonenal	C9H16O	M+NH4	158.1539	-2.8
	HMDB0034764	3-Nonen-2-one	C9H16O	M+NH4	158.1539	-2.8
	HMDB0034761	5-Nonen-2-one	C9H16O	M+NH4	158.1539	-2.8
	HMDB0033554	2-Methyl-2-octenal	C9H16O	M+NH4	158.1539	-2.8
	HMDB0035916	(E)-2-Nonen-4-one	C9H16O	M+NH4	158.1539	-2.8
	HMDB0038400	(2xi,4xi)-2,4-Nonadien-1-ol	C9H16O	M+NH4	158.1539	-2.8
	HMDB0031834	2,6-Dimethyl-5-heptenal	C9H16O	M+NH4	158.1539	-2.8
	HMDB0031262	2,6-Nonadien-1-ol	C9H16O	M+NH4	158.1539	-2.8
	HMDB0033794	2,2,6-Trimethylcyclohexanone	C9H16O	M+NH4	158.1539	-2.8
	HMDB0030958	(Z)-6-Nonenal	C9H16O	M+NH4	158.1539	-2.8
	HMDB0030957	(3Z,6Z)-3,6-Nonadien-1-ol	C9H16O	M+NH4	158.1539	-2.8
	HMDB0059828	3-Nonen-5-one	C9H16O	M+NH4	158.1539	-2.8
	HMDB0034758	8-Nonen-3-one	C9H16O	M+NH4	158.1539	-2.8
	HMDB0032535	trans-4-Nonenal	C9H16O	M+NH4	158.1539	-2.8
	HMDB0039461	7-Methyl-3-octen-2-one	C9H16O	M+NH4	158.1539	-2.8
159.0273	HMDB0014581	Allopurinol	C5H4N4O	M+Na	159.0277	-2.7
	HMDB0000157	Hypoxanthine	C5H4N4O	M+Na	159.0277	-2.7
	HMDB0033054	Ethyl isopropyl disulfide	C5H12S2	M+Na	159.0273	0.3
	HMDB0033053	Ethyl propyl disulfide	C5H12S2	M+Na	159.0273	0.3
	HMDB0031160	1-Pentanesulfenothioic acid	C5H12S2	M+Na	159.0273	0.3
159.0648	HMDB0163407	3-hydroxy-5-(2-hydroxyethyl)-4-methyl-2,5-dihydrofuran-2-one	C7H10O4	M+H	159.0652	-2.4
	HMDB0163406	3-hydroxy-5-(1-hydroxyethyl)-4-methyl-2,5-dihydrofuran-2-one	C7H10O4	M+H	159.0652	-2.4
	HMDB0163405	5-ethyl-3-hydroxy-4-(hydroxymethyl)-2,5-dihydrofuran-2-one	C7H10O4	M+H	159.0652	-2.4
	HMDB0163408	5-(1-hydroxyethyl)-4-methyloxolane-2,3-dione	C7H10O4	M+H	159.0652	-2.4
	HMDB0163409	5-(2-hydroxyethyl)-4-methyloxolane-2,3-dione	C7H10O4	M+H	159.0652	-2.4
	HMDB0012241	Isopropylmaleate	C7H10O4	M+H	159.0652	-2.4
	HMDB0036380	xi-2,3-Dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one	C7H10O4	M+H	159.0652	-2.4
	HMDB0059815	Ethyl 5-oxotetrahydro-2-furancarboxylate	C7H10O4	M+H	159.0652	-2.4
	HMDB0000635	Succinylacetone	C7H10O4	M+H	159.0652	-2.4
159.1012	HMDB0062788	isobutyric acid anhydride	C8H14O3	M+H	159.1016	-2.3
	HMDB0041616	Propyl levulinate	C8H14O3	M+H	159.1016	-2.3
	HMDB0158408	(2Z)-8-hydroxyoct-2-enoic acid	C8H14O3	M+H	159.1016	-2.3
	HMDB0158407	SCHEMBL63	C8H14O3	M+H	159.1016	-2.3
	HMDB0158406	(2Z)-7-hydroxyoct-2-enoic acid	C8H14O3	M+H	159.1016	-2.3
	HMDB0158405	(2Z)-4-hydroxyoct-2-enoic acid	C8H14O3	M+H	159.1016	-2.3
	HMDB0040447	Butyl acetoacetate	C8H14O3	M+H	159.1016	-2.3
	HMDB0030303	6-Ethyl-1-methyl-2,7,8-trioxabicyclo[3.2.1]octane	C8H14O3	M+H	159.1016	-2.3
	HMDB0031307	Ethyl 3-oxohexanoate	C8H14O3	M+H	159.1016	-2.3
	HMDB0036395	2-Methylpropyl 3-oxobutanoate	C8H14O3	M+H	159.1016	-2.3
	HMDB0036230	1-Methyl-2-oxopropyl butyrate	C8H14O3	M+H	159.1016	-2.3
	HMDB0038305	3-Methylbutyl 2-oxopropanoate	C8H14O3	M+H	159.1016	-2.3
	HMDB0031177	Tetrahydrofurfuryl propionate	C8H14O3	M+H	159.1016	-2.3
	HMDB0010721	3-Oxooctanoic acid	C8H14O3	M+H	159.1016	-2.3
	HMDB0000909	trans-4-Hydroxycyclohexylacetic acid	C8H14O3	M+H	159.1016	-2.3
	HMDB0013211	Alpha-Ketooctanoic acid	C8H14O3	M+H	159.1016	-2.3
	HMDB0059938	5-Butyl-1,4-dioxan-2-one	C8H14O3	M+H	159.1016	-2.3
	HMDB0059939	6-Butyl-1,4-dioxan-2-one	C8H14O3	M+H	159.1016	-2.3
	HMDB0060685	3-Oxovalproic acid	C8H14O3	M+H	159.1016	-2.3
	HMDB0060683	2-n-Propyl-4-oxopentanoic acid	C8H14O3	M+H	159.1016	-2.3
	HMDB0000451	cis-4-Hydroxycyclohexylacetic acid	C8H14O3	M+H	159.1016	-2.3
	HMDB0179988	Isononanoic acid	C9H18O2	M+H	159.1380	-1.6
	HMDB0163472	2-methyl-octanoic acid	C9H18O2	M+H	159.1380	-1.6

159.1377	HMDB0179809	9-hydroxynonan-2-one	C9H18O2	M+H	159.1380	-1.6
	HMDB0179811	2-nonanon-3-ol	C9H18O2	M+H	159.1380	-1.6
	HMDB0179810	1-hydroxy-2-nonanone	C9H18O2	M+H	159.1380	-1.6
	HMDB0179808	8-hydroxynonan-2-one	C9H18O2	M+H	159.1380	-1.6
	HMDB0179167	1-hydroxynonan-4-one	C9H18O2	M+H	159.1380	-1.6
	HMDB0171041	SCHEMBL926	C9H18O2	M+H	159.1380	-1.6
	HMDB0171042	SCHEMBL7123711	C9H18O2	M+H	159.1380	-1.6
	HMDB0171040	non-8-ene-2,7-diol	C9H18O2	M+H	159.1380	-1.6
	HMDB0163464	(2Z)-2-methyloct-2-ene-1,8-diol	C9H18O2	M+H	159.1380	-1.6
	HMDB0163461	(2Z)-2-methyloct-2-ene-1,4-diol	C9H18O2	M+H	159.1380	-1.6
	HMDB0163462	(2Z)-2-methyloct-2-ene-1,7-diol	C9H18O2	M+H	159.1380	-1.6
	HMDB0163460	2-Hexylidene-1,3-propanediol	C9H18O2	M+H	159.1380	-1.6
	HMDB0163463	(2-methyl-3-pentylloxiran-2-yl)methanol	C9H18O2	M+H	159.1380	-1.6
	HMDB0062123	2-methylpropyl pentanoate	C9H18O2	M+H	159.1380	-1.6
	HMDB0040295	Butyl pentanoate	C9H18O2	M+H	159.1380	-1.6
	HMDB0034606	Hexyl propionate	C9H18O2	M+H	159.1380	-1.6
	HMDB0036234	3-Methylbutyl 2-methylpropanoate	C9H18O2	M+H	159.1380	-1.6
	HMDB0031291	Methyl caprylate	C9H18O2	M+H	159.1380	-1.6
	HMDB0034165	Propyl hexanoate	C9H18O2	M+H	159.1380	-1.6
	HMDB0039216	Butyl 2-methylbutanoate	C9H18O2	M+H	159.1380	-1.6
	HMDB0034162	Pentyl butanoate	C9H18O2	M+H	159.1380	-1.6
	HMDB0031480	Heptyl acetate	C9H18O2	M+H	159.1380	-1.6
	HMDB0039219	1-Methylbutyl butanoate	C9H18O2	M+H	159.1380	-1.6
	HMDB0030331	xi-2-Ethylheptanoic acid	C9H18O2	M+H	159.1380	-1.6
	HMDB0031557	4-Methyloctanoic acid	C9H18O2	M+H	159.1380	-1.6
	HMDB0000847	Pelargonic acid	C9H18O2	M+H	159.1380	-1.6
	HMDB0038603	Octyl formate	C9H18O2	M+H	159.1380	-1.6
	HMDB0037288	4-Methyl-2-pentyl-1,3-dioxolane	C9H18O2	M+H	159.1380	-1.6
	HMDB0037164	3-(Hydroxymethyl)-2-octanone	C9H18O2	M+H	159.1380	-1.6
	HMDB0059822	Ethyl 5-methylhexanoate	C9H18O2	M+H	159.1380	-1.6
	HMDB0032454	3-Octyl formate	C9H18O2	M+H	159.1380	-1.6
	HMDB0032309	3-Heptyl acetate	C9H18O2	M+H	159.1380	-1.6
	HMDB0032406	5-Methylhexyl acetate	C9H18O2	M+H	159.1380	-1.6
	HMDB0038040	2-Methylpropyl 3-methylbutanoate	C9H18O2	M+H	159.1380	-1.6
	HMDB0040221	Isoamyl butyrate	C9H18O2	M+H	159.1380	-1.6
	HMDB0032042	Butyl 3-methylbutanoate	C9H18O2	M+H	159.1380	-1.6
	HMDB0040430	Isopropyl hexanoate	C9H18O2	M+H	159.1380	-1.6
	HMDB0037143	1-Hydroxy-3-nonanone	C9H18O2	M+H	159.1380	-1.6
	HMDB0000798	Oenanthic ether	C9H18O2	M+H	159.1380	-1.6
160.0964	HMDB0164725	4-hydroxy-4-(hydroxymethyl)cyclohex-2-en-1-one	C7H10O3	M+NH4	160.0968	-2.6
	HMDB0164726	5-hydroxy-5-methyl-7-oxabicyclo[4.1]heptan-2-one	C7H10O3	M+NH4	160.0968	-2.6
	HMDB0180324	(2E)-3-(3-ethyloxiran-2-yl)prop-2-enoic acid	C7H10O3	M+NH4	160.0968	-2.6
	HMDB0180325	(2E)-4,5-dihydroxyhepta-2,4-dienal	C7H10O3	M+NH4	160.0968	-2.6
	HMDB0172015	4-methoxy-5-methyl-2-methylideneoxolan-3-one	C7H10O3	M+NH4	160.0968	-2.6
	HMDB0165787	2-ethyl-5-methyloxolane-3,4-dione	C7H10O3	M+NH4	160.0968	-2.6
	HMDB0033551	5-Ethyl-3-hydroxy-4-methyl-2(5H)-furanone	C7H10O3	M+NH4	160.0968	-2.6
	HMDB0164727	4,6-dihydroxy-4-methylcyclohex-2-en-1-one	C7H10O3	M+NH4	160.0968	-2.6
	HMDB0034230	Mesifurane	C7H10O3	M+NH4	160.0968	-2.6
	HMDB0033736	Homofureanol	C7H10O3	M+NH4	160.0968	-2.6
	HMDB0041426	Erinapyrone A	C7H10O3	M+NH4	160.0968	-2.6
	HMDB0041427	Erinapyrone B	C7H10O3	M+NH4	160.0968	-2.6
	HMDB0163404	5-ethyl-4-methyloxolane-2,3-dione	C7H10O3	M+NH4	160.0968	-2.6
	HMDB0011757	N-Acetylvaline	C7H13NO3	M+H	160.0968	-2.6
	HMDB0029412	Betonidine	C7H13NO3	M+H	160.0968	-2.6
	HMDB0038593	Calystegin A3	C7H13NO3	M+H	160.0968	-2.6
	HMDB0031345	Calystegine A6	C7H13NO3	M+H	160.0968	-2.6
	HMDB0038625	Medicanine	C7H13NO3	M+H	160.0968	-2.6
	HMDB0036384	Calystegine A7	C7H13NO3	M+H	160.0968	-2.6
	HMDB0012175	5-Acetamidovalerate	C7H13NO3	M+H	160.0968	-2.6
	HMDB0012154	3-Dehydrocarnitine	C7H13NO3	M+H	160.0968	-2.6
	HMDB0000927	Valerylglycine	C7H13NO3	M+H	160.0968	-2.6
	HMDB0000678	Isovalerylglycine	C7H13NO3	M+H	160.0968	-2.6
	HMDB0000339	2-Methylbutyrylglycine	C7H13NO3	M+H	160.0968	-2.6
	HMDB0029230	4-Hydroxystachydrine	C7H13NO3	M+H	160.0968	-2.6
	HMDB0029409	Turicine	C7H13NO3	M+H	160.0968	-2.6

160.1328	HMDB0061678	Methyl 5-(hydroxymethyl)pyrrolidine-3-carboxylate	C7H13NO3	M+H	160.0968	-2.6
	HMDB0163316	(3E)-7-hydroxyoct-3-en-2-one	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0163318	(E)-8-Hydroxy-3-octene-2-one	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0163317	Ethanone, 1-(3-butyloxiranyl)-	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0163315	SCHEMBL17867	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0163319	(3E)-1-hydroxyoct-3-en-2-one	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0037624	Isopropyl tiglate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0031293	2,3-Octanedione	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0029761	Ethyl 2-methyl-4-pentenoate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0035422	4-Butyl-gamma-butyrolactone	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0031352	Cyclohexyl acetate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0031343	Methyl cyclohexanecarboxylate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0036212	2-Methylpropyl (2E)-butenoate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0032533	trans-3-Hexenyl acetate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0240301	3-Octenoic acid	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0032266	Ethyl (E)-3-hexenoate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0036236	2-Methylallyl butyrate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0032268	Ethyl 2E-hexenoate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0000392	2-Octenoic acid	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0001568	trans-2-Octenoic acid	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0039793	(E)-4-Octenoic acid	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0037630	xi-Tetrahydro-3-propyl-2H-pyran-2-one	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0038310	xi-Tetrahydro-6-propyl-2H-pyran-2-one	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0039872	Methyl 2-heptenoate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0037622	Ethyl 2-methyl-3-pentenoate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0040215	cis-3-Hexenyl acetate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0040212	2-Hexenyl acetate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0032164	Allyl valerate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0059908	Ethyl-3-hexanoate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0013903	(3Z)-2-Propylpent-3-enoic acid	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0061342	(3Z)-2-Propylpent-3-enoic acid	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0062077	6-methylheptan-2,4-dione	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0013902	2-ene-Valproic acid	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0032267	Ethyl 5-hexenoate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0062166	Vinyl hexanoate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0013904	(3E)-2-Propylpent-3-enoic acid	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0032207	cis-5-Octenoic acid	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0032278	Ethyl trans-2-methyl-2-pentenoate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0038036	2-Propenyl 3-methylbutanoate	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0031403	Cyclohexanecarboxylic acid	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0013897	4-ene-Valproic acid	C8H14O2	M+NH4	160.1332	-2.5
	HMDB0000991	DL-2-Aminooctanoic acid	C8H17NO2	M+H	160.1332	-2.5
	HMDB0240571	Valine betaine	C8H18NO2	M+H	160.1332	-2.5
	HMDB0014375	Pregabalin	C8H17NO2	M+H	160.1332	-2.5
	HMDB0240732	delta-Valerobetaine	C8H17NO2	M+H	160.1332	-2.5
161.0593	HMDB0036073	Viburtinal	C10H8O2	M+H	161.0597	-2.5
	HMDB0041009	7-Methyl-2-benzofurancarboxaldehyde	C10H8O2	M+H	161.0597	-2.5
	HMDB0032394	6-Methylcoumarin	C10H8O2	M+H	161.0597	-2.5
	HMDB0060497	Naphthalene-1,2-diol	C10H8O2	M+H	161.0597	-2.5
161.0804	HMDB0041605	Propyleneglycol diacetate	C7H12O4	M+H	161.0808	-2.7
	HMDB0165010	2-(acetyloxy)-3-methylbutanoic acid	C7H12O4	M+H	161.0808	-2.7
	HMDB0175388	ss-Acetoxyisovaleriansaure	C7H12O4	M+H	161.0808	-2.7
	HMDB0000555	3-Methyladipic acid	C7H12O4	M+H	161.0808	-2.7
	HMDB0002441	3,3-Dimethylglutaric acid	C7H12O4	M+H	161.0808	-2.7
	HMDB0029573	Diethyl malonate	C7H12O4	M+H	161.0808	-2.7
	HMDB0029167	2-Methyladipic acid	C7H12O4	M+H	161.0808	-2.7
	HMDB0059893	Ethyl methyl succinate	C7H12O4	M+H	161.0808	-2.7
	HMDB0059722	Mono-methyl-adipate	C7H12O4	M+H	161.0808	-2.7
	HMDB0059738	2-Ethylglutaric acid	C7H12O4	M+H	161.0808	-2.7
	HMDB0061239	2-Propylsuccinic acid	C7H12O4	M+H	161.0808	-2.7
	HMDB0061676	2,2-Dimethylglutaric acid	C7H12O4	M+H	161.0808	-2.7
	HMDB0000857	Pimelic acid	C7H12O4	M+H	161.0808	-2.7
	HMDB0172040	CTK8I1333	C8H16O3	M+H	161.1172	-2.6
	HMDB0061914	8-Hydroxyoctanoate	C8H16O3	M+H	161.1172	-2.6
	HMDB0062596	(7R)-7-hydroxyoctanoic acid	C8H16O3	M+H	161.1172	-2.6

161.1168	HMDB0164640	3,7-dihydroxyoctanal	C8H16O3	M+H	161.1172	-2.6
	HMDB0172041	SCHEMBL9153763	C8H16O3	M+H	161.1172	-2.6
	HMDB0172042	NSC616278	C8H16O3	M+H	161.1172	-2.6
	HMDB0172043	ethyl 3-(hydroxymethyl)pentanoate	C8H16O3	M+H	161.1172	-2.6
	HMDB0172044	SCHEMBL8569867	C8H16O3	M+H	161.1172	-2.6
	HMDB0000711	Hydroxyoctanoic acid	C8H16O3	M+H	161.1172	-2.6
	HMDB0002264	(R)-2-Hydroxycaprylic acid	C8H16O3	M+H	161.1172	-2.6
	HMDB0010722	(R)-3-Hydroxyoctanoic acid	C8H16O3	M+H	161.1172	-2.6
	HMDB0031509	Ethyl 3-hydroxyhexanoate	C8H16O3	M+H	161.1172	-2.6
	HMDB0032827	Peroxyoctanoic acid	C8H16O3	M+H	161.1172	-2.6
	HMDB0032270	(+/-)-Ethyl 2-hydroxy-3-methylvalerate	C8H16O3	M+H	161.1172	-2.6
	HMDB0013898	5-Hydroxyvalproic acid	C8H16O3	M+H	161.1172	-2.6
	HMDB0013900	4-Hydroxyvalproic acid	C8H16O3	M+H	161.1172	-2.6
	HMDB0013899	3-Hydroxyvalproic acid	C8H16O3	M+H	161.1172	-2.6
	HMDB0059825	Isoamyl lactate	C8H16O3	M+H	161.1172	-2.6
	HMDB0059867	Ethyl 2-hydroxy-4-methylpentanoate	C8H16O3	M+H	161.1172	-2.6
	HMDB0001954	(S)-3-hydroxyoctanoic acid	C8H16O3	M+H	161.1172	-2.6
	HMDB0000486	7-Hydroxyoctanoic acid	C8H16O3	M+H	161.1172	-2.6
161.1280	HMDB0030410	L-2-Amino-3-methylenehexanoic acid	C7H13NO2	M+NH4	161.1285	-2.8
	HMDB0004827	Proline betaine	C7H13NO2	M+NH4	161.1285	-2.8
	HMDB0038949	3beta,6beta-Dihydroxynortropine	C7H13NO2	M+NH4	161.1285	-2.8
	HMDB0240689	N2-Methyl-L-lysine	C7H16N2O2	M+H	161.1285	-2.8
	HMDB0006009	Isoputrescine	C7H16N2O2	M+H	161.1285	-2.8
	HMDB0002038	N(6)-Methyllysine	C7H16N2O2	M+H	161.1285	-2.8
161.1320	HMDB0061814	1-(1-methylethenyl)-3-(1-methylethyl)-benzene	C12H16	M+H	161.1325	-3.0
	HMDB0061813	1-(1-Methylethenyl)-4-(1-methylethyl)benzene	C12H16	M+H	161.1325	-3.0
162.0757	HMDB0240300	3-methylpent-2-enedioic acid	C6H8O4	M+NH4	162.0761	-2.4
	HMDB0000393	3-Hexenedioic acid	C6H8O4	M+NH4	162.0761	-2.4
	HMDB0040207	Ethyl hydrogen fumarate	C6H8O4	M+NH4	162.0761	-2.4
	HMDB0036232	Maleic acid homopolymer	C6H8O4	M+NH4	162.0761	-2.4
	HMDB0163709	(2Z)-3-(hydroxymethyl)-4-oxopent-2-enoic acid	C6H8O4	M+NH4	162.0761	-2.4
	HMDB0180627	2,4-Dioxohexanoic acid	C6H8O4	M+NH4	162.0761	-2.4
	HMDB0163710	3-acetyl-3-methyloxirane-2-carboxylic acid	C6H8O4	M+NH4	162.0761	-2.4
	HMDB0002266	(E)-2-Methylglutaconic acid	C6H8O4	M+NH4	162.0761	-2.4
	HMDB0013311	trans-2-Hexenedioic acid	C6H8O4	M+NH4	162.0761	-2.4
	HMDB0163711	(2Z)-5-hydroxy-3-methyl-4-oxopent-2-enoic acid	C6H8O4	M+NH4	162.0761	-2.4
	HMDB0000522	3-Methylglutaconic acid	C6H8O4	M+NH4	162.0761	-2.4
	HMDB0029171	3-Hydroxyadipic acid 3,6-lactone	C6H8O4	M+NH4	162.0761	-2.4
	HMDB0031257	Dimethyl fumarate	C6H8O4	M+NH4	162.0761	-2.4
	HMDB0161226	2-[(1,2-dihydroxy-2-methylpropylidene)amino]acetic acid	C6H11NO4	M+H	162.0761	-2.4
	HMDB0094716	hydroxybutyrylglycine	C6H11NO4	M+H	162.0761	-2.4
	HMDB0161227	SCHEMBL1642433	C6H11NO4	M+H	162.0761	-2.4
	HMDB0062660	N-methyl-L-glutamic Acid	C6H11NO4	M+H	162.0761	-2.4
	HMDB0000510	Aminoadipic acid	C6H11NO4	M+H	162.0761	-2.4
	HMDB0033747	2,2'-Iminobispropanoic acid	C6H11NO4	M+H	162.0761	-2.4
	HMDB0029423	Acetylhomoserine	C6H11NO4	M+H	162.0761	-2.4
	HMDB0062557	N-Acetylthreonine	C6H11NO4	M+H	162.0761	-2.4
	HMDB0061715	L-Glutamic acid 5-methyl ester	C6H11NO4	M+H	162.0761	-2.4
162.0878	HMDB0041946	N-Nitrosoproline	C5H8N2O3	M+NH4	162.0873	3.0
162.1121	HMDB0163403	5-ethyl-3-hydroxy-4-methyloxolan-2-one	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0164729	2,4-dihydroxy-4-methylcyclohexan-1-one	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0164728	4-hydroxy-4-(hydroxymethyl)cyclohexan-1-one	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0165786	2(5)-ethyl-4-hydroxy-5(2)-methyl-3(2H)-furanone (ethylfuranol)	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0166497	(4Z)-6-hydroxyhept-4-enoic acid	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0180327	(2E)-3-[3-(2-hydroxyethyl)oxiran-2-yl]prop-2-en-1-ol	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0180326	(2E)-3-[3-(1-hydroxyethyl)oxiran-2-yl]prop-2-en-1-ol	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0166501	(4Z)-2-hydroxyhept-4-enoic acid	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0180835	pentyl 2-oxoacetate	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0031176	Tetrahydrofurfuryl acetate	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0040433	Ethyl levulinate	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0036594	Botryodiplodin	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0037114	Methyl (R)-3-methyl-2-oxopentanoate	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0001988	4-Hydroxycyclohexylcarboxylic acid	C7H12O3	M+NH4	162.1125	-2.3

	HMDB0172013	4-methoxy-2,5-dimethyloxolan-3-one	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0166498	(4Z)-3-hydroxyhept-4-enoic acid	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0166499	SCHEMBL7994854	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0061990	2-hydroxycyclohexanecarboxylic acid	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0166500	SCHEMBL26282	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0166747	SCHEMBL088	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0166744	(2E)-4-hydroxyhept-2-enoic acid	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0166746	ACMC-mulz	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0166745	(2E)-6-hydroxyhept-2-enoic acid	C7H12O3	M+NH4	162.1125	-2.3
	HMDB0062496	L-Carnitine	C7H15NO3	M+H	162.1125	-2.3
162.1484	HMDB0145126	5-[(2-hydroxyethyl)amino]pentanoic acid	C7H15NO3	M+H	162.1125	-2.3
	HMDB0181105	8-hydroxyoctan-3-one	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0062151	Propyl 2-methylbutanoate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0061998	2-methylbutyl propanoate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0061931	Tetrahydro-2,5-dimethyl-2H-pyranmethanol	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0032272	Ethyl 4-methylpentanoate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0032225	1,1-Dimethoxy-trans-2-hexene	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0032335	3-Hydroxy-2-octanone	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0032203	cis- and trans-2-Isobutyl-4-methyl-1,3-dioxolane	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0032551	Valeraldehyde propyleneglycol acetal	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0181107	4-Hydroxyoctane-3-one	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0181104	7-hydroxyoctan-3-one	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0163320	7-hydroxyoctan-2-one	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0163321	8-Hydroxy-2-octanone	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0163323	1-hydroxy-2-octanone	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0181103	2-hydroxyoctan-3-one	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0031579	Ethyl 2-methylpentanoate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0034234	Ethyl 3-methylpentanoate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0034161	2-Methylpropyl butanoate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0031478	Methyl heptanoate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0040209	Ethyl hexanoate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0034164	3-Methylbutyl propanoate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0034459	Heptyl formate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0029980	Hexyl acetate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0036165	3-(Hydroxymethyl)-2-heptanone	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0030368	(3R,5Z)-5-Octene-1,3-diol	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0035457	5-Hydroxy-4-octanone	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0031290	1-Hydroxy-3-octanone	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0000482	Caprylic acid	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0062511	Caprylic acid	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0031703	2-Ethylbutyl acetate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0031587	2-Methylheptanoic acid	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0031588	6-Methylheptanoic acid	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0039217	Isopropyl 2-methylbutanoate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0039620	Butyl butyrate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0040298	Ethyl 2-ethylbutanoate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0040252	Isobutyl isobutyrate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0040251	Butyl isobutyrate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0032047	Propyl 3-methylbutanoate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0001877	Valproic acid	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0031638	Pentyl propanoate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0032046	Isopropyl 3-methylbutanoate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0040296	Propyl pentanoate	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0031230	2-Ethylhexanoic acid	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0062546	2-Ethylhexanoic acid	C8H16O2	M+NH4	162.1489	-2.8
	HMDB0031596	Methyl 5-methylhexanoate	C8H16O2	M+NH4	162.1489	-2.8
163.0385	HMDB0183677	3-(3-hydroxyphenyl)prop-2-ynoic acid	C9H6O3	M+H	163.0390	-2.9
	HMDB0183678	3-(4-hydroxyphenyl)prop-2-ynoic Acid	C9H6O3	M+H	163.0390	-2.9
	HMDB0136738	5-hydroxy-2H-chromen-2-one	C9H6O3	M+H	163.0390	-2.9
	HMDB0140948	6-hydroxy-2H-chromen-2-one	C9H6O3	M+H	163.0390	-2.9
	HMDB0140949	8-hydroxy-2H-chromen-2-one	C9H6O3	M+H	163.0390	-2.9
	HMDB0137904	4-hydroxy-2H-chromen-2-one	C9H6O3	M+H	163.0390	-2.9
	HMDB0029865	Umbelliferone	C9H6O3	M+H	163.0390	-2.9
	HMDB0002149	3 Hydroxycoumarin	C9H6O3	M+H	163.0390	-2.9
	HMDB0177509	2-(4-methoxyphenyl)-3-methylideneoxirane	C10H10O2	M+H	163.0754	-2.2

163.0750	HMDB0133504	4-(3-hydroxyphenyl)but-3-en-2-one	C10H10O2	M+H	163.0754	-2.2
	HMDB0133595	(2Z)-2-(hydroxymethyl)-3-phenylprop-2-enal	C10H10O2	M+H	163.0754	-2.2
	HMDB0157134	2-phenylbut-3-enoic acid	C10H10O2	M+H	163.0754	-2.2
	HMDB0151225	AKO17514298	C10H10O2	M+H	163.0754	-2.2
	HMDB0141158	1-hydroxy-4-phenylbut-3-en-2-one	C10H10O2	M+H	163.0754	-2.2
	HMDB0133755	1-phenylbutane-2,3-dione	C10H10O2	M+H	163.0754	-2.2
	HMDB0133751	(3E)-4-(2-hydroxyphenyl)but-3-en-2-one	C10H10O2	M+H	163.0754	-2.2
	HMDB0133750	1-(3-phenyloxiran-2-yl)ethan-1-one	C10H10O2	M+H	163.0754	-2.2
	HMDB0133749	(3E)-4-(4-hydroxyphenyl)but-3-en-2-one	C10H10O2	M+H	163.0754	-2.2
	HMDB0133752	(3Z)-3-hydroxy-4-phenylbut-3-en-2-one	C10H10O2	M+H	163.0754	-2.2
	HMDB0133748	(3E)-4-(3-hydroxyphenyl)but-3-en-2-one	C10H10O2	M+H	163.0754	-2.2
	HMDB0133747	(3E)-1-hydroxy-4-phenylbut-3-en-2-one	C10H10O2	M+H	163.0754	-2.2
	HMDB0133597	(2Z)-3-(4-hydroxyphenyl)-2-methylprop-2-enal	C10H10O2	M+H	163.0754	-2.2
	HMDB0133598	2-methyl-3-phenyloxirane-2-carbaldehyde	C10H10O2	M+H	163.0754	-2.2
	HMDB0133599	(2Z)-3-(2-hydroxyphenyl)-2-methylprop-2-enal	C10H10O2	M+H	163.0754	-2.2
	HMDB0133596	(2Z)-3-(3-hydroxyphenyl)-2-methylprop-2-enal	C10H10O2	M+H	163.0754	-2.2
	HMDB0133594	(2E)-2-methyl-3-phenylprop-2-enoic acid	C10H10O2	M+H	163.0754	-2.2
	HMDB0060335	1,2-Dihydronaphthalene-1,2-diol	C10H10O2	M+H	163.0754	-2.2
	HMDB0033830	Cassiastearoptene	C10H10O2	M+H	163.0754	-2.2
	HMDB0040577	Cinnamyl formate	C10H10O2	M+H	163.0754	-2.2
	HMDB0029714	4,5-Dihydro-1-benzoxepin-3(2H)-one	C10H10O2	M+H	163.0754	-2.2
	HMDB0033591	Safrole	C10H10O2	M+H	163.0754	-2.2
	HMDB0033833	Methyl cinnamate	C10H10O2	M+H	163.0754	-2.2
	HMDB0032611	3-(4-Methoxyphenyl)-2-propenal	C10H10O2	M+H	163.0754	-2.2
	HMDB0040592	Allyl benzoate	C10H10O2	M+H	163.0754	-2.2
	HMDB0141046	4-(4-hydroxyphenyl)but-3-en-2-one	C10H10O2	M+H	163.0754	-2.2
	HMDB0146627	3-(2-methoxyphenyl)prop-2-enal	C10H10O2	M+H	163.0754	-2.2
	HMDB0135643	3-(4-methoxyphenyl)prop-2-enal	C10H10O2	M+H	163.0754	-2.2
	HMDB0038893	3,6-Dimethyl-2(3H)-benzofuranone	C10H10O2	M+H	163.0754	-2.2
163.1073	HMDB0240326	N-(1-carboxypropyl)ethanecarboximidate	C6H10NO3	M+NH4	163.1077	-2.6
	HMDB0094698	N-PROPIONYLALANINE	C6H11NO3	M+NH4	163.1077	-2.6
	HMDB0012131	(S)-5-Amino-3-oxohexanoate	C6H11NO3	M+NH4	163.1077	-2.6
	HMDB0000808	N-Butyrylglycine	C6H11NO3	M+NH4	163.1077	-2.6
	HMDB0012151	2-Keto-6-aminocaproate	C6H11NO3	M+NH4	163.1077	-2.6
	HMDB0000730	Isobutyrylglycine	C6H11NO3	M+NH4	163.1077	-2.6
	HMDB0029425	L-cis-4-(Hydroxymethyl)-2-pyrrolidinecarboxylic acid	C6H11NO3	M+NH4	163.1077	-2.6
	HMDB0029426	L-trans-5-Hydroxy-2-piperidinecarboxylic acid	C6H11NO3	M+NH4	163.1077	-2.6
	HMDB0003681	4-Acetamidobutanoic acid	C6H11NO3	M+NH4	163.1077	-2.6
	HMDB0060265	4-Acetamidobutanoic acid	C6H11NO3	M+NH4	163.1077	-2.6
	HMDB0015127	Methyl aminolevulinate	C6H11NO3	M+NH4	163.1077	-2.6
	HMDB0061156	N-(2-Carboxymethyl)-morpholine	C6H11NO3	M+NH4	163.1077	-2.6
	HMDB0001263	(S)-2-amino-6-oxohexanoate	C6H11NO3	M+NH4	163.1077	-2.6
	HMDB0059595	(S)-2-amino-6-oxohexanoate	C6H11NO3	M+NH4	163.1077	-2.6
	HMDB0000450	5-Hydroxylysine	C6H14N2O3	M+H	163.1077	-2.6
163.1113	HMDB0062570	erythro-5-hydroxy-L-lysinium(1+)	C6H15N2O3	M+H	163.1077	-2.6
	HMDB0040245	2-Methyl-3-(2-methylphenyl)propanal	C11H14O	M+H	163.1117	-2.7
	HMDB0133676	3-methyl-4-phenylbutan-2-one	C11H14O	M+H	163.1117	-2.7
	HMDB0163601	3-Methyl-2-phenyl-3-buten-1-ol	C11H14O	M+H	163.1117	-2.7
	HMDB0032415	2-Methyl-4-phenylbutyraldehyde	C11H14O	M+H	163.1117	-2.7
	HMDB0033562	3-Methyl-2-phenylbutanal	C11H14O	M+H	163.1117	-2.7
	HMDB0039803	4,4alpha,5,6-Tetrahydro-7-methyl-2(3H)-naphthalenone	C11H14O	M+H	163.1117	-2.7
	HMDB0031856	2-Methyl-3-(4-methylphenyl)propanal	C11H14O	M+H	163.1117	-2.7
	HMDB0032025	4'-Isopropylacetophenone	C11H14O	M+H	163.1117	-2.7
	HMDB0031208	1-Phenyl-1-pentanone	C11H14O	M+H	163.1117	-2.7
	HMDB0036183	4-(4-Methylphenyl)-2-butanone	C11H14O	M+H	163.1117	-2.7
	HMDB0041493	4-Isopropylphenylacetaldehyde	C11H14O	M+H	163.1117	-2.7
163.1226	HMDB0032967	2,4-Dimethyl-1H-indole	C10H11N	M+NH4	163.1230	-2.3
	HMDB0001934	Nicotine	C10H14N2	M+H	163.1230	-2.3
	HMDB0004350	Anabasine	C10H14N2	M+H	163.1230	-2.3
	HMDB0039982	Trimethyl-2-propenylpyrazine	C10H14N2	M+H	163.1230	-2.3
	HMDB0014330	Nicotine	C10H14N2	M+H	163.1230	-2.3
163.1324	HMDB0033625	(3R,7R)-1,3,7-Octanetriol	C8H18O3	M+H	163.1329	-2.9
	HMDB0240327	2,3-dimethylbutanedioate	C6H8O4	M+NH4	164.0917	-2.6
	HMDB0161125	3-hydroxy-4-methyl-2-oxopentanoic acid	C6H10O4	M+NH4	164.0917	-2.6

164.0913	HMDB0161124	5-hydroxy-4-methyl-2-oxopentanoic acid	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0161123	SCHEMBL193563	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0159478	SCHEMBL3185864	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0159479	3-(hydroxymethyl)-2-oxopentanoic acid	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0159480	SCHEMBL85244	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0159477	3-Hydroxy-3-methyl-2-oxopentanoate	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0158748	SCHEMBL2592393	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0158747	2-(hydroxymethyl)-3-oxopentanoic acid	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0158746	SCHEMBL1268	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0158745	SCHEMBL143458	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0155922	Mevaldic acid	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0061930	4-Ethoxy-4-oxobutanoic acid	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0006900	(S)-2-Aceto-2-hydroxybutanoic acid	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0002173	Solerol	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0002074	2,2-Dimethylsuccinic acid	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0000858	Monomethyl glutaric acid	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0000752	Methylglutaric acid	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0000448	Adipic acid	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0033837	Dimethyl succinate	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0000422	2-Methylglutaric acid	C6H10O4	M+NH4	164.0917	-2.6
	HMDB0011727	Bicine	C6H13NO4	M+H	164.0917	-2.6
	HMDB0032862	2-Amino-4-ethoxy-3-hydroxybutanoic acid	C6H13NO4	M+H	164.0917	-2.6
	HMDB0035359	1-Deoxynojirimycin	C6H13NO4	M+H	164.0917	-2.6
164.1278	HMDB0165834	SCHEMBL934322	C7H14O3	M+NH4	164.1281	-1.9
	HMDB0165833	Ethyl 3-hydroxy-2-methylbutyrate	C7H14O3	M+NH4	164.1281	-1.9
	HMDB0165835	Ethyl 2-(hydroxymethyl)butanoate	C7H14O3	M+NH4	164.1281	-1.9
	HMDB0165836	SCHEMBL7861	C7H14O3	M+NH4	164.1281	-1.9
	HMDB0161032	6-hydroxyheptanoic acid	C7H14O3	M+NH4	164.1281	-1.9
	HMDB0002207	3-Hydroxyisoheptanoic acid	C7H14O3	M+NH4	164.1281	-1.9
	HMDB0036231	Methyl DL-Leucate	C7H14O3	M+NH4	164.1281	-1.9
	HMDB0039407	Methyl 3-hydroxyhexanoate	C7H14O3	M+NH4	164.1281	-1.9
	HMDB0040254	Butyl lactate	C7H14O3	M+NH4	164.1281	-1.9
	HMDB0032269	(+/-)-Ethyl 2-hydroxy-2-methylbutyrate	C7H14O3	M+NH4	164.1281	-1.9
	HMDB0059842	Ethyl 2-hydroxyisovalerate	C7H14O3	M+NH4	164.1281	-1.9
	HMDB0061653	3-hydroxyheptanoic acid	C7H14O3	M+NH4	164.1281	-1.9
	HMDB0161034	2-hydroxyheptanoic acid	C7H14O3	M+NH4	164.1281	-1.9
	HMDB0161033	7-Hydroxyheptanoic acid	C7H14O3	M+NH4	164.1281	-1.9
164.1641	HMDB0029359	(R)-1,3-Octanediol	C8H18O2	M+NH4	164.1645	-2.5
	HMDB0170960	1,7-Octanediol	C8H18O2	M+NH4	164.1645	-2.5
	HMDB0172313	octane-1,2-diol	C8H18O2	M+NH4	164.1645	-2.5
	HMDB0170961	octane-1,8-diol	C8H18O2	M+NH4	164.1645	-2.5
	HMDB0038679	1-Methoxy-1-pentyloxyethane	C8H18O2	M+NH4	164.1645	-2.5
	HMDB0037635	xi-1-Ethoxy-1-butoxyethane	C8H18O2	M+NH4	164.1645	-2.5
	HMDB0172312	19686-96-5	C8H18O2	M+NH4	164.1645	-2.5
165.0542	HMDB0126545	3-phenyloxirane-2-carboxylic acid	C9H8O3	M+H	165.0546	-2.5
	HMDB0129375	4-methoxy-1-benzofuran-6-ol	C9H8O3	M+H	165.0546	-2.5
	HMDB0150715	7-hydroxychroman-2-one	C9H8O3	M+H	165.0546	-2.5
	HMDB0128076	3-(4-hydroxyphenyl)prop-2-enoic acid	C9H8O3	M+H	165.0546	-2.5
	HMDB0062774	3-(3-hydroxyphenyl)prop-2-enoic acid	C9H8O3	M+H	165.0546	-2.5
	HMDB0125104	3-(3-hydroxyphenyl)prop-2-enoic acid	C9H8O3	M+H	165.0546	-2.5
	HMDB0134029	3-(2,3-dihydroxyphenyl)prop-2-enal	C9H8O3	M+H	165.0546	-2.5
	HMDB0134030	3-(2,5-dihydroxyphenyl)prop-2-enal	C9H8O3	M+H	165.0546	-2.5
	HMDB0134031	3-(2-hydroxyphenyl)oxirane-2-carbaldehyde	C9H8O3	M+H	165.0546	-2.5
	HMDB0166606	(2Z)-3-(3,4-dihydroxyphenyl)prop-2-enal	C9H8O3	M+H	165.0546	-2.5
	HMDB0150720	4-hydroxychroman-2-one	C9H8O3	M+H	165.0546	-2.5
	HMDB0150718	974-72-5	C9H8O3	M+H	165.0546	-2.5
	HMDB0150717	hydroxychromanone	C9H8O3	M+H	165.0546	-2.5
	HMDB0150719	5-hydroxychroman-2-one	C9H8O3	M+H	165.0546	-2.5
	HMDB0150716	2669-94-5	C9H8O3	M+H	165.0546	-2.5
	HMDB0141767	(2E)-3-(3,4-dihydroxyphenyl)prop-2-enal	C9H8O3	M+H	165.0546	-2.5
	HMDB0141768	3-(4-hydroxyphenyl)oxirane-2-carbaldehyde	C9H8O3	M+H	165.0546	-2.5
	HMDB0062655	Cis-2-coumarate	C9H8O3	M+H	165.0546	-2.5
	HMDB0134028	Cis-2-coumarate	C9H8O3	M+H	165.0546	-2.5
	HMDB0062148	2-oxo-2-phenylethyl formate	C9H8O3	M+H	165.0546	-2.5
	HMDB0163003	cis-3-coumaric acid	C9H8O3	M+H	165.0546	-2.5

	HMDB0041592	Coumarinic acid	C9H8O3	M+H	165.0546	-2.5
	HMDB0030677	cis-p-Coumaric acid	C9H8O3	M+H	165.0546	-2.5
	HMDB0012225	Enol-phenylpyruvate	C9H8O3	M+H	165.0546	-2.5
	HMDB0001713	m-Coumaric acid	C9H8O3	M+H	165.0546	-2.5
	HMDB0002035	4-Hydroxycinnamic acid	C9H8O3	M+H	165.0546	-2.5
	HMDB0000205	Phenylpyruvic acid	C9H8O3	M+H	165.0546	-2.5
	HMDB0031629	Phenylpyruvic acid	C9H8O3	M+H	165.0546	-2.5
	HMDB0062605	methyl phenylglyoxalate	C9H8O3	M+H	165.0546	-2.5
165.0670	HMDB0002641	2-Hydroxycinnamic acid	C9H8O3	M+H	165.0546	-2.5
	HMDB0062000	2-Methylnaphthalene	C11H10	M+Na	165.0675	-2.8
	HMDB0032860	1-Methylnaphthalene	C11H10	M+Na	165.0675	-2.8
165.1270	HMDB0036816	Norecasantalal	C11H16O	M+H	165.1274	-2.4
	HMDB0029653	1-(1-Methoxy-1-methylethyl)-4-methylbenzene	C11H16O	M+H	165.1274	-2.4
	HMDB0031625	1-Phenyl-2-pentanol	C11H16O	M+H	165.1274	-2.4
	HMDB0031624	5-Phenyl-1-pentanol	C11H16O	M+H	165.1274	-2.4
	HMDB0036814	Santalone	C11H16O	M+H	165.1274	-2.4
	HMDB0035601	(Z)-3-Methyl-2-(2-pentenyl)-2-cyclopenten-1-one	C11H16O	M+H	165.1274	-2.4
	HMDB0031311	Benzyl butyl ether	C11H16O	M+H	165.1274	-2.4
	HMDB0035989	Thymol methyl ether	C11H16O	M+H	165.1274	-2.4
	HMDB0036719	Norbicycloekasantalal	C11H16O	M+H	165.1274	-2.4
	HMDB0032060	2-Butyl-4-methylphenol	C11H16O	M+H	165.1274	-2.4
	HMDB0031866	2-Methyl-4-phenyl-2-butanol	C11H16O	M+H	165.1274	-2.4
	HMDB0037294	2-Methyl-3-(2-pentenyl)-2-cyclopenten-1-one	C11H16O	M+H	165.1274	-2.4
	HMDB0031454	trans-Jasmone	C11H16O	M+H	165.1274	-2.4
	HMDB0163591	3-methyl-2-phenylbutan-1-ol	C11H16O	M+H	165.1274	-2.4
166.0710	HMDB0160407	3-ethoxy-2-hydroxy-3-oxopropanoic acid	C5H8O5	M+NH4	166.0710	0.0
	HMDB0160406	SCHEMBL41920	C5H8O5	M+NH4	166.0710	0.0
	HMDB0160667	SCHEMBL6374585	C5H8O5	M+NH4	166.0710	0.0
	HMDB0160666	SCHEMBL1124153	C5H8O5	M+NH4	166.0710	0.0
	HMDB0160668	Aethyltartroisaur	C5H8O5	M+NH4	166.0710	0.0
	HMDB0161319	Itamalic acid	C5H8O5	M+NH4	166.0710	0.0
	HMDB0000428	3-Hydroxyglutaric acid	C5H8O5	M+NH4	166.0710	0.0
	HMDB0000426	Citramalic acid	C5H8O5	M+NH4	166.0710	0.0
	HMDB0000606	D-2-Hydroxyglutaric acid	C5H8O5	M+NH4	166.0710	0.0
	HMDB0001900	Ribonolactone	C5H8O5	M+NH4	166.0710	0.0
	HMDB0011676	D-Xylono-1,5-lactone	C5H8O5	M+NH4	166.0710	0.0
	HMDB0059655	2-Hydroxyglutarate	C5H8O5	M+NH4	166.0710	0.0
	HMDB0061190	3-methylmalate(2-)	C5H8O5	M+NH4	166.0710	0.0
	HMDB0062739	3-methylmalate(2-)	C5H8O5	M+NH4	166.0710	0.0
	HMDB0000694	L-2-Hydroxyglutaric acid	C5H8O5	M+NH4	166.0710	0.0
166.0858	HMDB0135274	(2E)-3-(3-hydroxyphenyl)prop-2-enal	C9H8O2	M+NH4	166.0863	-2.7
	HMDB0135648	3-(4-hydroxyphenyl)prop-2-enal	C9H8O2	M+NH4	166.0863	-2.7
	HMDB0134039	3-(2-hydroxyphenyl)prop-2-enal	C9H8O2	M+NH4	166.0863	-2.7
	HMDB0135275	3-phenyloxirane-2-carbaldehyde	C9H8O2	M+NH4	166.0863	-2.7
	HMDB0135273	(2Z)-2-hydroxy-3-phenylprop-2-enal	C9H8O2	M+NH4	166.0863	-2.7
	HMDB0128078	3-phenylprop-2-enoic acid	C9H8O2	M+NH4	166.0863	-2.7
	HMDB0000567	Cinnamic acid	C9H8O2	M+NH4	166.0863	-2.7
	HMDB0036626	3,4-Dihydro-2H-1-benzopyran-2-one	C9H8O2	M+NH4	166.0863	-2.7
	HMDB0032947	Di-2-furanylmethane	C9H8O2	M+NH4	166.0863	-2.7
	HMDB0035243	1-Phenyl-1,2-propanedione	C9H8O2	M+NH4	166.0863	-2.7
	HMDB0000930	trans-Cinnamic acid	C9H8O2	M+NH4	166.0863	-2.7
	HMDB0040986	(E)-3-(4-Hydroxyphenyl)-2-propenal	C9H8O2	M+NH4	166.0863	-2.7
	HMDB0031725	(E)-3-(2-Hydroxyphenyl)-2-propenal	C9H8O2	M+NH4	166.0863	-2.7
	HMDB0062407	5-(3-Pyridyl)-2-hydroxytetrahydrofuran	C9H11NO2	M+H	166.0863	-2.7
	HMDB0033589	Ethyl 2-aminobenzoate	C9H11NO2	M+H	166.0863	-2.7
	HMDB0000159	L-Phenylalanine	C9H11NO2	M+H	166.0863	-2.7
	HMDB0159744	L-Phenylalanine	C9H11NO2	M+H	166.0863	-2.7
	HMDB0033485	Gentiatibetine	C9H11NO2	M+H	166.0863	-2.7
	HMDB0034169	Methyl N-methylanthranilate	C9H11NO2	M+H	166.0863	-2.7
	HMDB0006044	Norsalsolinol	C9H11NO2	M+H	166.0863	-2.7
	HMDB0001007	3-Pyridinebutanoic acid	C9H11NO2	M+H	166.0863	-2.7
	HMDB0059934	Benzyl glycinate	C9H11NO2	M+H	166.0863	-2.7
	HMDB0062402	4-Hydroxy-1-(3-pyridinyl)-1-butanone	C9H11NO2	M+H	166.0863	-2.7
	HMDB0004992	Benzocaine	C9H11NO2	M+H	166.0863	-2.7
	HMDB0015145	Edrophonium	C10H16NO	M+H	166.1232	-2.3

166.1228	HMDB0181325	AKO14925411	C10H15NO	M+H	166.1226	1.0
	HMDB0181326	5-(2-pyridyl)-1-pentanol	C10H15NO	M+H	166.1226	1.0
	HMDB0181238	3-pentyl-1位?pyridin-1-one	C10H15NO	M+H	166.1226	1.0
	HMDB0181237	1-(pyridin-3-yl)pentan-1-ol	C10H15NO	M+H	166.1226	1.0
	HMDB0181234	5-(pyridin-3-yl)pentan-2-ol	C10H15NO	M+H	166.1226	1.0
	HMDB0181235	3-pyridinepentanol	C10H15NO	M+H	166.1226	1.0
	HMDB0060767	4-Hydroxymethamphetamine	C10H15NO	M+H	166.1226	1.0
	HMDB0039678	3-Methyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one	C10H15NO	M+H	166.1226	1.0
	HMDB0001943	Pseudoephedrine	C10H15NO	M+H	166.1226	1.0
	HMDB0015451	Ephedrine	C10H15NO	M+H	166.1226	1.0
	HMDB0039682	2,3,4,5,6,7-Hexahydro-7-methylcyclopent[b]azepin-8(1H)-one	C10H15NO	M+H	166.1226	1.0
	HMDB0038597	Nepetalactam	C10H15NO	M+H	166.1226	1.0
	HMDB0039666	6-Ethyl-1,2,3,4,5,6-hexahydro-7H-cyclopenta[b]pyridin-7-one	C10H15NO	M+H	166.1226	1.0
	HMDB0004366	Hordenine	C10H15NO	M+H	166.1226	1.0
	HMDB0035652	Perilla sugar	C10H15NO	M+H	166.1226	1.0
	HMDB0039836	2-(5-Methyl-2-furanyl)piperidine	C10H15NO	M+H	166.1226	1.0
	HMDB0039665	5-Ethyl-1,2,3,4,5,6-hexahydro-7H-cyclopenta[b]pyridin-7-one	C10H15NO	M+H	166.1226	1.0
	HMDB0039679	5-Methyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one	C10H15NO	M+H	166.1226	1.0
	HMDB0040049	1-[(5-Methyl-2-furanyl)methyl]pyrrolidine	C10H15NO	M+H	166.1226	1.0
	HMDB0031616	4-Phenyl-3-buten-2-ol	C10H12O	M+NH4	166.1226	1.0
	HMDB0180475	SCHEMBL295411	C10H12O	M+NH4	166.1226	1.0
	HMDB0133593	(2E)-2-methyl-3-phenylprop-2-en-1-ol	C10H12O	M+NH4	166.1226	1.0
	HMDB0002214	Cuminaldehyde	C10H12O	M+NH4	166.1226	1.0
	HMDB0032014	2,3,6-Trimethylbenzaldehyde	C10H12O	M+NH4	166.1226	1.0
	HMDB0033382	2-(4-Methylphenyl)propanal	C10H12O	M+NH4	166.1226	1.0
	HMDB0061997	2-Methyl-3-phenylpropanal	C10H12O	M+NH4	166.1226	1.0
	HMDB0032015	Duryl aldehyde	C10H12O	M+NH4	166.1226	1.0
	HMDB0030837	Anethole	C10H12O	M+NH4	166.1226	1.0
	HMDB0133746	4-phenylbutan-2-one	C10H12O	M+NH4	166.1226	1.0
	HMDB0034121	1-Methoxy-4-(2-propenyl)benzene	C10H12O	M+NH4	166.1226	1.0
	HMDB0032140	2',4'-Dimethylacetophenone	C10H12O	M+NH4	166.1226	1.0
	HMDB0032017	3,4,5-Trimethylbenzaldehyde	C10H12O	M+NH4	166.1226	1.0
	HMDB0032016	2,4,6-Trimethylbenzaldehyde	C10H12O	M+NH4	166.1226	1.0
	HMDB0059845	p-Ethylacetophenone	C10H12O	M+NH4	166.1226	1.0
166.1591	HMDB0059834	Pentylbenzene	C11H16	M+NH4	166.1590	0.5
	HMDB0061810	2,4-Dimethyl-1-(1-methylethyl)-benzene	C11H16	M+NH4	166.1590	0.5
	HMDB0061809	1-Methyl-4-(1-methylpropyl)-benzene	C11H16	M+NH4	166.1590	0.5
167.0335	HMDB0032613	3,4-Methylenedioxybenzoic acid	C8H6O4	M+H	167.0339	-2.3
	HMDB0002428	Terephthalic acid	C8H6O4	M+H	167.0339	-2.3
	HMDB0061917	Terephthalic acid	C8H6O4	M+H	167.0339	-2.3
	HMDB0002334	Benzoquinoneacetic acid	C8H6O4	M+H	167.0339	-2.3
	HMDB0002107	Phthalic acid	C8H6O4	M+H	167.0339	-2.3
167.0550	HMDB0000539	Arabinonic acid	C5H10O6	M+H	167.0550	-0.1
	HMDB0060255	欽蟻-欽蟻xonic acid	C5H10O6	M+H	167.0550	-0.1
	HMDB0059750	欽婦-欽婦ylonic acid	C5H10O6	M+H	167.0550	-0.1
	HMDB0060256	欽蟻-Xylonic acid	C5H10O6	M+H	167.0550	-0.1
	HMDB0000867	Ribonic acid	C5H10O6	M+H	167.0550	-0.1
167.0892	HMDB0038183	3-(4-Methyl-3-pentenyl)thiophene	C10H14S	M+H	167.0889	1.8
	HMDB0041584	3-Hydroxy-p-mentha-1,8-dien-7-al	C10H14O2	M+H	167.1067	-2.7
	HMDB0163097	(2E,4Z)-6-(3-ethyloxiran-2-yl)hexa-2,4-dienal	C10H14O2	M+H	167.1067	-2.7
	HMDB0163096	4,5-epoxy-(e,z)-2,7-decadienal	C10H14O2	M+H	167.1067	-2.7
	HMDB0179459	5-methyl-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O2	M+H	167.1067	-2.7
	HMDB0179460	NSC143559	C10H14O2	M+H	167.1067	-2.7
	HMDB0180472	2-(4-methylphenyl)propane-1,2-diol	C10H14O2	M+H	167.1067	-2.7
	HMDB0180473	2-[4-(hydroxymethyl)phenyl]propan-1-ol	C10H14O2	M+H	167.1067	-2.7
	HMDB0180474	p-Cymene-9,-diol	C10H14O2	M+H	167.1067	-2.7
	HMDB0181685	3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M+H	167.1067	-2.7
	HMDB0181686	2-(hydroxymethyl)-3-methyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M+H	167.1067	-2.7
	HMDB0181689	4-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M+H	167.1067	-2.7

167.1062	HMDB0181687	5-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M+H	167.1067	-2.7
	HMDB0181688	1-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M+H	167.1067	-2.7
	HMDB0163095	3-[(1Z,4Z)-hepta-1,4-dien-1-yl]oxirane-2-carbaldehyde	C10H14O2	M+H	167.1067	-2.7
	HMDB0163098	(4Z,7Z)--hydroxydeca-2,4,7-trienal	C10H14O2	M+H	167.1067	-2.7
	HMDB0163093	SCHEMBL36924	C10H14O2	M+H	167.1067	-2.7
	HMDB0062603	2-(4-methoxyphenyl)propan-2-ol	C10H14O2	M+H	167.1067	-2.7
	HMDB0127496	1-ethyl-3,5-dimethoxybenzene	C10H14O2	M+H	167.1067	-2.7
	HMDB0135742	3-(4-methoxyphenyl)propan-1-ol	C10H14O2	M+H	167.1067	-2.7
	HMDB0146631	3-(2-methoxyphenyl)propan-1-ol	C10H14O2	M+H	167.1067	-2.7
	HMDB0163094	(2E,7Z)-9-hydroxydeca-2,4,7-trienal	C10H14O2	M+H	167.1067	-2.7
	HMDB0004586	Perillic acid	C10H14O2	M+H	167.1067	-2.7
	HMDB0032615	1,1-Dimethoxy-2-phenylethane	C10H14O2	M+H	167.1067	-2.7
	HMDB0037044	Rotundifolone	C10H14O2	M+H	167.1067	-2.7
	HMDB0037012	2-Hydroxy-p-mentha-1,8-dien-6-one	C10H14O2	M+H	167.1067	-2.7
	HMDB0040176	4-Ethyl-1,2-dimethoxybenzene	C10H14O2	M+H	167.1067	-2.7
	HMDB0032462	Pentyl 2-furyl ketone	C10H14O2	M+H	167.1067	-2.7
	HMDB0036878	1,4-Epidioxy-p-mentha-2,8-diene	C10H14O2	M+H	167.1067	-2.7
	HMDB0035328	Perilla ketone	C10H14O2	M+H	167.1067	-2.7
	HMDB0035063	Epinepetalactone	C10H14O2	M+H	167.1067	-2.7
	HMDB0032135	2-Methoxy-4-propylphenol	C10H14O2	M+H	167.1067	-2.7
	HMDB0036042	Marmelolactone A	C10H14O2	M+H	167.1067	-2.7
	HMDB0034922	alpha-Teresantalic acid	C10H14O2	M+H	167.1067	-2.7
	HMDB0039382	(1xi,4xi,6xi)-Carvone oxide	C10H14O2	M+H	167.1067	-2.7
	HMDB0041000	Karahana lactone	C10H14O2	M+H	167.1067	-2.7
	HMDB0032062	2-tert-Butyl-1,4-benzenediol	C10H14O2	M+H	167.1067	-2.7
	HMDB0037011	5-Hydroxy-p-mentha-6,8-dien-2-one	C10H14O2	M+H	167.1067	-2.7
	HMDB0031085	6-Pentyl-2H-pyran-2-one	C10H14O2	M+H	167.1067	-2.7
	HMDB0029691	Wine lactone	C10H14O2	M+H	167.1067	-2.7
	HMDB0036084	Isomintlactone	C10H14O2	M+H	167.1067	-2.7
	HMDB0035235	2,4,7-Decatrienoic acid	C10H14O2	M+H	167.1067	-2.7
	HMDB0036879	1,2:3,4-Diepoxy-p-menth-8-ene	C10H14O2	M+H	167.1067	-2.7
	HMDB0179461	2-methyl-5-(propan-2-yl)benzene-1,4-diol	C10H14O2	M+H	167.1067	-2.7
167.1426	HMDB0033546	2,5-Undecadienal	C11H18O	M+H	167.1430	-2.6
	HMDB0036815	Norecasantalol	C11H18O	M+H	167.1430	-2.6
	HMDB0036190	2-Heptylfuran	C11H18O	M+H	167.1430	-2.6
	HMDB0031728	2-Hexylidenecyclopentanone	C11H18O	M+H	167.1430	-2.6
	HMDB0031359	2,4-Undecadienal	C11H18O	M+H	167.1430	-2.6
	HMDB0030002	(-)-Nopol	C11H18O	M+H	167.1430	-2.6
	HMDB0030252	Limonene aldehyde	C11H18O	M+H	167.1430	-2.6
	HMDB0031565	Dihydrojasmane	C11H18O	M+H	167.1430	-2.6
	HMDB0032540	2,6,6-Trimethyl-1-cyclohexen-1-acetaldehyde	C11H18O	M+H	167.1430	-2.6
168.0053	HMDB0031004	Diatretin 2	C8H3NO2	M+Na	168.0056	-1.8
168.1227	HMDB0062045	hexane-1,2,5,6-tetrol	C6H14O4	M+NH4	168.1230	-2.0
	HMDB0062118	hexane-1,2,5,6-tetrol	C6H14O4	M+NH4	168.1230	-2.0
169.0258	HMDB0001218	Coumarin	C9H6O2	M+Na	169.0260	-1.2
	HMDB0032938	Chromone	C9H6O2	M+Na	169.0260	-1.2
	HMDB0033183	2-Benzofurancarboxaldehyde	C9H6O2	M+Na	169.0260	-1.2
	HMDB0002359	Phenylpropionic acid	C9H6O2	M+Na	169.0260	-1.2
169.0579	HMDB0000641	L-Glutamine	C5H10N2O3	M+Na	169.0584	-2.7
	HMDB0006899	Alanylglycine	C5H10N2O3	M+Na	169.0584	-2.7
	HMDB0240333	4-[(C-hydroxycarbonimidoyl)amino]butanoate	C5H9N2O3	M+Na	169.0584	-2.7
	HMDB0003423	D-Glutamine	C5H10N2O3	M+Na	169.0584	-2.7
	HMDB0028687	Alanylglycine	C5H10N2O3	M+Na	169.0584	-2.7
	HMDB0002031	Ureidoisobutyric acid	C5H10N2O3	M+Na	169.0584	-2.7
169.0855	HMDB0131223	3,5-dimethoxy-2-methylphenol	C9H12O3	M+H	169.0859	-2.5
	HMDB0168685	2-(4-(Hydroxymethyl)phenoxy)ethanol	C9H12O3	M+H	169.0859	-2.5
	HMDB0151518	SCHEMBL1954	C9H12O3	M+H	169.0859	-2.5
	HMDB0126600	5-methoxy-2,4-dimethylbenzene-1,3-diol	C9H12O3	M+H	169.0859	-2.5
	HMDB0125541	4-ethyl-2-methoxybenzene-1,3-diol	C9H12O3	M+H	169.0859	-2.5
	HMDB0125531	5-ethyl-3-methoxybenzene-1,2-diol	C9H12O3	M+H	169.0859	-2.5
	HMDB0125521	4-ethyl-6-methoxybenzene-1,3-diol	C9H12O3	M+H	169.0859	-2.5
	HMDB0059963	1,3,5-Trimethoxybenzene	C9H12O3	M+H	169.0859	-2.5
	HMDB0032252	Epoxyoxophorone	C9H12O3	M+H	169.0859	-2.5

	HMDB0030473	1-Ipomeanol	C9H12O3	M+H	169.0859	-2.5
	HMDB0038925	(4-Hydroxy-3-methoxyphenyl)ethanol	C9H12O3	M+H	169.0859	-2.5
	HMDB0030472	4-Ipomeanol	C9H12O3	M+H	169.0859	-2.5
	HMDB0029680	2,6-Dimethoxy-4-methylphenol	C9H12O3	M+H	169.0859	-2.5
	HMDB0037729	2-Furanylmethyl butanoate	C9H12O3	M+H	169.0859	-2.5
169.0954	HMDB0032921	Ethyl 2-furanpropionate	C9H12O3	M+H	169.0859	-2.5
	HMDB0062809	L-lysinium(1+)	C6H15N2O2	M+Na	169.0953	0.6
169.1218	HMDB0169534	geranic acid	C10H16O2	M+H	169.1223	-3.0
	HMDB0176281	6-hydroxycamphor	C10H16O2	M+H	169.1223	-3.0
	HMDB0182619	2-[2-(hydroxymethyl)-2,3-dimethylcyclopent-3-en-1-yl]acetaldehyde	C10H16O2	M+H	169.1223	-3.0
	HMDB0182618	2-hydroxy-2-(2,2,3-trimethylcyclopent-3-en-1-yl)acetaldehyde	C10H16O2	M+H	169.1223	-3.0
	HMDB0182617	25435-53-4	C10H16O2	M+H	169.1223	-3.0
	HMDB0181693	3-(hydroxymethyl)-2,3-dimethyltricyclo[2.2.1,heptan-1-ol	C10H16O2	M+H	169.1223	-3.0
	HMDB0181692	7-(hydroxymethyl)-1,7-dimethyltricyclo[2.2.1,heptan-3-ol	C10H16O2	M+H	169.1223	-3.0
	HMDB0181691	[7-(hydroxymethyl)-7-methyltricyclo[2.2.1,heptan-1-yl]methanol	C10H16O2	M+H	169.1223	-3.0
	HMDB0181690	[3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptan-3-yl]methanol	C10H16O2	M+H	169.1223	-3.0
	HMDB0181639	5-(1-hydroxypropan-2-yl)-2-methylbicyclo[3.1]hex-3-en-2-ol	C10H16O2	M+H	169.1223	-3.0
	HMDB0181638	2-methyl-5-(propan-2-yl)bicyclo[3.1]hex-3-ene-2,6-	C10H16O2	M+H	169.1223	-3.0
	HMDB0181635	5-(2-hydroxypropan-2-yl)-2-methylbicyclo[3.1]hex-3-en-2-ol	C10H16O2	M+H	169.1223	-3.0
	HMDB0182621	SCHEMBL14359771	C10H16O2	M+H	169.1223	-3.0
	HMDB0182620	2-[3-(hydroxymethyl)-2,2-dimethylcyclopent-3-en-1-yl]acetaldehyde	C10H16O2	M+H	169.1223	-3.0
	HMDB0240639	(1S,4R,6R)-1,3,3-Trimethyl-6-hydroxybicyclo[2.2.1]heptane-2-one	C10H16O2	M+H	169.1223	-3.0
	HMDB0182798	(1S,4R,6S)-1,3,3-Trimethyl-6-hydroxybicyclo[2.2.1]heptane-2-one	C10H16O2	M+H	169.1223	-3.0
	HMDB0182799	5-hydroxy-1,3,3-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O2	M+H	169.1223	-3.0
	HMDB0182797	7-hydroxy-1,3,3-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O2	M+H	169.1223	-3.0
	HMDB0182796	3-(hydroxymethyl)-1,3-dimethylbicyclo[2.2.1]heptan-2-one	C10H16O2	M+H	169.1223	-3.0
	HMDB0182685	6-Hydroxycarvotanacetone	C10H16O2	M+H	169.1223	-3.0
	HMDB0182684	SCHEMBL6689811	C10H16O2	M+H	169.1223	-3.0
	HMDB0182680	2-(hydroxymethyl)-5-(propan-2-yl)cyclohex-2-en-1-	C10H16O2	M+H	169.1223	-3.0
	HMDB0182683	1-methyl-4-(propan-2-yl)-7-oxabicyclo[4.1]heptan-2-one	C10H16O2	M+H	169.1223	-3.0
	HMDB0181634	2-(hydroxymethyl)-5-(propan-2-yl)bicyclo[3.1]hex-3-en-2-ol	C10H16O2	M+H	169.1223	-3.0
	HMDB0181636	5-methyl-1-(propan-2-yl)-3-oxatricyclo[4.1,heptan-5-ol	C10H16O2	M+H	169.1223	-3.0
	HMDB0163100	(7Z)-9-hydroxydeca-4,7-dienal	C10H16O2	M+H	169.1223	-3.0
	HMDB0163101	3-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}propanal	C10H16O2	M+H	169.1223	-3.0
	HMDB0163099	(4Z,7Z)-3-hydroxydeca-4,7-dienal	C10H16O2	M+H	169.1223	-3.0
	HMDB0163102	(4Z)-6-(3-ethyloxiran-2-yl)hex-4-enal	C10H16O2	M+H	169.1223	-3.0
	HMDB0182795	ACMC-mnpl	C10H16O2	M+H	169.1223	-3.0
	HMDB0136694	6-hydroxy-3,7-dimethylocta-2,7-dienal	C10H16O2	M+H	169.1223	-3.0
	HMDB0163104	(4Z,7Z)-2-hydroxydeca-4,7-dienal	C10H16O2	M+H	169.1223	-3.0
	HMDB0163106	(4Z,7Z)-deca-2,4,7-triene-1,-diol	C10H16O2	M+H	169.1223	-3.0
	HMDB0181637	2-methyl-5-(propan-2-yl)bicyclo[3.1]hex-3-ene-1,2-	C10H16O2	M+H	169.1223	-3.0
	HMDB0179485	14-64-6	C10H16O2	M+H	169.1223	-3.0
	HMDB0179394	2E,4Z-decadienoic acid	C10H16O2	M+H	169.1223	-3.0
	HMDB0178761	SCHEMBL7756279	C10H16O2	M+H	169.1223	-3.0
	HMDB0163117	(z,z)-4,7-decadienoic acid	C10H16O2	M+H	169.1223	-3.0
	HMDB0163109	(2E)-3-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}prop-2-en-1-ol	C10H16O2	M+H	169.1223	-3.0
	HMDB0163110	(2E,4Z)-6-(3-ethyloxiran-2-yl)hexa-2,4-dien-1-ol	C10H16O2	M+H	169.1223	-3.0
	HMDB0163108	{3-[(1Z,4Z)-hepta-1,4-dien-1-yl]oxiran-2-yl}methanol	C10H16O2	M+H	169.1223	-3.0
	HMDB0163103	(4Z,7Z)--hydroxydeca-4,7-dienal	C10H16O2	M+H	169.1223	-3.0
	HMDB0163105	(2E,7Z)-deca-2,4,7-triene-1,9-diol	C10H16O2	M+H	169.1223	-3.0

	HMDB0182681	8-Hydroxycarvotanacetone	C10H16O2	M+H	169.1223	-3.0
	HMDB0032313	2,4-Hexadienyl isobutyrate	C10H16O2	M+H	169.1223	-3.0
	HMDB0032312	2,4-Hexadienyl butyrate	C10H16O2	M+H	169.1223	-3.0
	HMDB0033700	(-)-(Z)-Tetrahydro-6-(2-pentenyl)-2H-pyran-2-one	C10H16O2	M+H	169.1223	-3.0
	HMDB0031273	Methyl octynecarboxylate	C10H16O2	M+H	169.1223	-3.0
	HMDB0031156	Ethyl (4Z)-4,7-octadienoate	C10H16O2	M+H	169.1223	-3.0
	HMDB0035714	Epoxycarvotanacetone	C10H16O2	M+H	169.1223	-3.0
	HMDB0040639	(xi)-(Z)-5-(3-Hexenyl)dihydro-2(3H)-furanone	C10H16O2	M+H	169.1223	-3.0
	HMDB0037175	4-Isopropyl-3-cyclohexene-1-carboxylic acid	C10H16O2	M+H	169.1223	-3.0
	HMDB0036067	Epoxycampholenic aldehyde	C10H16O2	M+H	169.1223	-3.0
	HMDB0037821	xi-1,8,8-Trimethyl-2-oxabicyclo[3.2.1]octan-3-one	C10H16O2	M+H	169.1223	-3.0
	HMDB0034452	5,6-Dihydro-6-pentyl-2H-pyran-2-one	C10H16O2	M+H	169.1223	-3.0
	HMDB0036103	Geranic acid	C10H16O2	M+H	169.1223	-3.0
	HMDB0032219	(+/-)-Dihydromintlactone	C10H16O2	M+H	169.1223	-3.0
	HMDB0032319	cis-3-Hexenyl crotonate	C10H16O2	M+H	169.1223	-3.0
	HMDB0032434	(+/-)-2-(5-Methyl-5-vinyltetrahydrofuran-2-yl)propionaldehyde	C10H16O2	M+H	169.1223	-3.0
	HMDB0035829	Dihydronepetalactone	C10H16O2	M+H	169.1223	-3.0
	HMDB0034670	6-Hydroxy-2,6-dimethyl-2,7-octadien-4-one	C10H16O2	M+H	169.1223	-3.0
	HMDB0037014	gamma-Diosphenol	C10H16O2	M+H	169.1223	-3.0
	HMDB0013105	trans-4,5-epoxy-2(E)-decenal	C10H16O2	M+H	169.1223	-3.0
	HMDB0035766	Ascaridole	C10H16O2	M+H	169.1223	-3.0
	HMDB0182682	4-hydroxy-2-methyl-5-(propan-2-yl)cyclohex-2-en-1-one	C10H16O2	M+H	169.1223	-3.0
169.1583	HMDB0040247	2-Undecenal	C11H20O	M+H	169.1587	-2.3
	HMDB0163220	(2E,5Z)-2,5-undecadien-1-ol	C11H20O	M+H	169.1587	-2.3
	HMDB0163219	(Z)-5-Undecenal	C11H20O	M+H	169.1587	-2.3
	HMDB0035417	(1R,2R)-1,2,7,7-Tetramethylbicyclo[2.2.1]heptan-2-ol	C11H20O	M+H	169.1587	-2.3
	HMDB0033577	-Undecen-2-one	C11H20O	M+H	169.1587	-2.3
	HMDB0031128	-Undecenal	C11H20O	M+H	169.1587	-2.3
	HMDB0037807	9-Undecenal	C11H20O	M+H	169.1587	-2.3
	HMDB0032238	(+/-)-trans- and cis-4,8-Dimethyl-3,7-nonadien-2-ol	C11H20O	M+H	169.1587	-2.3
	HMDB0061995	2-Methyl-3-decen-5-one	C11H20O	M+H	169.1587	-2.3
170.0420	HMDB0156263	glutamate(1-)	C5H8NO4	M+Na	170.0424	-2.2
	HMDB0000148	L-Glutamic acid	C5H9NO4	M+Na	170.0424	-2.2
	HMDB0062183	N-lactoyl-glycine	C5H9NO4	M+Na	170.0424	-2.2
	HMDB0002931	N-Acetylserine	C5H9NO4	M+Na	170.0424	-2.2
	HMDB0002393	N-Methyl-D-aspartic acid	C5H9NO4	M+Na	170.0424	-2.2
	HMDB0003011	O-Acetylserine	C5H9NO4	M+Na	170.0424	-2.2
	HMDB0003339	D-Glutamic acid	C5H9NO4	M+Na	170.0424	-2.2
	HMDB0006556	L-4-Hydroxyglutamate semialdehyde	C5H9NO4	M+Na	170.0424	-2.2
	HMDB0060475	DL-Glutamate	C5H9NO4	M+Na	170.0424	-2.2
	HMDB0033550	3-(Carboxymethylamino)propanoic acid	C5H9NO4	M+Na	170.0424	-2.2
170.0490	HMDB0015167	Mercaptopurine	C5H4N4S	M+NH4	170.0495	-2.9
170.0573	HMDB0172056	3-(2-hydroxyphenyl)propanenitrile	C9H9NO	M+Na	170.0576	-2.0
	HMDB0159223	5-Hydroxy-3-methylindole	C9H9NO	M+Na	170.0576	-2.0
	HMDB0159222	3-methyl-1H-indol-6-ol	C9H9NO	M+Na	170.0576	-2.0
	HMDB0159224	1125-35-5	C9H9NO	M+Na	170.0576	-2.0
	HMDB0159225	3-Methyl-1H-indol-4-ol	C9H9NO	M+Na	170.0576	-2.0
	HMDB0172057	3-Hydroxy-3-phenylpropanenitrile	C9H9NO	M+Na	170.0576	-2.0
	HMDB0172058	3-(3-hydroxyphenyl)propanenitrile	C9H9NO	M+Na	170.0576	-2.0
	HMDB0172059	3-(4-Hydroxyphenyl)propionitrile	C9H9NO	M+Na	170.0576	-2.0
	HMDB0040011	3-(2-Furanylmethyl)-1H-pyrrole	C9H9NO	M+Na	170.0576	-2.0
	HMDB0040009	4-(2-Furanylmethylene)-3,4-dihydro-2H-pyrrole	C9H9NO	M+Na	170.0576	-2.0
	HMDB0030204	1-(2-Furanylmethyl)-1H-pyrrole	C9H9NO	M+Na	170.0576	-2.0
	HMDB0005785	Indole-3-carbinol	C9H9NO	M+Na	170.0576	-2.0
	HMDB0060244	Phosphodimethylethanolamine	C4H12NO4P	M+H	170.0577	-2.2
	HMDB0166108	5-hydroxy-2-methoxybenzaldehyde	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0171094	ortho-vanillin	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0172092	3-Hydroxy-4-methoxybenzaldehyde	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0168664	Methyl 3-hydroxybenzoate	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0150437	6-methylsalicylic acid	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0166107	4-hydroxy-2-methoxybenzaldehyde	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0182861	SCHEMBL437438	C8H8O3	M+NH4	170.0812	-2.2

170.0808	HMDB0166109	3-hydroxy-2-methoxybenzaldehyde	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0166106	2-hydroxy-6-methoxybenzaldehyde	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0146889	SCHEMBL2128735	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0146870	SCHEMBL3679957	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0137457	4-[(E)-2-hydroxyethenyl]benzene-1,2-diol	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0125528	5-ethenylbenzene-1,2,3-triol	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0183904	mandelate	C8H7O3	M+NH4	170.0812	-2.2
	HMDB0183905	4-hydroxyphenylacetate	C8H7O3	M+NH4	170.0812	-2.2
	HMDB0000703	Mandelic acid	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0032604	2-Methoxybenzoic acid	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0034172	Methyl 2-hydroxybenzoate	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0032606	3-Methoxybenzoic acid	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0029657	2,4'-Dihydroxyacetophenone	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0041283	1-(2-Furanyl)-1,3-butanedione	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0032919	Ethyl 2-furanyl diketone	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0036907	2-Propenyl 2-furancarboxylate	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0012308	Vanillin	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0004815	4-Hydroxy-3-methylbenzoic acid	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0029661	3',4'-Dihydroxyacetophenone	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0003791	3,4-Dihydroxyphenylacetaldehyde	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0002390	3-Cresotinic acid	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0000669	ortho-Hydroxyphenylacetic acid	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0000440	3-Hydroxyphenylacetic acid	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0000020	p-Hydroxyphenylacetic acid	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0001101	p-Anisic acid	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0029662	3',5'-Dihydroxyacetophenone	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0032572	Methylparaben	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0032629	2',5'-Dihydroxyacetophenone	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0032399	Methyl furfuracrylate	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0172091	2-Hydroxy-4-methoxybenzaldehyde	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0060390	4-Hydroxyphenyl acetate	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0029660	2',6'-Dihydroxyacetophenone	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0029659	2',4'-Dihydroxyacetophenone	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0029658	2',3'-Dihydroxyacetophenone	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0062005	Dihydroxyacetophenone	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0031609	Phenoxyacetic acid	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0032594	2-(Hydroxymethyl)benzoic acid	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0124926	Mandelic acid	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0033003	1-(5-Methyl-2-furanyl)-1,2-propanedione	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0062635	(R)-mandelic Acid	C8H8O3	M+NH4	170.0812	-2.2
	HMDB0001537	6-Hydroxydopamine	C8H11NO3	M+H	170.0812	-2.2
	HMDB0000216	Norepinephrine	C8H11NO3	M+H	170.0812	-2.2
	HMDB0000239	Pyridoxine	C8H11NO3	M+H	170.0812	-2.2
	HMDB0035178	6-Acetyl-2,3-dihydro-2-(hydroxymethyl)-4(1H)-pyridinone	C8H11NO3	M+H	170.0812	-2.2
	HMDB0155164	2-Hydroxydopamine	C8H11NO3	M+H	170.0812	-2.2
	HMDB0037685	xi-Norepinephrine	C8H11NO3	M+H	170.0812	-2.2
	HMDB0004817	5-Hydroxydopamine	C8H11NO3	M+H	170.0812	-2.2
170.1171	HMDB0150177	3-phenylpropane-1,2-diol	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0150180	2-(3-hydroxypropyl)phenol	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0175244	4-(1-hydroxypropan-2-yl)phenol	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0175243	SCHEMBL9169343	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0175240	2-Phenyl-1,2-propanediol	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0175241	2-PHENYL-1,3-PROPANEDIOL	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0173825	1-[4-(Hydroxymethyl)phenyl]ethanol	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0173826	1-(4-methylphenyl)ethane-1,2-diol	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0150178	1-Phenylpropane-1,3-diol	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0150179	3-(3-hydroxypropyl)phenol	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0146637	4-ETHYL-3-METHOXYPHENOL	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0125537	3-ethyl-5-methoxyphenol	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0041804	2-Isopropoxyphenol	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0040175	4-Ethyl-2-methoxyphenol	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0032132	2-Isopropyl-1,4-benzenediol	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0032599	3-(4-Hydroxyphenyl)-1-propanol	C9H12O2	M+NH4	170.1176	-2.7
	HMDB0040216	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	C9H12O2	M+NH4	170.1176	-2.7

HMDB0039801	1-(2-Furanyl)-1-pentanone	C9H12O2	M+NH4	170.1176	-2.7
HMDB0036227	2-Propenyl 2,4-hexadienoate	C9H12O2	M+NH4	170.1176	-2.7
HMDB0039956	4-(Ethoxymethyl)phenol	C9H12O2	M+NH4	170.1176	-2.7
HMDB0036169	3-(5-Methyl-2-furanyl)butanal	C9H12O2	M+NH4	170.1176	-2.7
HMDB0041326	(Dimethoxymethyl)benzene	C9H12O2	M+NH4	170.1176	-2.7
HMDB0040449	2-(Ethoxymethyl)phenol	C9H12O2	M+NH4	170.1176	-2.7
HMDB0059853	3,5-Dimethoxytoluene	C9H12O2	M+NH4	170.1176	-2.7
HMDB0168680	(4-ethoxyphenyl)methanol	C9H12O2	M+NH4	170.1176	-2.7
HMDB0038321	Homoarecoline	C9H15NO2	M+H	170.1176	-2.7
HMDB0176883	1-hydroxy-9-methyl-9-azabicyclo[3.3.1]nonan-3-one	C9H15NO2	M+H	170.1176	-2.7
HMDB0176884	9-methyl-9-aza-bicyclo[3.3.1]nonan-3-one-9-oxide	C9H15NO2	M+H	170.1176	-2.7
HMDB0176882	2-hydroxy-9-methyl-9-azabicyclo[3.3.1]nonan-3-one	C9H15NO2	M+H	170.1176	-2.7
HMDB0182523	p-Menth-1(7)-en-2-one	C10H16O	M+NH4	170.1539	-2.6
HMDB0187618	isopiperitenol	C10H16O	M+NH4	170.1539	-2.6
HMDB0187619	2-methyl-2-(4-methylcyclohex-3-en-1-yl)oxirane	C10H16O	M+NH4	170.1539	-2.6
HMDB0182597	SCHEMBL13931696	C10H16O	M+NH4	170.1539	-2.6
HMDB0182548	2-[(1R)-4-methylcyclohexa-2,4-dien-1-yl]propan-1-ol	C10H16O	M+NH4	170.1539	-2.6
HMDB0182544	SCHEMBL4374431	C10H16O	M+NH4	170.1539	-2.6
HMDB0182545	(6S)-3-methyl-6-(propan-2-yl)cyclohexa-2,4-dien-1-ol	C10H16O	M+NH4	170.1539	-2.6
HMDB0182547	(5S)-2-methyl-5-(propan-2-yl)-7-oxabicyclo[4.1]hept-2-ene	C10H16O	M+NH4	170.1539	-2.6
HMDB0182546	(4S)-1-methyl-4-(propan-2-yl)-7-oxabicyclo[4.1]hept-2-ene	C10H16O	M+NH4	170.1539	-2.6
HMDB0182543	(R)-p-Mentha-1,5-diene-8-ol	C10H16O	M+NH4	170.1539	-2.6
HMDB0182542	ZINC321828	C10H16O	M+NH4	170.1539	-2.6
HMDB0181808	(1S)-4-methylidene-1-(propan-2-yl)bicyclo[3.1]hexan-6-ol	C10H16O	M+NH4	170.1539	-2.6
HMDB0181809	2-[(1R)-4-methylidenebicyclo[3.1]hexan-1-yl]propan-1-ol	C10H16O	M+NH4	170.1539	-2.6
HMDB0181807	(5S)-2-methylidene-5-(propan-2-yl)bicyclo[3.1]hexan-1-ol	C10H16O	M+NH4	170.1539	-2.6
HMDB0181806	(1R)-4-methylidene-1-(propan-2-yl)bicyclo[3.1]hexan-2-ol	C10H16O	M+NH4	170.1539	-2.6
HMDB0181804	2-[(1R)-4-methylidenebicyclo[3.1]hexan-1-yl]propan-2-ol	C10H16O	M+NH4	170.1539	-2.6
HMDB0181805	AC1O5B2Q	C10H16O	M+NH4	170.1539	-2.6
HMDB0163091	(4Z,7Z)-deca-4,7-dienal	C10H16O	M+NH4	170.1539	-2.6
HMDB0163092	SCHEMBL5863926	C10H16O	M+NH4	170.1539	-2.6
HMDB0035158	1,2-Epoxy-p-menth-8-ene	C10H16O	M+NH4	170.1539	-2.6
HMDB0037009	Terpinolene oxide	C10H16O	M+NH4	170.1539	-2.6
HMDB0035744	(-)-Isopinocampnone	C10H16O	M+NH4	170.1539	-2.6
HMDB0036115	(-)-3-Isothujone	C10H16O	M+NH4	170.1539	-2.6
HMDB0036598	(E,E)-2,4-Decadienal	C10H16O	M+NH4	170.1539	-2.6
HMDB0035656	3-Pinanone	C10H16O	M+NH4	170.1539	-2.6
HMDB0035737	(R)-Piperitone	C10H16O	M+NH4	170.1539	-2.6
HMDB0035738	(R)-Piperitone	C10H16O	M+NH4	170.1539	-2.6
HMDB0038290	Photocitral A	C10H16O	M+NH4	170.1539	-2.6
HMDB0035743	Pinocarveol	C10H16O	M+NH4	170.1539	-2.6
HMDB0037025	Hop ether	C10H16O	M+NH4	170.1539	-2.6
HMDB0032120	2,6-Dimethyl-1,7-octadien-3-one	C10H16O	M+NH4	170.1539	-2.6
HMDB0036127	(-)-Pinocampnone	C10H16O	M+NH4	170.1539	-2.6
HMDB0036128	(-)-trans-Pinocarveol	C10H16O	M+NH4	170.1539	-2.6
HMDB0034975	Piperitone	C10H16O	M+NH4	170.1539	-2.6
HMDB0036087	(R)-p-Mentha-1,8-dien-7-ol	C10H16O	M+NH4	170.1539	-2.6
HMDB0036088	(R)-p-Mentha-1,8-dien-7-ol	C10H16O	M+NH4	170.1539	-2.6
HMDB0039008	3,4-Epoxy-p-menth-1(7)-ene	C10H16O	M+NH4	170.1539	-2.6
HMDB0030893	Isocitral	C10H16O	M+NH4	170.1539	-2.6
HMDB0037024	4-Acetyl-1,4-dimethyl-1-cyclohexene	C10H16O	M+NH4	170.1539	-2.6
HMDB0034974	(R)-Carvotanacetone	C10H16O	M+NH4	170.1539	-2.6
HMDB0040766	Anethofuran	C10H16O	M+NH4	170.1539	-2.6
HMDB0035092	cis-Citral	C10H16O	M+NH4	170.1539	-2.6
HMDB0037280	Junionone	C10H16O	M+NH4	170.1539	-2.6
HMDB0036129	Verbenol	C10H16O	M+NH4	170.1539	-2.6
HMDB0034973	(R)-Campholenic aldehyde	C10H16O	M+NH4	170.1539	-2.6
HMDB0034985	(+)-Fenchone	C10H16O	M+NH4	170.1539	-2.6

170.1535	HMDB0035741	(-)-trans-Isopulegone	C10H16O	M+NH4	170.1539	-2.6
	HMDB0038557	xi-3,6-Dihydro-4-methyl-2-(2-methyl-1-propenyl)-2H-pyran	C10H16O	M+NH4	170.1539	-2.6
	HMDB0035622	(+)-cis-Carveol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0036080	(1S,4S)-Dihydrocarvone	C10H16O	M+NH4	170.1539	-2.6
	HMDB0036114	(-)-3-Thujone	C10H16O	M+NH4	170.1539	-2.6
	HMDB0035054	(1S,4R)-p-Mentha-2,8-dien-1-ol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0035077	(1R,4R)-p-Mentha-2,8-dien-1-ol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0003667	Alpha-Pinene-oxide	C10H16O	M+NH4	170.1539	-2.6
	HMDB0003634	Perillyl alcohol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0003450	(-)-trans-Carveol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0035600	(S)-Phellandral	C10H16O	M+NH4	170.1539	-2.6
	HMDB0035120	Dehydrolinalool	C10H16O	M+NH4	170.1539	-2.6
	HMDB0034715	p-Mentha-1(6),8-dien-3-ol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0037015	p-Mentha-1,8-dien-4-ol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0037303	xi-p-Mentha-1(7),2-dien-4-ol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0038251	xi-Pinol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0035241	(Z)-2-Methyl-6-methylene-2,7-octadien-1-ol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0037010	(2S,4R)-p-Mentha-1(7),8-dien-2-ol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0035277	(2S,4R)-p-Mentha-1(7),5-dien-2-ol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0036044	Marmelo oxide A	C10H16O	M+NH4	170.1539	-2.6
	HMDB0035203	(S)-9,-Cyclo-p-menth-1-en-4-ol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0037302	xi-p-Mentha-3,8-dien-1-ol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0059827	3-Cyclohexene-1-carboxaldehyde, 1,3,4-trimethyl-	C10H16O	M+NH4	170.1539	-2.6
	HMDB0059761	4-(1-Methylethyl)-1-cyclohexene-4-carboxaldehyde	C10H16O	M+NH4	170.1539	-2.6
	HMDB0041631	3-Thujanone	C10H16O	M+NH4	170.1539	-2.6
	HMDB0059608	(+)-trans-Carveol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0032242	(E)-3,7-Dimethyl-1,5,7-octatrien-3-ol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0032536	2-(trans-2-Pentenyl)cyclopentanone	C10H16O	M+NH4	170.1539	-2.6
	HMDB0059838	Camphor	C10H16O	M+NH4	170.1539	-2.6
	HMDB0059875	Carvotanacetone	C10H16O	M+NH4	170.1539	-2.6
	HMDB0035604	Pulegone	C10H16O	M+NH4	170.1539	-2.6
	HMDB0061794	Pulegone	C10H16O	M+NH4	170.1539	-2.6
	HMDB0061292	SCHEMBL6943113	C10H16O	M+NH4	170.1539	-2.6
	HMDB0059885	p-Menth-1-en-9-al	C10H16O	M+NH4	170.1539	-2.6
	HMDB0036085	Dehydro-1,8-cineole	C10H16O	M+NH4	170.1539	-2.6
	HMDB0031854	3-Methyl-5-propyl-2-cyclohexen-1-one	C10H16O	M+NH4	170.1539	-2.6
	HMDB0041013	Isocyclocitral	C10H16O	M+NH4	170.1539	-2.6
	HMDB0035100	2-Pinen--ol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0035125	Darwinol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0035280	Teresantalol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0036083	Carveol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0035078	Geranial	C10H16O	M+NH4	170.1539	-2.6
	HMDB0037008	6,8-Epoxy-p-menth-2-ene	C10H16O	M+NH4	170.1539	-2.6
	HMDB0036082	(-)-cis-Carveol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0037017	(R)-p-Mentha-1,8-dien--ol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0030892	p-Menth-3-en-9-al	C10H16O	M+NH4	170.1539	-2.6
	HMDB0036079	Dihydrocarvone	C10H16O	M+NH4	170.1539	-2.6
	HMDB0035706	alpha-Cyclocitral	C10H16O	M+NH4	170.1539	-2.6
	HMDB0036113	(+)-3-Thujone	C10H16O	M+NH4	170.1539	-2.6
	HMDB0039816	2-Hexylfuran	C10H16O	M+NH4	170.1539	-2.6
	HMDB0041011	beta-Cyclocitral	C10H16O	M+NH4	170.1539	-2.6
	HMDB0034916	cis-2-Thujen-4-ol	C10H16O	M+NH4	170.1539	-2.6
	HMDB0037172	Tetrahydro-5-isopropenyl-2-methyl-2-vinylfuran	C10H16O	M+NH4	170.1539	-2.6
171.0048	HMDB0001112	Glyceraldehyde-3-Phosphate	C3H7O6P	M+H	171.0053	-2.9
	HMDB0001473	Dihydroxyacetone phosphate	C3H7O6P	M+H	171.0053	-2.9
	HMDB0156243	phospholactic acid	C3H7O6P	M+H	171.0053	-2.9
171.0414	HMDB0135274	(2E)-3-(3-hydroxyphenyl)prop-2-enal	C9H8O2	M+Na	171.0416	-1.4
	HMDB0135648	3-(4-hydroxyphenyl)prop-2-enal	C9H8O2	M+Na	171.0416	-1.4
	HMDB0128078	3-phenylprop-2-enoic acid	C9H8O2	M+Na	171.0416	-1.4
	HMDB0135273	(2Z)-2-hydroxy-3-phenylprop-2-enal	C9H8O2	M+Na	171.0416	-1.4
	HMDB0135275	3-phenyloxirane-2-carbaldehyde	C9H8O2	M+Na	171.0416	-1.4
	HMDB0134039	3-(2-hydroxyphenyl)prop-2-enal	C9H8O2	M+Na	171.0416	-1.4
	HMDB0000930	trans-Cinnamic acid	C9H8O2	M+Na	171.0416	-1.4
	HMDB0040986	(E)-3-(4-Hydroxyphenyl)-2-propenal	C9H8O2	M+Na	171.0416	-1.4

	HMDB0031725	(E)-3-(2-Hydroxyphenyl)-2-propenal	C9H8O2	M+Na	171.0416	-1.4
	HMDB0035243	1-Phenyl-1,2-propanedione	C9H8O2	M+Na	171.0416	-1.4
	HMDB0032947	Di-2-furanylmethane	C9H8O2	M+Na	171.0416	-1.4
	HMDB0036626	3,4-Dihydro-2H-1-benzopyran-2-one	C9H8O2	M+Na	171.0416	-1.4
	HMDB0000567	Cinnamic acid	C9H8O2	M+Na	171.0416	-1.4
171.1011	HMDB0164922	1,3-bis(hydroxymethyl)bicyclo[2.2.1]heptan-2-one	C9H14O3	M+H	171.1016	-2.7
	HMDB0164925	6-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M+H	171.1016	-2.7
	HMDB0164926	5-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M+H	171.1016	-2.7
	HMDB0164923	3-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M+H	171.1016	-2.7
	HMDB0164924	7-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M+H	171.1016	-2.7
	HMDB0167053	(2E,6Z)-5-hydroxynona-2,6-dienoic acid	C9H14O3	M+H	171.1016	-2.7
	HMDB0167051	(2E,6Z)-4-hydroxynona-2,6-dienoic acid	C9H14O3	M+H	171.1016	-2.7
	HMDB0167052	(2E,6Z)-8-hydroxynona-2,6-dienoic acid	C9H14O3	M+H	171.1016	-2.7
	HMDB0167054	3-[(3Z)-hex-3-en-1-yl]oxirane-2-carboxylic acid	C9H14O3	M+H	171.1016	-2.7
	HMDB0167055	(2E)-5-(3-ethyloxiran-2-yl)pent-2-enoic acid	C9H14O3	M+H	171.1016	-2.7
	HMDB0167056	(2E,6Z)-9-hydroxynona-2,6-dienoic acid	C9H14O3	M+H	171.1016	-2.7
	HMDB0038276	cis-3-Hexenyl pyruvate	C9H14O3	M+H	171.1016	-2.7
	HMDB0030471	1,4-Ipomeadiol	C9H14O3	M+H	171.1016	-2.7
	HMDB0182601	4-Hydroxypiperitone	C10H18O2	M+H	171.1380	-2.7
	HMDB0182595	8-hydroxy-p-menthan-3-one	C10H18O2	M+H	171.1380	-2.7
	HMDB0182599	(+)-4-hydroxy-p-menth-3-one	C10H18O2	M+H	171.1380	-2.7
	HMDB0182598	2-hydroxy-p-menthanone-(3)	C10H18O2	M+H	171.1380	-2.7
	HMDB0182600	5-(hydroxymethyl)-2-(propan-2-yl)cyclohexan-1-one	C10H18O2	M+H	171.1380	-2.7
	HMDB0182594	5-Hydroxy-2-isopropyl-5-methylcyclohexanone	C10H18O2	M+H	171.1380	-2.7
	HMDB0182596	2-(2-Hydroxy-1-methylethyl)-5-methylcyclohexanone	C10H18O2	M+H	171.1380	-2.7
	HMDB0182528	SCHEMBL12683693	C10H18O2	M+H	171.1380	-2.7
	HMDB0182525	2-(hydroxymethyl)-5-(propan-2-yl)cyclohexan-1-one	C10H18O2	M+H	171.1380	-2.7
	HMDB0182527	4-hydroxy-2-methyl-5-(propan-2-yl)cyclohexan-1-one	C10H18O2	M+H	171.1380	-2.7
	HMDB0182526	Oxytetrahydrocarvon	C10H18O2	M+H	171.1380	-2.7
	HMDB0182524	2-hydroxy-6-methyl-3-(propan-2-yl)cyclohexan-1-one	C10H18O2	M+H	171.1380	-2.7
	HMDB0182521	5-(2-hydroxypropan-2-yl)-2-methylcyclohexan-1-one	C10H18O2	M+H	171.1380	-2.7
	HMDB0182520	SCHEMBL12683689	C10H18O2	M+H	171.1380	-2.7
	HMDB0182602	SCHEMBL16581455	C10H18O2	M+H	171.1380	-2.7
	HMDB0182625	5-(2-hydroxyethyl)-3,4,4-trimethylcyclopent-2-en-1-ol	C10H18O2	M+H	171.1380	-2.7
	HMDB0182701	(1S)-1,7,7-trimethylbicyclo[2.2.1]heptane-2,5-diol	C10H18O2	M+H	171.1380	-2.7
	HMDB0182700	1,7,7-trimethylbicyclo[2.2.1]heptane-2,6-diol	C10H18O2	M+H	171.1380	-2.7
	HMDB0182698	(1S)-1,7,7-trimethylbicyclo[2.2.1]heptane-2,3-diol	C10H18O2	M+H	171.1380	-2.7
	HMDB0182697	(1S)-7-(hydroxymethyl)-1,7-dimethylbicyclo[2.2.1]heptan-2-ol	C10H18O2	M+H	171.1380	-2.7
	HMDB0182699	(1S)-1,7,7-trimethylbicyclo[2.2.1]heptane-2,2-diol	C10H18O2	M+H	171.1380	-2.7
	HMDB0182696	SCHEMBL15462834	C10H18O2	M+H	171.1380	-2.7
	HMDB0182626	2-{1,2,2-trimethyl-6-oxabicyclo[3.1]hexan-3-yl}ethan-1-ol	C10H18O2	M+H	171.1380	-2.7
	HMDB0182624	SCHEMBL5398	C10H18O2	M+H	171.1380	-2.7
	HMDB0182622	2-[2-(hydroxymethyl)-2,3-dimethylcyclopent-3-en-1-yl]ethan-1-ol	C10H18O2	M+H	171.1380	-2.7
	HMDB0182623	2-[3-(hydroxymethyl)-2,2-dimethylcyclopent-3-en-1-yl]ethan-1-ol	C10H18O2	M+H	171.1380	-2.7
	HMDB0182522	AC1LCBYF	C10H18O2	M+H	171.1380	-2.7
	HMDB0181920	AC1MS2IY	C10H18O2	M+H	171.1380	-2.7
	HMDB0180492	6-hydroxydec-9-enal	C10H18O2	M+H	171.1380	-2.7
	HMDB0180107	8-METHYL-8-NONENOIC ACID	C10H18O2	M+H	171.1380	-2.7
	HMDB0161937	(2Z)-3,7-Dimethyl-6,7-epoxy-2-octene-1-ol	C10H18O2	M+H	171.1380	-2.7
	HMDB0161936	2,3-Epoxy-3,7-dimethyloct-6-enol	C10H18O2	M+H	171.1380	-2.7
	HMDB0161935	(2Z)-3,7-dimethylocta-2,6-diene-1,5-diol	C10H18O2	M+H	171.1380	-2.7
	HMDB0161933	SCHEMBL15361567	C10H18O2	M+H	171.1380	-2.7
	HMDB0161932	SCHEMBL9863268	C10H18O2	M+H	171.1380	-2.7
	HMDB0161931	(2Z)-3,7-dimethylocta-2,6-diene-1,4-diol	C10H18O2	M+H	171.1380	-2.7
	HMDB0161934	8-hydroxyneryl	C10H18O2	M+H	171.1380	-2.7
	HMDB0179965	3-exo-hydroxy-1,8-cineole	C10H18O2	M+H	171.1380	-2.7
	HMDB0131081	(2E)-7-hydroxy-3,6,6-trimethylhept-2-enal	C10H18O2	M+H	171.1380	-2.7

171.1375

HMDB0180491	5-hydroxydec-9-enal	C10H18O2	M+H	171.1380	-2.7
HMDB0180489	3-hydroxydec-9-enal	C10H18O2	M+H	171.1380	-2.7
HMDB0181921	1,3,3-trimethylbicyclo[2.2.1]heptane-2,5-diol	C10H18O2	M+H	171.1380	-2.7
HMDB0181919	1,3,3-trimethylbicyclo[2.2.1]heptane-2,7-diol	C10H18O2	M+H	171.1380	-2.7
HMDB0181917	3-(hydroxymethyl)-1,3-dimethylbicyclo[2.2.1]heptan-2-ol	C10H18O2	M+H	171.1380	-2.7
HMDB0181918	1,3,3-trimethylbicyclo[2.2.1]heptane-2,2-diol	C10H18O2	M+H	171.1380	-2.7
HMDB0181916	62853-86-5	C10H18O2	M+H	171.1380	-2.7
HMDB0180591	4-methylnon-8-enoic acid	C10H18O2	M+H	171.1380	-2.7
HMDB0180590	4-methylidenenonanoic acid	C10H18O2	M+H	171.1380	-2.7
HMDB0180494	SCHEMBL186654	C10H18O2	M+H	171.1380	-2.7
HMDB0180495	SCHEMBL58664	C10H18O2	M+H	171.1380	-2.7
HMDB0180496	2-hydroxydec-9-enal	C10H18O2	M+H	171.1380	-2.7
HMDB0180493	7-hydroxydec-9-enal	C10H18O2	M+H	171.1380	-2.7
HMDB0180490	4-hydroxydec-9-enal	C10H18O2	M+H	171.1380	-2.7
HMDB0030031	6-Methyl-5-hepten-2-yl acetate	C10H18O2	M+H	171.1380	-2.7
HMDB0040213	cis-3-Hexenyl isobutyrate	C10H18O2	M+H	171.1380	-2.7
HMDB0036990	2,6-Dimethyl-3,7-octadiene-2,6-diol	C10H18O2	M+H	171.1380	-2.7
HMDB0031362	Cyclohexylethyl acetate	C10H18O2	M+H	171.1380	-2.7
HMDB0036211	Hexyl crotonate	C10H18O2	M+H	171.1380	-2.7
HMDB0035365	Cnidol C	C10H18O2	M+H	171.1380	-2.7
HMDB0040330	Menthone lactone	C10H18O2	M+H	171.1380	-2.7
HMDB0040530	Isopentyl 3-methyl-2-butenate	C10H18O2	M+H	171.1380	-2.7
HMDB0031003	9-Decenoic acid	C10H18O2	M+H	171.1380	-2.7
HMDB0040194	Methyl 2-nonenate	C10H18O2	M+H	171.1380	-2.7
HMDB0033377	cis-3-Hexenyl butyrate	C10H18O2	M+H	171.1380	-2.7
HMDB0031297	2-Octenyl acetate	C10H18O2	M+H	171.1380	-2.7
HMDB0039768	5-Decenoic acid	C10H18O2	M+H	171.1380	-2.7
HMDB0035907	Linalyl oxide	C10H18O2	M+H	171.1380	-2.7
HMDB0031441	Linalool oxide III	C10H18O2	M+H	171.1380	-2.7
HMDB0041630	Linalool oxide III	C10H18O2	M+H	171.1380	-2.7
HMDB0031440	Linalool oxide (trans-pyranoid)	C10H18O2	M+H	171.1380	-2.7
HMDB0032393	2-Methylbutyl 3-methyl-2-butenate	C10H18O2	M+H	171.1380	-2.7
HMDB0032452	1-Octen-3-yl acetate	C10H18O2	M+H	171.1380	-2.7
HMDB0032275	Ethyl 3-octenoate	C10H18O2	M+H	171.1380	-2.7
HMDB0029859	Methyl (xi)-3-nonenate	C10H18O2	M+H	171.1380	-2.7
HMDB0034880	3-Methyl-2,4-nonanedione	C10H18O2	M+H	171.1380	-2.7
HMDB0035837	Citronellic acid	C10H18O2	M+H	171.1380	-2.7
HMDB0040208	2-Propenyl heptanoate	C10H18O2	M+H	171.1380	-2.7
HMDB0039795	Ethyl 4Z-octenoate	C10H18O2	M+H	171.1380	-2.7
HMDB0036992	1-Cyclopropyl-4-methyl-1,3-cyclohexanediol	C10H18O2	M+H	171.1380	-2.7
HMDB0061293	1-p-Menthene-8,9-diol	C10H18O2	M+H	171.1380	-2.7
HMDB0035122	(S,E)-2,6-Dimethyl-5,7-octadiene-2,3-diol	C10H18O2	M+H	171.1380	-2.7
HMDB0037632	xi-Tetrahydro-3-pentyl-2H-pyran-2-one	C10H18O2	M+H	171.1380	-2.7
HMDB0037217	xi-5-Hexyldihydro-2(3H)-furanone	C10H18O2	M+H	171.1380	-2.7
HMDB0035839	(E)-3-(Tetrahydro-5,5-dimethyl-2-furanyl)-2-buten-1-ol	C10H18O2	M+H	171.1380	-2.7
HMDB0038744	9-Hydroxygeraniol	C10H18O2	M+H	171.1380	-2.7
HMDB0039149	(+)-6-Hydroxy-2,6-dimethyl-7-octen-4-one	C10H18O2	M+H	171.1380	-2.7
HMDB0012183	8-Methylnonenoate	C10H18O2	M+H	171.1380	-2.7
HMDB0010726	trans-Dec-2-enoic acid	C10H18O2	M+H	171.1380	-2.7
HMDB0037116	delta-Decalactone	C10H18O2	M+H	171.1380	-2.7
HMDB0034581	2-Hexenyl butanoate	C10H18O2	M+H	171.1380	-2.7
HMDB0034427	Cyclohexyl butanoate	C10H18O2	M+H	171.1380	-2.7
HMDB0037021	trans-p-Menth-2-ene-1,4-diol	C10H18O2	M+H	171.1380	-2.7
HMDB0032119	4-Hydroxy-2,6-dimethyl-7-octen-3-one	C10H18O2	M+H	171.1380	-2.7
HMDB0029358	5Z-Octenyl acetate	C10H18O2	M+H	171.1380	-2.7
HMDB0041012	6-Decenoic acid	C10H18O2	M+H	171.1380	-2.7
HMDB0036099	Lilac alcohol	C10H18O2	M+H	171.1380	-2.7
HMDB0040726	cis-Linalyl oxide	C10H18O2	M+H	171.1380	-2.7
HMDB0031002	3-Decenoic acid	C10H18O2	M+H	171.1380	-2.7
HMDB0033203	6-Decanolide	C10H18O2	M+H	171.1380	-2.7
HMDB0040727	trans-Linalyl oxide	C10H18O2	M+H	171.1380	-2.7
HMDB0037497	Ethyl (E)-2-octenoate	C10H18O2	M+H	171.1380	-2.7
HMDB0004980	cis-4-Decenoic acid	C10H18O2	M+H	171.1380	-2.7
HMDB0164952	4-methyl-1-(propan-2-yl)bicyclo[3.1]hexane-2,4-diol	C10H18O2	M+H	171.1380	-2.7

	HMDB0062152	Propyl cyclohexanecarboxylate	C10H18O2	M+H	171.1380	-2.7
	HMDB0059852	2-Hydroxycineol	C10H18O2	M+H	171.1380	-2.7
	HMDB0059610	2-Exo-hydroxy-1,8-cineole	C10H18O2	M+H	171.1380	-2.7
171.1488	HMDB0037878	4-Ethyl-5-methyl-2-(1-methylethyl)oxazole	C9H15NO	M+NH4	171.1492	-2.3
	HMDB0037881	4-Ethyl-5-methyl-2-propyloxazole	C9H15NO	M+NH4	171.1492	-2.3
	HMDB0037880	2-Isobutyl-4,5-dimethyloxazole	C9H15NO	M+NH4	171.1492	-2.3
	HMDB0034580	psi-Pelletierine	C9H15NO	M+NH4	171.1492	-2.3
	HMDB0037856	2-Methyl-4-pentyloxazole	C9H15NO	M+NH4	171.1492	-2.3
	HMDB0037879	4-Butyl-2,5-dimethyloxazole	C9H15NO	M+NH4	171.1492	-2.3
	HMDB0037873	4-Ethyl-2-methyl-5-propyloxazole	C9H15NO	M+NH4	171.1492	-2.3
	HMDB0037875	2-Butyl-4,5-dimethyloxazole	C9H15NO	M+NH4	171.1492	-2.3
	HMDB0037882	5-Butyl-2,4-dimethyloxazole	C9H15NO	M+NH4	171.1492	-2.3
	HMDB0037857	4-Methyl-2-pentyloxazole	C9H15NO	M+NH4	171.1492	-2.3
	HMDB0037872	2-Ethyl-4-methyl-5-propyloxazole	C9H15NO	M+NH4	171.1492	-2.3
	HMDB0037862	5-Butyl-2-ethyloxazole	C9H15NO	M+NH4	171.1492	-2.3
	HMDB0037874	5-Ethyl-4-methyl-2-(1-methylethyl)oxazole	C9H15NO	M+NH4	171.1492	-2.3
	HMDB0037876	5-Ethyl-2-methyl-4-propyloxazole	C9H15NO	M+NH4	171.1492	-2.3
172.0366	HMDB0240351	1H-Indole-2,5-diol	C8H7NO2	M+Na	172.0369	-1.7
	HMDB0060318	(S)-4-Hydroxymandelonitrile	C8H7NO2	M+Na	172.0369	-1.7
	HMDB0004058	5,6-Dihydroxyindole	C8H7NO2	M+Na	172.0369	-1.7
	HMDB0178041	trans-2,3-Dehydroacyl-CoA	C8H7NO2	M+Na	172.0369	-1.7
	HMDB0060946	NAPQI	C8H7NO2	M+Na	172.0369	-1.7
172.0966	HMDB0131232	5-methoxy-2-methylbenzene-1,3-diol	C8H10O3	M+NH4	172.0968	-1.3
	HMDB0131231	5-methoxy-4-methylbenzene-1,3-diol	C8H10O3	M+NH4	172.0968	-1.3
	HMDB0169080	2-Hydroxy-3-methoxybenzyl alcohol	C8H10O3	M+NH4	172.0968	-1.3
	HMDB0146894	4-Ethylpyrogallol	C8H10O3	M+NH4	172.0968	-1.3
	HMDB0146874	SCHEMBL093	C8H10O3	M+NH4	172.0968	-1.3
	HMDB0125534	5-ethylbenzene-1,2,3-triol	C8H10O3	M+NH4	172.0968	-1.3
	HMDB0126617	2,4-dimethylbenzene-1,3,5-triol	C8H10O3	M+NH4	172.0968	-1.3
	HMDB0131479	2,3-dimethoxyphenol	C8H10O3	M+NH4	172.0968	-1.3
	HMDB0059966	3,5-Dimethoxyphenol	C8H10O3	M+NH4	172.0968	-1.3
	HMDB0135785	1-(4-hydroxyphenyl)ethane-1,2-diol	C8H10O3	M+NH4	172.0968	-1.3
	HMDB0037724	Propyl 2-furoate	C8H10O3	M+NH4	172.0968	-1.3
	HMDB0034158	2,6-Dimethoxyphenol	C8H10O3	M+NH4	172.0968	-1.3
	HMDB0037728	2-Furanylmethyl propanoate	C8H10O3	M+NH4	172.0968	-1.3
	HMDB0032012	4-Hydroxy-3-methoxybenzenemethanol	C8H10O3	M+NH4	172.0968	-1.3
	HMDB0030570	Sylvopinol	C8H10O3	M+NH4	172.0968	-1.3
	HMDB0005784	Hydroxytyrosol	C8H10O3	M+NH4	172.0968	-1.3
172.1327	HMDB0180434	(2E,4E)-9-hydroxynona-2,4-dienal	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0180433	trans-4,5-Epoxy-(E)-nonenal	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0180431	SCHEMBL179742	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0180432	3-[(1E)-hex-1-en-1-yl]oxirane-2-carbaldehyde	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0180430	(2E,4E)-6-hydroxynona-2,4-dienal	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0167038	(2E,6Z)-9-hydroxynona-2,6-dienal	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0167036	3-[(3Z)-hex-3-en-1-yl]oxirane-2-carbaldehyde	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0167034	(2E,6Z)-8-hydroxynona-2,6-dienal	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0167035	(2E,6Z)-5-hydroxynona-2,6-dienal	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0167037	(2E)-5-(3-ethyloxiran-2-yl)pent-2-enal	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0167032	2E,6Z-nonadienoic acid	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0167033	(2E,6Z)-4-hydroxynona-2,6-dienal	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0164921	1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0163467	(2Z)-2-methylocta-2,7-dienoic acid	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0060285	4-Oxo-2-nonenal	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0032442	2-Nonenoic acid gamma-lactone	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0032314	2,4-Hexadienyl propionate	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0040285	Anapear	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0036177	3,5,5-Trimethyl-1,2-cyclohexanedione	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0036239	3,5,5-Trimethyl-1,2-cyclohexanedione	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0037276	Octahydro-2H-1-benzopyran-2-one	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0031302	Methyl 2-octynoate	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0038268	Allyl hexenoate	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0038697	xi-2,2,6-Trimethyl-1,4-cyclohexanedione	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0035135	(E)-2,6-Dimethyl-2,5-heptadienoic acid	C9H14O2	M+NH4	172.1332	-2.9
	HMDB0005015	Gabapentin	C9H17NO2	M+H	172.1332	-2.9
	HMDB0061802	5-Methyl-2-(1-methylethyl)-cyclohexanone	C10H18O	M+NH4	172.1696	-2.8

HMDB0187564	CTK8I1689	C10H18O	M+NH4	172.1696	-2.8
HMDB0163116	(4Z,7Z)-deca-4,7-dien-1-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0032530	(+)-thujan-3-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0035815	(+)-Isoborneol	C10H18O	M+NH4	172.1696	-2.8
HMDB0037006	cis-Isopulegone	C10H18O	M+NH4	172.1696	-2.8
HMDB0037048	m-Menth-1-en-8-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0035825	(-)-Dihydrocarveol	C10H18O	M+NH4	172.1696	-2.8
HMDB0035783	(+)-Menthone	C10H18O	M+NH4	172.1696	-2.8
HMDB0037016	p-Menth-1-en-5-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0035954	(1R*,3R*,6S*)-3-Caranol	C10H18O	M+NH4	172.1696	-2.8
HMDB0035820	(R)-Citronellal	C10H18O	M+NH4	172.1696	-2.8
HMDB0035842	(R)-Citronellal	C10H18O	M+NH4	172.1696	-2.8
HMDB0034848	9-Decenal	C10H18O	M+NH4	172.1696	-2.8
HMDB0037019	6,8-Epoxy-p-menthane	C10H18O	M+NH4	172.1696	-2.8
HMDB0036077	p-Menth-8-en-3-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0036096	1,4-Cineole	C10H18O	M+NH4	172.1696	-2.8
HMDB0037133	Linaloyl oxide	C10H18O	M+NH4	172.1696	-2.8
HMDB0036100	3,7-Dimethyl-1,6-octadien-3-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0032118	2,6-Dimethyl-7-octen-3-one	C10H18O	M+NH4	172.1696	-2.8
HMDB0035841	Citronellal	C10H18O	M+NH4	172.1696	-2.8
HMDB0037007	p-Menth-1-en-9-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0036991	delta-Terpineol	C10H18O	M+NH4	172.1696	-2.8
HMDB0036993	gamma-Terpineol	C10H18O	M+NH4	172.1696	-2.8
HMDB0036097	Rose oxide	C10H18O	M+NH4	172.1696	-2.8
HMDB0034976	(-)-Borneol	C10H18O	M+NH4	172.1696	-2.8
HMDB0035818	(-)-Borneol	C10H18O	M+NH4	172.1696	-2.8
HMDB0035819	(-)-Isoborneol	C10H18O	M+NH4	172.1696	-2.8
HMDB0041034	(4Z,7Z)-4,7-Decadien-1-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0031410	3-Decen-2-one	C10H18O	M+NH4	172.1696	-2.8
HMDB0037049	(R)-m-Menth-1(6)-en-8-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0038025	xi-p-Menth-3-en-1-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0035861	trans-(-)-p-Menth-1-en-3-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0005812	Geraniol	C10H18O	M+NH4	172.1696	-2.8
HMDB0004043	alpha-Terpineol	C10H18O	M+NH4	172.1696	-2.8
HMDB0036126	(-)-Pinocampheol	C10H18O	M+NH4	172.1696	-2.8
HMDB0036112	(1R,4S,5R)-4-Thujanol	C10H18O	M+NH4	172.1696	-2.8
HMDB0037047	(-)-trans-m-Menth-8-en-1-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0036068	Campholenic alcohol	C10H18O	M+NH4	172.1696	-2.8
HMDB0035955	(1R*,2S*,3S*,6S*)-2-Caranol	C10H18O	M+NH4	172.1696	-2.8
HMDB0036196	(2E,4E)-2,4-Decadien-1-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0004472	Eucalyptol	C10H18O	M+NH4	172.1696	-2.8
HMDB0059869	p-tert-Butylcyclohexanone	C10H18O	M+NH4	172.1696	-2.8
HMDB0035833	p-Menth-1-en-4-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0035272	p-Menth-2-one	C10H18O	M+NH4	172.1696	-2.8
HMDB0059881	Ocimenol	C10H18O	M+NH4	172.1696	-2.8
HMDB0036086	(S)-alpha-Terpineol	C10H18O	M+NH4	172.1696	-2.8
HMDB0034932	Fenchol	C10H18O	M+NH4	172.1696	-2.8
HMDB0035162	(-)-Menthone	C10H18O	M+NH4	172.1696	-2.8
HMDB0059864	(-)-Menthone	C10H18O	M+NH4	172.1696	-2.8
HMDB0034972	Isomenthone	C10H18O	M+NH4	172.1696	-2.8
HMDB0036041	(R)-Lavandulol	C10H18O	M+NH4	172.1696	-2.8
HMDB0036107	Myrcenol	C10H18O	M+NH4	172.1696	-2.8
HMDB0036101	(R)-3,7-Dimethyl-1,6-octadien-3-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0036102	(R)-3,7-Dimethyl-1,6-octadien-3-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0030999	2-Decenal	C10H18O	M+NH4	172.1696	-2.8
HMDB0035155	beta-Geraniol	C10H18O	M+NH4	172.1696	-2.8
HMDB0041014	4-Decenal	C10H18O	M+NH4	172.1696	-2.8
HMDB0037215	trans-beta-Terpineol	C10H18O	M+NH4	172.1696	-2.8
HMDB0037161	2-Isopropyl-5-methyl-2-hexenal	C10H18O	M+NH4	172.1696	-2.8
HMDB0040448	2-(1-Methylpropyl)cyclohexanone	C10H18O	M+NH4	172.1696	-2.8
HMDB0035823	(S)-p-Menth-1-en-4-ol	C10H18O	M+NH4	172.1696	-2.8
HMDB0035838	Piperitol	C10H18O	M+NH4	172.1696	-2.8
HMDB0038185	Ocimen quintoxide	C10H18O	M+NH4	172.1696	-2.8
HMDB0036078	(-)-Isopulegol	C10H18O	M+NH4	172.1696	-2.8
HMDB0034969	(-)-Carvomenthone	C10H18O	M+NH4	172.1696	-2.8

	HMDB0036996	cis-beta-Terpineol	C10H18O	M+NH4	172.1696	-2.8
	HMDB0037214	cis-beta-Terpineol	C10H18O	M+NH4	172.1696	-2.8
	HMDB0036195	N,2,3-Trimethyl-2-(1-methylethyl)butanamide	C10H21NO	M+H	172.1696	-2.8
173.0570	HMDB0135239	4-(prop-2-en-1-yl)benzene-1,2-diol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0176418	2-Nonene-4,6-diyne-1,9-diol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0170980	4-[(1Z)-prop-1-en-1-yl]benzene-1,2-diol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0170763	4-(oxiran-2-ylmethyl)phenol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0146657	2-hydroxycinnamyl alcohol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0146635	4-vinyl-3-methoxyphenol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0135279	3-(4-hydroxyphenyl)propanal	C9H10O2	M+Na	173.0573	-1.7
	HMDB0135281	(3-phenyloxiran-2-yl)methanol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0135280	3-[(1E)-3-hydroxyprop-1-en-1-yl]phenol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0135278	3-(3-hydroxyphenyl)propanal	C9H10O2	M+Na	173.0573	-1.7
	HMDB0135276	2-hydroxy-3-phenylpropanal	C9H10O2	M+Na	173.0573	-1.7
	HMDB0135277	3-hydroxy-3-phenylpropanal	C9H10O2	M+Na	173.0573	-1.7
	HMDB0134027	2-(3-hydroxyprop-1-en-1-yl)phenol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0134026	3-(2-hydroxyphenyl)propanal	C9H10O2	M+Na	173.0573	-1.7
	HMDB0125532	3-ethenyl-5-methoxyphenol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0062349	4-Chromanol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0177508	4-(3-methyloxiran-2-yl)phenol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0032592	2'-Hydroxy-5'-methylacetophenone	C9H10O2	M+Na	173.0573	-1.7
	HMDB0033967	Ethyl benzoate	C9H10O2	M+Na	173.0573	-1.7
	HMDB0032570	4'-Methoxyacetophenone	C9H10O2	M+Na	173.0573	-1.7
	HMDB0032075	p-Tolyl acetate	C9H10O2	M+Na	173.0573	-1.7
	HMDB0040428	2-Phenylethyl formate	C9H10O2	M+Na	173.0573	-1.7
	HMDB0032073	o-Tolyl acetate	C9H10O2	M+Na	173.0573	-1.7
	HMDB0032569	2'-Methoxyacetophenone	C9H10O2	M+Na	173.0573	-1.7
	HMDB0033970	4-Ethoxybenzaldehyde	C9H10O2	M+Na	173.0573	-1.7
	HMDB0031310	Benzyl acetate	C9H10O2	M+Na	173.0573	-1.7
	HMDB0011743	2-Phenylpropionate	C9H10O2	M+Na	173.0573	-1.7
	HMDB0003654	4-Coumaryl alcohol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0002237	3,4-Dimethylbenzoic acid	C9H10O2	M+Na	173.0573	-1.7
	HMDB0002222	3-Methylphenylacetic acid	C9H10O2	M+Na	173.0573	-1.7
	HMDB0002097	4-Ethylbenzoic acid	C9H10O2	M+Na	173.0573	-1.7
	HMDB0013744	2-Methoxy-4-vinylphenol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0032617	Methyl phenylacetate	C9H10O2	M+Na	173.0573	-1.7
	HMDB0040925	2-(2-Furanyl)-3-methyl-2-butenal	C9H10O2	M+Na	173.0573	-1.7
	HMDB0135644	4-(3-hydroxyprop-1-en-1-yl)phenol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0176419	6-(3-methyloxiran-2-yl)hexa-3,5-diyne-1-ol	C9H10O2	M+Na	173.0573	-1.7
	HMDB0059824	4-Hydroxy-3-methylacetophenone	C9H10O2	M+Na	173.0573	-1.7
	HMDB0037715	1-Phenylethyl formate	C9H10O2	M+Na	173.0573	-1.7
	HMDB0038355	2-Ethyl-4-(2-furanyl)-2-propenal	C9H10O2	M+Na	173.0573	-1.7
	HMDB0000764	Hydrocinnamic acid	C9H10O2	M+Na	173.0573	-1.7
173.0804	HMDB0000341	2-Octenedioic acid	C8H12O4	M+H	173.0808	-2.5
	HMDB0159134	2-(3-hydroxy-4-oxocyclohexyl)acetic acid	C8H12O4	M+H	173.0808	-2.5
	HMDB0159135	2-hydroxy-2-(4-oxocyclohexyl)acetic acid	C8H12O4	M+H	173.0808	-2.5
	HMDB0173107	2,5-dimethoxycyclohexane-1,4-dione	C8H12O4	M+H	173.0808	-2.5
	HMDB0013312	trans-3-Octenedioic acid	C8H12O4	M+H	173.0808	-2.5
	HMDB0032352	3-Isopropenylpentanedioic acid	C8H12O4	M+H	173.0808	-2.5
	HMDB0038601	Diethyl fumarate	C8H12O4	M+H	173.0808	-2.5
	HMDB0034851	Ethyl 2,4-dioxohexanoate	C8H12O4	M+H	173.0808	-2.5
	HMDB0004982	cis-4-Octenedioic acid	C8H12O4	M+H	173.0808	-2.5
173.1168	HMDB0179168	3-caproyl propionic acid	C9H16O3	M+H	173.1172	-2.4
	HMDB0094711	9-oxononanoic acid	C9H16O3	M+H	173.1172	-2.4
	HMDB0163465	(2Z)-7-hydroxy-2-methyloct-2-enoic acid	C9H16O3	M+H	173.1172	-2.4
	HMDB0163466	(2Z)-8-hydroxy-2-methyloct-2-enoic acid	C9H16O3	M+H	173.1172	-2.4
	HMDB0163468	SCHEMBL7173369	C9H16O3	M+H	173.1172	-2.4
	HMDB0163470	2-methyl-3-pentyloxirane-2-carboxylic acid	C9H16O3	M+H	173.1172	-2.4
	HMDB0163469	(2Z)-4-hydroxy-2-methyloct-2-enoic acid	C9H16O3	M+H	173.1172	-2.4
	HMDB0169421	2-ethenyl-4,6-diethyl-1,3,5-trioxane	C9H16O3	M+H	173.1172	-2.4
	HMDB0040203	2-Methylpropyl 3-hydroxy-2-methylidenebutanoate	C9H16O3	M+H	173.1172	-2.4
	HMDB0036213	cis-3-Hexenyl lactate	C9H16O3	M+H	173.1172	-2.4
	HMDB0036188	Tetrahydrofurfuryl butyrate	C9H16O3	M+H	173.1172	-2.4
	HMDB0040165	Butyl levulinate	C9H16O3	M+H	173.1172	-2.4
	HMDB0036396	3-Methylbutyl 3-oxobutanoate	C9H16O3	M+H	173.1172	-2.4

	HMDB0059937	6-Pentyl-1,4-dioxan-2-one	C9H16O3	M+H	173.1172	-2.4
	HMDB0059936	5-Pentyl-1,4-dioxan-2-one	C9H16O3	M+H	173.1172	-2.4
	HMDB0060287	4-Hydroperoxy-2-nonenal	C9H16O3	M+H	173.1172	-2.4
	HMDB0062081	9-oxononanoate	C9H15O3	M+H	173.1172	-2.4
	HMDB0040202	Butyl 3-hydroxy-2-methylidenobutanoate	C9H16O3	M+H	173.1172	-2.4
173.1532	HMDB0171175	3,7-dimethyloct-6-ene-1,3-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0180497	9-Decene-1,2-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0180498	dec-9-ene-1,3-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0180500	dec-9-ene-1,5-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0180501	dec-9-ene-1,6-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0180503	1-decene-3,-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0180504	8-Oxiranyl-1-octanol	C10H20O2	M+H	173.1536	-2.3
	HMDB0180502	dec-9-ene-1,7-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0180499	dec-9-ene-1,4-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0179927	3,7-dimethyl-5-octene-1,7-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0179212	2-(4-methylcyclohexyl)propane-1,2-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0094654	propan-2-yl heptanoate	C10H20O2	M+H	173.1536	-2.3
	HMDB0171178	Citronellol epoxide	C10H20O2	M+H	173.1536	-2.3
	HMDB0171179	2-(4-methylpent-3-en-1-yl)butane-1,4-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0171177	3,7-Dimethyl-6-octene-1,5-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0171176	2,6-dimethyloct-2-ene-1,8-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0179213	7,8-dihydroxy-p-menthane	C10H20O2	M+H	173.1536	-2.3
	HMDB0031264	Methyl nonanoate	C10H20O2	M+H	173.1536	-2.3
	HMDB0031739	7-Hydroxy-3,7-dimethyloctanal	C10H20O2	M+H	173.1536	-2.3
	HMDB0040529	3-Methylbutyl pentanoate	C10H20O2	M+H	173.1536	-2.3
	HMDB0032045	Pentyl 3-methylbutanoate	C10H20O2	M+H	173.1536	-2.3
	HMDB0033620	Hexyl butyrate	C10H20O2	M+H	173.1536	-2.3
	HMDB0029760	1,1-Diethoxy-2-hexene	C10H20O2	M+H	173.1536	-2.3
	HMDB0040211	Butyl hexanoate	C10H20O2	M+H	173.1536	-2.3
	HMDB0036145	p-Menthane-3,8-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0041216	2,6-Dimethyl-7-octene-2,6-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0040195	Ethyl octanoate	C10H20O2	M+H	173.1536	-2.3
	HMDB0034457	Propyl heptanoate	C10H20O2	M+H	173.1536	-2.3
	HMDB0062146	Pentyl pentanoate	C10H20O2	M+H	173.1536	-2.3
	HMDB0000511	Capric acid	C10H20O2	M+H	173.1536	-2.3
	HMDB0037387	(1S,3R,4R)-p-Menthane-1,3-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0035723	(1R,2S,3S,4R)-p-Menthane-2,3-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0036136	4-Ethyl octanoic acid	C10H20O2	M+H	173.1536	-2.3
	HMDB0040167	3-Octyl acetate	C10H20O2	M+H	173.1536	-2.3
	HMDB0036228	2-Methylpropyl hexanoate	C10H20O2	M+H	173.1536	-2.3
	HMDB0038038	2-Methylbutyl 3-methylbutanoate	C10H20O2	M+H	173.1536	-2.3
	HMDB0032070	Isooctyl acetate	C10H20O2	M+H	173.1536	-2.3
	HMDB0035595	trans-p-Menthane-1,8-diol	C10H20O2	M+H	173.1536	-2.3
	HMDB0032302	Heptanal propyleneglycol acetal	C10H20O2	M+H	173.1536	-2.3
	HMDB0180097	Isocaproic acid	C10H20O2	M+H	173.1536	-2.3
	HMDB0061805	(2S)-2-Ethylhexyl acetate	C10H20O2	M+H	173.1536	-2.3
	HMDB0187563	2-(1-hydroxypropan-2-yl)-5-methylcyclohexan-1-ol	C10H20O2	M+H	173.1536	-2.3
	HMDB0061987	2-ethylhexyl acetate	C10H20O2	M+H	173.1536	-2.3
	HMDB0032155	Acetaldehyde 1,3-octanediol acetal	C10H20O2	M+H	173.1536	-2.3
	HMDB0032264	Ethyl 2-ethylhexanoate	C10H20O2	M+H	173.1536	-2.3
	HMDB0032315	Hexanal butane-2,3-diol acetal	C10H20O2	M+H	173.1536	-2.3
	HMDB0040157	3-Methylbutyl 2-methylbutanoate	C10H20O2	M+H	173.1536	-2.3
	HMDB0037849	Hexyl 2-methylpropanoate	C10H20O2	M+H	173.1536	-2.3
	HMDB0034849	4-Methylnonanoic acid	C10H20O2	M+H	173.1536	-2.3
	HMDB0030029	Isopentyl isopentanoate	C10H20O2	M+H	173.1536	-2.3
	HMDB0038602	Octyl acetate	C10H20O2	M+H	173.1536	-2.3
	HMDB0039218	2-Methylbutyl 2-methylbutanoate	C10H20O2	M+H	173.1536	-2.3
	HMDB0038783	(Z)-1-(1-Ethoxyethoxy)-3-hexene	C10H20O2	M+H	173.1536	-2.3
174.1121	HMDB0032232	2,5-Dimethyl-4-ethoxy-3(2H)-furanone	C8H12O3	M+NH4	174.1125	-2.1
	HMDB0031101	8-Hydroxy-5,6-octadienoic acid	C8H12O3	M+NH4	174.1125	-2.1
	HMDB0159132	2-(4-oxocyclohexyl)acetic Acid	C8H12O3	M+NH4	174.1125	-2.1
	HMDB0061684	N-Acetylisoleucine	C8H15NO3	M+H	174.1125	-2.1
	HMDB0000701	Hexanoylglycine	C8H15NO3	M+H	174.1125	-2.1
	HMDB0000747	Isovalerylalanine	C8H15NO3	M+H	174.1125	-2.1
	HMDB0002087	Isovalerylsarcosine	C8H15NO3	M+H	174.1125	-2.1

174.1484	HMDB0011756	N-Acetyl-leucine	C8H15NO3	M+H	174.1125	-2.1
	HMDB0163454	SCHEMBL11263	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0163455	(2Z)-2-(hydroxymethyl)oct-2-enal	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0163456	(2Z)-4-hydroxy-2-methyloct-2-enal	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0163458	2-methyl-3-pentylloxiran-2-carbaldehyde	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0163457	(2Z)-7-hydroxy-2-methyloct-2-enal	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0163459	(2Z)-8-hydroxy-2-methyloct-2-enal	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0166519	6-(hydroxymethyl)-2,2-dimethylcyclohexan-1-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0166518	2-(hydroxymethyl)-2,6-dimethylcyclohexan-1-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0167040	(6Z)-5-hydroxynon-6-enal	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0167039	(6Z)-8-hydroxynon-6-enal	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0167041	5-(3-ethyloxiran-2-yl)pentanal	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0167044	(2E,6Z)-nona-2,6-diene-1,8-diol	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0167042	(6Z)-9-hydroxynon-6-enal	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0167043	(6Z)-2-hydroxynon-6-enal	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0167045	(2E,6Z)-nona-2,6-diene-1,9-diol	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179788	(5E)-3-hydroxynon-5-en-2-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179787	(5E)-1-hydroxynon-5-en-2-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179803	(3Z)-5-hydroxynon-3-en-2-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179804	(3Z)-8-hydroxynon-3-en-2-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179806	(3Z)-9-hydroxynon-3-en-2-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179805	Ethanone, 1-(3-pentylloxiran-2-yl)-	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179807	(3Z)-1-hydroxynon-3-en-2-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0180000	7-METHYL-7-OCTENOIC ACID	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0180427	{3-[(1E)-hex-1-en-1-yl]oxiran-2-yl}methanol	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0180425	(2E,4E)-nona-2,4-diene-1,6-diol	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0180426	(2E,4E)-nona-2,4-diene-1,8-diol	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0180428	(2E)-3-(3-butyloxiran-2-yl)prop-2-en-1-ol	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0180429	(2E,4E)-nona-2,4-diene-1,9-diol	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179786	(5E)-9-hydroxynon-5-en-2-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179785	4-(3-propyloxiran-2-yl)butan-2-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0167049	{3-[(3Z)-hex-3-en-1-yl]oxiran-2-yl}methanol	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0167047	(2E,6Z)-nona-2,6-diene-1,4-diol	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0167048	(2E,6Z)-nona-2,6-diene-1,5-diol	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0167050	(2E)-5-(3-ethyloxiran-2-yl)pent-2-en-1-ol	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0167057	6Z-Nonenoic acid	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179750	7-hydroxynon-8-en-3-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179752	7-(oxiran-2-yl)heptan-3-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179754	4-hydroxynon-8-en-3-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179751	2-hydroxynon-8-en-3-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179753	SCHEMBL18838844	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179782	(5E)-7-hydroxynon-5-en-2-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179784	(5E)-8-hydroxynon-5-en-2-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0179783	4-Hydroxynon-5-en-2-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0031271	2-Nonenoic acid	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0038272	trans-2-Hexenyl propanoate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0036208	2-Propenyl 2-ethylbutanoate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0032491	Prenyl isobutyrate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0032265	cis-Ethyl 4-heptenoate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0032307	Hept-trans-2-en-1-yl acetate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0059728	Methyl 3-Octenoate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0059817	(Z)-Oak lactone	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0059894	(Z)-Oak lactone	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0059840	(E)-2-Ethyl heptenoate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0060286	3,4-Epoxy-nonanal	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0032413	Methyl 2-octenoate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0038275	cis-3-Hexenyl propanoate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0039794	Methyl 4Z-octenoate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0037629	Isobutyl angelate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0004362	4-Hydroxynonenal	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0035307	Quercuslactone a	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0037618	(E)-3-Heptenyl acetate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0037023	2-Hydroxy-2,6,6-trimethylcyclohexanone	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0031531	Dihydro-5-pentyl-2(3H)-furanone	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0039736	6-Hydroxy-4,6-dimethyl-3-hepten-2-one	C9H16O2	M+NH4	174.1489	-2.6

	HMDB0031263	2,4-Nonanedione	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0034716	4-Oxononanal	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0033167	Ethyl cyclohexanecarboxylate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0040210	2-Propenyl hexanoate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0037496	Methyl (E)-2-octenoate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0031514	6-Butyltetrahydro-2H-pyran-2-one	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0036222	Cyclohexyl propionate	C9H16O2	M+NH4	174.1489	-2.6
	HMDB0170941	8-nonylenic acid	C9H16O2	M+NH4	174.1489	-2.6
175.0361	HMDB0150437	6-methylsalicylic acid	C8H8O3	M+Na	175.0366	-2.6
	HMDB0171094	ortho-vanillin	C8H8O3	M+Na	175.0366	-2.6
	HMDB0166108	5-hydroxy-2-methoxybenzaldehyde	C8H8O3	M+Na	175.0366	-2.6
	HMDB0172092	3-Hydroxy-4-methoxybenzaldehyde	C8H8O3	M+Na	175.0366	-2.6
	HMDB0168664	Methyl 3-hydroxybenzoate	C8H8O3	M+Na	175.0366	-2.6
	HMDB0182861	SCHEMBL437438	C8H8O3	M+Na	175.0366	-2.6
	HMDB0166109	3-hydroxy-2-methoxybenzaldehyde	C8H8O3	M+Na	175.0366	-2.6
	HMDB0166106	2-hydroxy-6-methoxybenzaldehyde	C8H8O3	M+Na	175.0366	-2.6
	HMDB0146889	SCHEMBL2128735	C8H8O3	M+Na	175.0366	-2.6
	HMDB0146870	SCHEMBL3679957	C8H8O3	M+Na	175.0366	-2.6
	HMDB0137457	4-[(E)-2-hydroxyethenyl]benzene-1,2-diol	C8H8O3	M+Na	175.0366	-2.6
	HMDB0125528	5-ethenylbenzene-1,2,3-triol	C8H8O3	M+Na	175.0366	-2.6
	HMDB0166107	4-hydroxy-2-methoxybenzaldehyde	C8H8O3	M+Na	175.0366	-2.6
	HMDB0183904	mandelate	C8H7O3	M+Na	175.0366	-2.6
	HMDB0183905	4-hydroxyphenylacetate	C8H7O3	M+Na	175.0366	-2.6
	HMDB0029661	3',4'-Dihydroxyacetophenone	C8H8O3	M+Na	175.0366	-2.6
	HMDB0032604	2-Methoxybenzoic acid	C8H8O3	M+Na	175.0366	-2.6
	HMDB0034172	Methyl 2-hydroxybenzoate	C8H8O3	M+Na	175.0366	-2.6
	HMDB0032606	3-Methoxybenzoic acid	C8H8O3	M+Na	175.0366	-2.6
	HMDB0029657	2,4'-Dihydroxyacetophenone	C8H8O3	M+Na	175.0366	-2.6
	HMDB0041283	1-(2-Furanyl)-1,3-butanedione	C8H8O3	M+Na	175.0366	-2.6
	HMDB0032919	Ethyl 2-furanyl diketone	C8H8O3	M+Na	175.0366	-2.6
	HMDB0036907	2-Propenyl 2-furancarboxylate	C8H8O3	M+Na	175.0366	-2.6
	HMDB0012308	Vanillin	C8H8O3	M+Na	175.0366	-2.6
	HMDB0004815	4-Hydroxy-3-methylbenzoic acid	C8H8O3	M+Na	175.0366	-2.6
	HMDB0003791	3,4-Dihydroxyphenylacetaldehyde	C8H8O3	M+Na	175.0366	-2.6
	HMDB0002390	3-Cresotinic acid	C8H8O3	M+Na	175.0366	-2.6
	HMDB0000669	ortho-Hydroxyphenylacetic acid	C8H8O3	M+Na	175.0366	-2.6
	HMDB0000440	3-Hydroxyphenylacetic acid	C8H8O3	M+Na	175.0366	-2.6
	HMDB0000020	p-Hydroxyphenylacetic acid	C8H8O3	M+Na	175.0366	-2.6
	HMDB0001101	p-Anisic acid	C8H8O3	M+Na	175.0366	-2.6
	HMDB0029662	3',5'-Dihydroxyacetophenone	C8H8O3	M+Na	175.0366	-2.6
	HMDB0032572	Methylparaben	C8H8O3	M+Na	175.0366	-2.6
	HMDB0124926	Mandelic acid	C8H8O3	M+Na	175.0366	-2.6
	HMDB0062005	Dihydroxyacetophenone	C8H8O3	M+Na	175.0366	-2.6
	HMDB0060390	4-Hydroxyphenyl acetate	C8H8O3	M+Na	175.0366	-2.6
	HMDB0062635	(R)-mandelic Acid	C8H8O3	M+Na	175.0366	-2.6
	HMDB0032399	Methyl furfuracrylate	C8H8O3	M+Na	175.0366	-2.6
	HMDB0172091	2-Hydroxy-4-methoxybenzaldehyde	C8H8O3	M+Na	175.0366	-2.6
	HMDB0029660	2',6'-Dihydroxyacetophenone	C8H8O3	M+Na	175.0366	-2.6
	HMDB0029659	2',4'-Dihydroxyacetophenone	C8H8O3	M+Na	175.0366	-2.6
	HMDB0029658	2',3'-Dihydroxyacetophenone	C8H8O3	M+Na	175.0366	-2.6
	HMDB0031609	Phenoxyacetic acid	C8H8O3	M+Na	175.0366	-2.6
	HMDB0032594	2-(Hydroxymethyl)benzoic acid	C8H8O3	M+Na	175.0366	-2.6
	HMDB0033003	1-(5-Methyl-2-furanyl)-1,2-propanedione	C8H8O3	M+Na	175.0366	-2.6
	HMDB0032629	2',5'-Dihydroxyacetophenone	C8H8O3	M+Na	175.0366	-2.6
	HMDB0000703	Mandelic acid	C8H8O3	M+Na	175.0366	-2.6
175.0750	HMDB0031845	3-Propylidene-1(3H)-isobenzofuranone	C11H10O2	M+H	175.0754	-2.0
	HMDB0032727	4-Methoxy-1-naphthol	C11H10O2	M+H	175.0754	-2.0
	HMDB0166920	Menadiol	C11H10O2	M+H	175.0754	-2.0
175.0961	HMDB0041606	Dimethyl adipate	C8H14O4	M+H	175.0965	-2.2
	HMDB0159133	2-hydroxy-2-(4-hydroxycyclohexyl)acetic acid	C8H14O4	M+H	175.0965	-2.2
	HMDB0059727	2,4-Dimethyladipic acid	C8H14O4	M+H	175.0965	-2.2
	HMDB0033838	Diethyl succinate	C8H14O4	M+H	175.0965	-2.2
	HMDB0002023	Ethyladipic acid	C8H14O4	M+H	175.0965	-2.2
	HMDB0060684	2-Propylglutaric acid	C8H14O4	M+H	175.0965	-2.2
	HMDB0059757	3-Methylpimelic acid	C8H14O4	M+H	175.0965	-2.2

	HMDB0000893	Suberic acid	C8H14O4	M+H	175.0965	-2.2
175.1113	HMDB0040823	(S)-11,12,13-Trinor-7-calamenone	C12H14O	M+H	175.1117	-2.5
	HMDB0031622	6-Phenyl-3-hexen-2-one	C12H14O	M+H	175.1117	-2.5
	HMDB0037281	4-Methyl-2-phenyl-2-pentenal	C12H14O	M+H	175.1117	-2.5
	HMDB0039153	(R)-11,12,13-Trinor-1(5),6,9-guaiatrien-8-one	C12H14O	M+H	175.1117	-2.5
	HMDB0171339	4-(4-methylphenyl)pent-4-en-2-one	C12H14O	M+H	175.1117	-2.5
175.1185	HMDB0000517	L-Arginine	C6H14N4O2	M+H	175.1190	-2.6
	HMDB0003416	D-Arginine	C6H14N4O2	M+H	175.1190	-2.6
175.1324	HMDB0170940	2-hydroxynonanoic acid	C9H18O3	M+H	175.1329	-2.7
	HMDB0179169	1,8-dihydroxynonan-4-one	C9H18O3	M+H	175.1329	-2.7
	HMDB0179170	SCHEMBL1635	C9H18O3	M+H	175.1329	-2.7
	HMDB0179172	1,5-dihydroxynonan-4-one	C9H18O3	M+H	175.1329	-2.7
	HMDB0179171	1,3-dihydroxynonan-4-one	C9H18O3	M+H	175.1329	-2.7
	HMDB0179997	SCHEMBL3537	C9H18O3	M+H	175.1329	-2.7
	HMDB0179998	SCHEMBL9379	C9H18O3	M+H	175.1329	-2.7
	HMDB0034040	2,4,6-Triethyl-1,3,5-trioxane	C9H18O3	M+H	175.1329	-2.7
	HMDB0031513	3-Hydroxynonanoic acid	C9H18O3	M+H	175.1329	-2.7
	HMDB0170939	9-Hydroxynonanoic acid	C9H18O3	M+H	175.1329	-2.7
	HMDB0170938	8-hydroxy-nonanoic acid	C9H18O3	M+H	175.1329	-2.7
	HMDB0179999	2-hydroxy-7-methyloctanoic acid	C9H18O3	M+H	175.1329	-2.7
175.1439	HMDB0014447	Tranexamic Acid	C8H15NO2	M+NH4	175.1441	-1.2
	HMDB0033433	(S)-Homostachydrine	C8H15NO2	M+NH4	175.1441	-1.2
	HMDB0013287	Ne,Ne dimethyllysine	C8H18N2O2	M+H	175.1441	-1.2
175.1477	HMDB0036683	5,7alpha-Dihydro-1,4,4,7a-tetramethyl-4H-indene	C13H18	M+H	175.1481	-2.4
	HMDB0059826	alpha-Ionene	C13H18	M+H	175.1481	-2.4
	HMDB0059696	1,2,3,4-Tetrahydro-1,5,7-trimethylnaphthalene	C13H18	M+H	175.1481	-2.4
	HMDB0061824	1-Methyl-4-(1-methyl-2-propenyl)-benzene	C13H18	M+H	175.1481	-2.4
175.9983	HMDB0000996	3-Sulfinioalanine	C3H7NO4S	M+Na	175.9988	-2.8
	HMDB0060179	3-Sulfinioalanine	C3H7NO4S	M+Na	175.9988	-2.8
176.0549	HMDB0060348	2-Maleylacetate	C6H6O5	M+NH4	176.0553	-2.5
	HMDB0031210	Zymonic acid	C6H6O5	M+NH4	176.0553	-2.5
	HMDB0137818	benzene-1,2,3,4,5-pentol	C6H6O5	M+NH4	176.0553	-2.5
	HMDB0037759	2-Methylene-4-oxopentanedioic acid	C6H6O5	M+NH4	176.0553	-2.5
	HMDB0183470	3-[(1E)-2-carboxyeth-1-en-1-yl]oxirane-2-carboxylic acid	C6H6O5	M+NH4	176.0553	-2.5
	HMDB0060273	2-Amino-3-oxoadipate	C6H9NO5	M+H	176.0553	-2.5
	HMDB0039163	D-N-(Carboxyacetyl)alanine	C6H9NO5	M+H	176.0553	-2.5
	HMDB0003470	N-Formyl-L-glutamic acid	C6H9NO5	M+H	176.0553	-2.5
	HMDB0000812	N-Acetyl-L-aspartic acid	C6H9NO5	M+H	176.0553	-2.5
176.0913	HMDB0163407	3-hydroxy-5-(2-hydroxyethyl)-4-methyl-2,5-dihydrofuran-2-one	C7H10O4	M+NH4	176.0917	-2.5
	HMDB0163406	3-hydroxy-5-(1-hydroxyethyl)-4-methyl-2,5-dihydrofuran-2-one	C7H10O4	M+NH4	176.0917	-2.5
	HMDB0163405	5-ethyl-3-hydroxy-4-(hydroxymethyl)-2,5-dihydrofuran-2-one	C7H10O4	M+NH4	176.0917	-2.5
	HMDB0163408	5-(1-hydroxyethyl)-4-methyloxolane-2,3-dione	C7H10O4	M+NH4	176.0917	-2.5
	HMDB0163409	5-(2-hydroxyethyl)-4-methyloxolane-2,3-dione	C7H10O4	M+NH4	176.0917	-2.5
	HMDB0012241	Isopropylmaleate	C7H10O4	M+NH4	176.0917	-2.5
	HMDB0036380	xi-2,3-Dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one	C7H10O4	M+NH4	176.0917	-2.5
	HMDB0059815	Ethyl 5-oxotetrahydro-2-furancarboxylate	C7H10O4	M+NH4	176.0917	-2.5
	HMDB0000635	Succinylacetone	C7H10O4	M+NH4	176.0917	-2.5
	HMDB0034252	2-Aminoheptanedioic acid	C7H13NO4	M+H	176.0917	-2.5
	HMDB0094717	hydroxyvaleryl glycine	C7H13NO4	M+H	176.0917	-2.5
	HMDB0036383	Calystegine B5	C7H13NO4	M+H	176.0917	-2.5
	HMDB0002201	N-Carboxyethyl-g-aminobutyric acid	C7H13NO4	M+H	176.0917	-2.5
	HMDB0038594	Calystegine B2	C7H13NO4	M+H	176.0917	-2.5
	HMDB0062788	isobutyric acid anhydride	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0158408	(2Z)-8-hydroxyoct-2-enoic acid	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0158407	SCHEMBL63	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0158406	(2Z)-7-hydroxyoct-2-enoic acid	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0158405	(2Z)-4-hydroxyoct-2-enoic acid	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0041616	Propyl levulinate	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0000451	cis-4-Hydroxycyclohexylacetic acid	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0060685	3-Oxovalproic acid	C8H14O3	M+NH4	176.1281	-2.9

176.1276	HMDB0060683	2-n-Propyl-4-oxopentanoic acid	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0059939	6-Butyl-1,4-dioxan-2-one	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0059938	5-Butyl-1,4-dioxan-2-one	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0013211	Alpha-Ketooctanoic acid	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0040447	Butyl acetoacetate	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0030303	6-Ethyl-1-methyl-2,7,8-trioxabicyclo[3.2.1]octane	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0031307	Ethyl 3-oxohexanoate	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0036395	2-Methylpropyl 3-oxobutanoate	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0036230	1-Methyl-2-oxopropyl butyrate	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0038305	3-Methylbutyl 2-oxopropanoate	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0031177	Tetrahydrofurfuryl propionate	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0010721	3-Oxo-octanoic acid	C8H14O3	M+NH4	176.1281	-2.9
177.0542	HMDB0000909	trans-4-Hydroxycyclohexylacetic acid	C8H14O3	M+NH4	176.1281	-2.9
	HMDB0128615	3-(hydroxymethyl)-1H-isochromen-1-one	C10H8O3	M+H	177.0546	-2.4
	HMDB0129369	1-(4-hydroxy-1-benzofuran-5-yl)ethan-1-one	C10H8O3	M+H	177.0546	-2.4
	HMDB0135530	6-(hydroxymethyl)-2H-chromen-2-one	C10H8O3	M+H	177.0546	-2.4
	HMDB0135531	8-hydroxy-6-methyl-2H-chromen-2-one	C10H8O3	M+H	177.0546	-2.4
	HMDB0135532	5-hydroxy-6-methyl-2H-chromen-2-one	C10H8O3	M+H	177.0546	-2.4
	HMDB0135533	3-hydroxy-6-methyl-2H-chromen-2-one	C10H8O3	M+H	177.0546	-2.4
	HMDB0059622	4-Methylumbelliferone	C10H8O3	M+H	177.0546	-2.4
	HMDB0029758	Herniarin	C10H8O3	M+H	177.0546	-2.4
	HMDB0032990	7-Hydroxy-6-methyl-2H-1-benzopyran-2-one	C10H8O3	M+H	177.0546	-2.4
	HMDB0163660	beta-Hydrojuglone	C10H8O3	M+H	177.0546	-2.4
	HMDB0033813	3-(3,4-Methylenedioxyphenyl)propenal	C10H8O3	M+H	177.0546	-2.4
177.0906	HMDB0032883	1,4,5-Naphthalenetriol	C10H8O3	M+H	177.0546	-2.4
	HMDB0031054	-Hydroxy-2,8-decadiene-4,6-diynoic acid	C10H8O3	M+H	177.0546	-2.4
	HMDB0126379	2,2-dimethyl-2H-chromen-5-ol	C11H12O2	M+H	177.0910	-2.3
	HMDB0126467	2-[(1E)-3-methylbuta-1,3-dien-1-yl]benzene-1,3-diol	C11H12O2	M+H	177.0910	-2.3
	HMDB0163608	alpha-Isopropenylbenzeneacetic acid	C11H12O2	M+H	177.0910	-2.3
	HMDB0151237	119711-59	C11H12O2	M+H	177.0910	-2.3
	HMDB0151231	2-(4-methoxybenzyl)acrylaldehyde	C11H12O2	M+H	177.0910	-2.3
	HMDB0133681	1-(2-methyl-3-phenyloxiran-2-yl)ethan-1-one	C11H12O2	M+H	177.0910	-2.3
	HMDB0133680	4-(4-hydroxyphenyl)-3-methylbut-3-en-2-one	C11H12O2	M+H	177.0910	-2.3
	HMDB0133677	1-hydroxy-3-methyl-4-phenylbut-3-en-2-one	C11H12O2	M+H	177.0910	-2.3
	HMDB0133678	3-(hydroxymethyl)-4-phenylbut-3-en-2-one	C11H12O2	M+H	177.0910	-2.3
	HMDB0133679	4-(3-hydroxyphenyl)-3-methylbut-3-en-2-one	C11H12O2	M+H	177.0910	-2.3
177.1119	HMDB0133466	4-(3-methoxyphenyl)but-3-en-2-one	C11H12O2	M+H	177.0910	-2.3
	HMDB0132973	(1E)-1-(4-hydroxyphenyl)pent-1-en-3-one	C11H12O2	M+H	177.0910	-2.3
	HMDB0033834	Ethyl cinnamate	C11H12O2	M+H	177.0910	-2.3
	HMDB0037145	3-(4-Methoxyphenyl)-2-methyl-2-propenal	C11H12O2	M+H	177.0910	-2.3
	HMDB0037142	2-(Phenylethenyl)-1,3-dioxolane	C11H12O2	M+H	177.0910	-2.3
	HMDB0029699	Cinnamyl acetate	C11H12O2	M+H	177.0910	-2.3
	HMDB0036905	2-Propenyl phenylacetate	C11H12O2	M+H	177.0910	-2.3
	HMDB0132267	5-benzylloxolan-2-one	C11H12O2	M+H	177.0910	-2.3
	HMDB0164642	2,3,7-trihydroxyoctanal	C8H16O4	M+H	177.1121	-1.3
	HMDB0164641	3,7,8-trihydroxyoctanal	C8H16O4	M+H	177.1121	-1.3
	HMDB0161158	2,8-dihydroxy-octanoic acid	C8H16O4	M+H	177.1121	-1.3
	HMDB0159450	2,7-dihydroxyoctanoic acid	C8H16O4	M+H	177.1121	-1.3
177.1270	HMDB0159449	7,8-dihydroxyoctanoic acid	C8H16O4	M+H	177.1121	-1.3
	HMDB0036021	Rhubafuran	C12H16O	M+H	177.1274	-2.2
	HMDB0031569	4-Methyl-1-phenyl-2-pentanone	C12H16O	M+H	177.1274	-2.2
	HMDB0036171	3-(4-Isopropylphenyl)propanal	C12H16O	M+H	177.1274	-2.2
	HMDB0034177	(S)-4-(4-Methylphenyl)-2-pentanone	C12H16O	M+H	177.1274	-2.2
177.1633	HMDB0094661	1-phenylhexan-2-one	C12H16O	M+H	177.1274	-2.2
	HMDB0035180	(6E,8E)-4,6,8-Megastigmatriene	C13H20	M+H	177.1638	-2.7
	HMDB0061825	1-Phenylheptane	C13H20	M+H	177.1638	-2.7
	HMDB0061826	1-Methyl-2-n-hexylbenzene	C13H20	M+H	177.1638	-2.7
178.0582	HMDB0034267	L-2-Amino-3-(1-pyrazolyl)propanoic acid	C6H9N3O2	M+Na	178.0587	-2.8
	HMDB0000177	L-Histidine	C6H9N3O2	M+Na	178.0587	-2.8
	HMDB0154888	L-Histidine	C6H9N3O2	M+Na	178.0587	-2.8
	HMDB0041605	Propyleneglycol diacetate	C7H12O4	M+NH4	178.1074	-2.1
	HMDB0165010	2-(acetyloxy)-3-methylbutanoic acid	C7H12O4	M+NH4	178.1074	-2.1
	HMDB0175388	ss-Acetoxyisovaleriansaure	C7H12O4	M+NH4	178.1074	-2.1
	HMDB0000857	Pimelic acid	C7H12O4	M+NH4	178.1074	-2.1
	HMDB0059738	2-Ethylglutaric acid	C7H12O4	M+NH4	178.1074	-2.1

178.1070	HMDB0059722	Mono-methyl-adipate	C7H12O4	M+NH4	178.1074	-2.1
	HMDB0059893	Ethyl methyl succinate	C7H12O4	M+NH4	178.1074	-2.1
	HMDB0061676	2,2-Dimethylglutaric acid	C7H12O4	M+NH4	178.1074	-2.1
	HMDB0061239	2-Propylsuccinic acid	C7H12O4	M+NH4	178.1074	-2.1
	HMDB0029167	2-Methyladipic acid	C7H12O4	M+NH4	178.1074	-2.1
	HMDB0029573	Diethyl malonate	C7H12O4	M+NH4	178.1074	-2.1
	HMDB0002441	3,3-Dimethylglutaric acid	C7H12O4	M+NH4	178.1074	-2.1
	HMDB0000555	3-Methyladipic acid	C7H12O4	M+NH4	178.1074	-2.1
178.1433	HMDB0035360	N-Methyl-1-deoxynojirimycin	C7H15NO4	M+H	178.1074	-2.2
	HMDB0000486	7-Hydroxyoctanoic acid	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0172040	CTK8I1333	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0061914	8-Hydroxyoctanoate	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0062596	(7R)-7-hydroxyoctanoic acid	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0164640	3,7-dihydroxyoctanal	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0172043	ethyl 3-(hydroxymethyl)pentanoate	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0172042	NSC616278	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0172041	SCHEMBL9153763	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0000711	Hydroxyoctanoic acid	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0002264	(R)-2-Hydroxycaprylic acid	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0010722	(R)-3-Hydroxyoctanoic acid	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0031509	Ethyl 3-hydroxyhexanoate	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0032827	Peroxyoctanoic acid	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0032270	(+/-)-Ethyl 2-hydroxy-3-methylvalerate	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0013898	5-Hydroxyvalproic acid	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0013900	4-Hydroxyvalproic acid	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0013899	3-Hydroxyvalproic acid	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0059825	Isoamyl lactate	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0059867	Ethyl 2-hydroxy-4-methylpentanoate	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0001954	(S)-3-hydroxyoctanoic acid	C8H16O3	M+NH4	178.1438	-2.6
	HMDB0172044	SCHEMBL8569867	C8H16O3	M+NH4	178.1438	-2.6
179.0482	HMDB0000078	Cysteinylglycine	C5H10N2O3S	M+H	179.0485	-1.6
	HMDB0028775	2-[(2-amino-1-hydroxy-3-sulfanylpropylidene)amino]acetic acid	C5H10N2O3S	M+H	179.0485	-1.6
	HMDB0028838	Glycyl-Cysteine	C5H10N2O3S	M+H	179.0485	-1.6
179.1062	HMDB0126149	2-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C11H14O2	M+H	179.1067	-2.5
	HMDB0126449	2-[(1E)-3-methylbut-1-en-1-yl]benzene-1,3-diol	C11H14O2	M+H	179.1067	-2.5
	HMDB0132981	1-(4-hydroxyphenyl)pentan-3-one	C11H14O2	M+H	179.1067	-2.5
	HMDB0163598	SCHEMBL9714564	C11H14O2	M+H	179.1067	-2.5
	HMDB0163594	4-hydroxy-3-methyl-2-phenylbutanal	C11H14O2	M+H	179.1067	-2.5
	HMDB0163597	SCHEMBL9714781	C11H14O2	M+H	179.1067	-2.5
	HMDB0163596	2-hydroxy-3-methyl-2-phenylbutanal	C11H14O2	M+H	179.1067	-2.5
	HMDB0163592	38-94-9	C11H14O2	M+H	179.1067	-2.5
	HMDB0163593	SCHEMBL11476137	C11H14O2	M+H	179.1067	-2.5
	HMDB0151222	3-(4-methoxyphenyl)-2-methylprop-2-en-1-ol	C11H14O2	M+H	179.1067	-2.5
	HMDB0151221	3-(4-methoxyphenyl)-2-methylpropanal	C11H14O2	M+H	179.1067	-2.5
	HMDB0133686	3-benzyl-4-hydroxybutan-2-one	C11H14O2	M+H	179.1067	-2.5
	HMDB0133685	4-(4-hydroxyphenyl)-3-methylbutan-2-one	C11H14O2	M+H	179.1067	-2.5
	HMDB0133687	1-hydroxy-3-methyl-4-phenylbutan-2-one	C11H14O2	M+H	179.1067	-2.5
	HMDB0133684	4-(3-hydroxyphenyl)-3-methylbutan-2-one	C11H14O2	M+H	179.1067	-2.5
	HMDB0133682	3-hydroxy-3-methyl-4-phenylbutan-2-one	C11H14O2	M+H	179.1067	-2.5
	HMDB0133683	4-hydroxy-3-methyl-4-phenylbutan-2-one	C11H14O2	M+H	179.1067	-2.5
	HMDB0133469	4-(3-methoxyphenyl)butan-2-one	C11H14O2	M+H	179.1067	-2.5
	HMDB0133181	4-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C11H14O2	M+H	179.1067	-2.5
	HMDB0040287	1-Phenylethyl propanoate	C11H14O2	M+H	179.1067	-2.5
	HMDB0037708	p-Tolyl isobutyrate	C11H14O2	M+H	179.1067	-2.5
	HMDB0040356	Osmorhizole	C11H14O2	M+H	179.1067	-2.5
	HMDB0036235	alpha, alpha-Dimethylphenethyl formate	C11H14O2	M+H	179.1067	-2.5
	HMDB0031864	Methyleugenol	C11H14O2	M+H	179.1067	-2.5
	HMDB0033597	4-(4-Methoxyphenyl)-2-butanone	C11H14O2	M+H	179.1067	-2.5
	HMDB0036385	Methyl 4-phenylbutanoate	C11H14O2	M+H	179.1067	-2.5
	HMDB0040800	2-Ethoxy-5-(1-propenyl)phenol	C11H14O2	M+H	179.1067	-2.5
	HMDB0040426	Isopropyl phenylacetate	C11H14O2	M+H	179.1067	-2.5
	HMDB0038179	3-(2-Hydroxy-4-methylphenyl)-2-butanone	C11H14O2	M+H	179.1067	-2.5

	HMDB0037680	2-Methylphenyl 2-methylpropanoate	C11H14O2	M+H	179.1067	-2.5
	HMDB0040411	Ethyl 3-phenylpropanoate	C11H14O2	M+H	179.1067	-2.5
	HMDB0035013	2-Phenylethyl propanoate	C11H14O2	M+H	179.1067	-2.5
	HMDB0041553	Methylisoeugenol	C11H14O2	M+H	179.1067	-2.5
	HMDB0040425	Propyl phenylacetate	C11H14O2	M+H	179.1067	-2.5
	HMDB0031250	Phenylmethyl 2-methylpropanoate	C11H14O2	M+H	179.1067	-2.5
	HMDB0033376	Phenylmethyl butanoate	C11H14O2	M+H	179.1067	-2.5
	HMDB0033386	3-Phenylpropyl acetate	C11H14O2	M+H	179.1067	-2.5
	HMDB0040583	2-Methylpropyl benzoate	C11H14O2	M+H	179.1067	-2.5
	HMDB0002043	5-Phenylvaleric acid	C11H14O2	M+H	179.1067	-2.5
179.1426	HMDB0032579	2,5-Diisopropylphenol	C12H18O	M+H	179.1430	-2.5
	HMDB0037272	2-Ethoxy-1-methyl-4-(1-methylethyl)benzene	C12H18O	M+H	179.1430	-2.5
	HMDB0038107	Quinceoxepine	C12H18O	M+H	179.1430	-2.5
	HMDB0031731	3-Methyl-1-phenyl-3-pentanol	C12H18O	M+H	179.1430	-2.5
	HMDB0035055	Photocitral A	C12H18O	M+H	179.1430	-2.5
	HMDB0036681	7-Isopropyl-5-methylbicyclo[2.2.2]oct-5-en-2-one	C12H18O	M+H	179.1430	-2.5
	HMDB0031194	Tricycloekasantal	C12H18O	M+H	179.1430	-2.5
	HMDB0031568	4-Methyl-1-phenyl-2-pentanol	C12H18O	M+H	179.1430	-2.5
	HMDB0038194	Geijerone	C12H18O	M+H	179.1430	-2.5
180.0862	HMDB0014956	Propofol	C12H18O	M+H	179.1430	-2.5
	HMDB0029169	(2S,3R)-3-hydroxy-2-methylpentanedioic acid	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0166864	Butanedioic acid, 2-hydroxy-, 1-ethyl ester	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0166863	4-ethoxy-2-hydroxy-4-oxobutanoic acid	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0166862	21583-38	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0158873	2-Hydroxy-2-methylglutaric acid	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0158875	2-hydroxy-4-methylpentanedioic acid	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0158874	2-(hydroxymethyl)pentanedioic acid	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0061362	(2R)-1-(formyloxy)-3-hydroxypropan-2-yl acetate	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0000345	3-Hydroxyadipic acid	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0000368	2(R)-Hydroxyadipic acid	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0059758	2-Hydroxy-2-ethylsuccinic acid	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0000640	Levogluconan	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0000355	3-Hydroxymethylglutaric acid	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0059737	3-Hydroxymethylglutaric acid	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0029934	D-1-Deoxy-erythro-hexo-2,3-diulose	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0032873	Diethyl dicarbonate	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0166857	1,4-dimethyl 2-hydroxybutanedioate	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0000321	2-Hydroxyadipic acid	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0041561	D-1,5-Anhydrofructose	C6H10O5	M+NH4	180.0866	-2.5
	HMDB0002030	Fructosamine	C6H13NO5	M+H	180.0866	-2.5
	HMDB0001514	Glucosamine	C6H13NO5	M+H	180.0866	-2.5
	HMDB0030091	beta-D-Glucosamine	C6H13NO5	M+H	180.0866	-2.5
180.1016	HMDB0146627	3-(2-methoxyphenyl)prop-2-enal	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0135643	3-(4-methoxyphenyl)prop-2-enal	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0141046	4-(4-hydroxyphenyl)but-3-en-2-one	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0177509	2-(4-methoxyphenyl)-3-methylideneoxirane	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0133597	(2Z)-3-(4-hydroxyphenyl)-2-methylprop-2-enal	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0033833	Methyl cinnamate	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0133594	(2E)-2-methyl-3-phenylprop-2-enoic acid	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0133748	(3E)-4-(3-hydroxyphenyl)but-3-en-2-one	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0040592	Allyl benzoate	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0133752	(3Z)-3-hydroxy-4-phenylbut-3-en-2-one	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0133749	(3E)-4-(4-hydroxyphenyl)but-3-en-2-one	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0038893	3,6-Dimethyl-2(3H)-benzofuranone	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0133750	1-(3-phenyloxiran-2-yl)ethan-1-one	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0133751	(3E)-4-(2-hydroxyphenyl)but-3-en-2-one	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0133755	1-phenylbutane-2,3-dione	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0141158	1-hydroxy-4-phenylbut-3-en-2-one	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0032611	3-(4-Methoxyphenyl)-2-propenal	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0151225	AKO17514298	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0157134	2-phenylbut-3-enoic acid	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0133598	2-methyl-3-phenyloxirane-2-carbaldehyde	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0033591	Saffrole	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0060335	1,2-Dihydronaphthalene-1,2-diol	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0133599	(2Z)-3-(2-hydroxyphenyl)-2-methylprop-2-enal	C10H10O2	M+NH4	180.1019	-1.7

	HMDB0133504	4-(3-hydroxyphenyl)but-3-en-2-one	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0133596	(2Z)-3-(3-hydroxyphenyl)-2-methylprop-2-enal	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0033830	Cassiastearoptene	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0040577	Cinnamyl formate	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0133747	(3E)-1-hydroxy-4-phenylbut-3-en-2-one	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0029714	4,5-Dihydro-1-benzoxepin-3(2H)-one	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0133595	(2Z)-2-(hydroxymethyl)-3-phenylprop-2-enal	C10H10O2	M+NH4	180.1019	-1.7
	HMDB0041931	3,4-Methylenedioxyamphetamine	C10H13NO2	M+H	180.1019	-1.7
	HMDB0029223	alpha-Methylphenylalanine	C10H13NO2	M+H	180.1019	-1.7
	HMDB0029224	N-methylphenylalanine	C10H13NO2	M+H	180.1019	-1.7
	HMDB0042012	Salsolinol	C10H13NO2	M+H	180.1019	-1.7
	HMDB0030372	Maltozazine	C10H13NO2	M+H	180.1019	-1.7
	HMDB0040021	2,3-Dihydro-5-(3-hydroxypropanoyl)-1H-pyrrolizine	C10H13NO2	M+H	180.1019	-1.7
	HMDB0033763	Ethyl N-methylantranilate	C10H13NO2	M+H	180.1019	-1.7
	HMDB0001189	2(N)-Methyl-norsalsolinol	C10H13NO2	M+H	180.1019	-1.7
	HMDB0005199	(R)-Salsolinol	C10H13NO2	M+H	180.1019	-1.7
	HMDB0031811	3,5-Dimethylphenyl methylcarbamate	C10H13NO2	M+H	180.1019	-1.7
	HMDB0039655	1,2,3,4,5,6-Hexahydro-5-(1-hydroxyethylidene)-7H-cyclopenta[b]pyridin-7-one	C10H13NO2	M+H	180.1019	-1.7
180.1381	HMDB0033562	3-Methyl-2-phenylbutanal	C11H14O	M+NH4	180.1383	-1.0
	HMDB0036183	4-(4-Methylphenyl)-2-butanone	C11H14O	M+NH4	180.1383	-1.0
	HMDB0041493	4-Isopropylphenylacetaldehyde	C11H14O	M+NH4	180.1383	-1.0
	HMDB0031856	2-Methyl-3-(4-methylphenyl)propanal	C11H14O	M+NH4	180.1383	-1.0
	HMDB0039803	4,4alpha,5,6-Tetrahydro-7-methyl-2(3H)-naphthalenone	C11H14O	M+NH4	180.1383	-1.0
	HMDB0163601	3-Methyl-2-phenyl-3-buten-1-ol	C11H14O	M+NH4	180.1383	-1.0
	HMDB0133676	3-methyl-4-phenylbutan-2-one	C11H14O	M+NH4	180.1383	-1.0
	HMDB0032415	2-Methyl-4-phenylbutyraldehyde	C11H14O	M+NH4	180.1383	-1.0
	HMDB0032025	4'-Isopropylacetophenone	C11H14O	M+NH4	180.1383	-1.0
	HMDB0031208	1-Phenyl-1-pentanone	C11H14O	M+NH4	180.1383	-1.0
	HMDB0040245	2-Methyl-3-(2-methylphenyl)propanal	C11H14O	M+NH4	180.1383	-1.0
	HMDB0014523	Mexiletine	C11H17NO	M+H	180.1383	-1.1
	HMDB0039683	7-Ethyl-2,3,4,5,6,7-hexahydrocyclopent[b]azepin-8(1H)-one	C11H17NO	M+H	180.1383	-1.1
	HMDB0039686	trans-4,5-Dimethyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one	C11H17NO	M+H	180.1383	-1.1
	HMDB0039676	5-Ethyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one	C11H17NO	M+H	180.1383	-1.1
	HMDB0039675	3-Ethyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one	C11H17NO	M+H	180.1383	-1.1
	HMDB0039677	3,4-Dimethyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one	C11H17NO	M+H	180.1383	-1.1
	HMDB0041930	Methoxyphenamine	C11H17NO	M+H	180.1383	-1.1
	HMDB0041932	Methylephedrine	C11H17NO	M+H	180.1383	-1.1
	HMDB0039684	2,3,4,5,6,7-Hexahydro-6,7-dimethylcyclopent[b]azepin-8(1H)-one	C11H17NO	M+H	180.1383	-1.1
180.1590	HMDB0033625	(3R,7R)-1,3,7-Octanetriol	C8H18O3	M+NH4	180.1594	-2.3
181.0620	HMDB0060303	(2-Naphthyl)methanol	C11H10O	M+Na	181.0624	-2.1
	HMDB0060322	1-Hydroxymethylnaphthalene	C11H10O	M+Na	181.0624	-2.1
	HMDB0061285	1-Hydroxymethylnaphthalene	C11H10O	M+Na	181.0624	-2.1
	HMDB0032861	2-Methoxynaphthalene	C11H10O	M+Na	181.0624	-2.1
	HMDB0141019	3-(2-hydroxyphenyl)butanoic acid	C10H12O3	M+H	181.0859	-2.3
	HMDB0135740	3-hydroxy-3-(4-methoxyphenyl)propanal	C10H12O3	M+H	181.0859	-2.3
	HMDB0135739	2-hydroxy-3-(4-methoxyphenyl)propanal	C10H12O3	M+H	181.0859	-2.3
	HMDB0135646	[3-(4-methoxyphenyl)oxiran-2-yl]methanol	C10H12O3	M+H	181.0859	-2.3
	HMDB0135645	2-(3-hydroxyprop-1-en-1-yl)-5-methoxyphenol	C10H12O3	M+H	181.0859	-2.3
	HMDB0135242	2-methoxy-4-(prop-2-en-1-yl)benzene-1,3-diol	C10H12O3	M+H	181.0859	-2.3
	HMDB0135243	4-methoxy-6-(prop-2-en-1-yl)benzene-1,3-diol	C10H12O3	M+H	181.0859	-2.3
	HMDB0135241	2-methoxy-4-[(oxiran-2-yl)methyl]phenol	C10H12O3	M+H	181.0859	-2.3
	HMDB0141020	3-hydroxy-3-phenylbutanoic acid	C10H12O3	M+H	181.0859	-2.3
	HMDB0141022	4-hydroxy-3-phenylbutanoic acid	C10H12O3	M+H	181.0859	-2.3
	HMDB0142085	dimethoxy-4-vinyl phenol	C10H12O3	M+H	181.0859	-2.3
	HMDB0141179	4-hydroxy-4-(4-hydroxyphenyl)butan-2-one	C10H12O3	M+H	181.0859	-2.3
	HMDB0141159	1-hydroxy-4-(4-hydroxyphenyl)butan-2-one	C10H12O3	M+H	181.0859	-2.3
	HMDB0141138	4-(2,4-dihydroxyphenyl)butan-2-one	C10H12O3	M+H	181.0859	-2.3
	HMDB0141118	3-hydroxy-4-(4-hydroxyphenyl)butan-2-one	C10H12O3	M+H	181.0859	-2.3
	HMDB0141021	3-(4-hydroxyphenyl)butanoic acid	C10H12O3	M+H	181.0859	-2.3
	HMDB0141023	2-hydroxy-3-phenylbutanoic acid	C10H12O3	M+H	181.0859	-2.3

HMDB0134076	2-(3-hydroxyprop-1-en-1-yl)-6-methoxyphenol	C10H12O3	M+H	181.0859	-2.3
HMDB0134065	3-(2-hydroxy-3-methoxyphenyl)propanal	C10H12O3	M+H	181.0859	-2.3
HMDB0133505	4-(3,4-dihydroxyphenyl)butan-2-one	C10H12O3	M+H	181.0859	-2.3
HMDB0160084	4-Hydroxy-4-phenyl-butyric acid	C10H12O3	M+H	181.0859	-2.3
HMDB0062773	-hydroxy-(2E,8E)-decadien-4-ynoic acid	C10H12O3	M+H	181.0859	-2.3
HMDB0145926	5-ethenyl-2,3-dimethoxyphenol	C10H12O3	M+H	181.0859	-2.3
HMDB0177512	2-Hydroxy-1-(4-methoxyphenyl)propan-1-one	C10H12O3	M+H	181.0859	-2.3
HMDB0177507	1-(4-methoxyphenyl)prop-1-ene-1,2-diol	C10H12O3	M+H	181.0859	-2.3
HMDB0175295	Formic acid 3-(4-hydroxyphenyl)propyl ester	C10H12O3	M+H	181.0859	-2.3
HMDB0175293	3-hydroxy-3-phenylpropyl formate	C10H12O3	M+H	181.0859	-2.3
HMDB0175292	3-(2-hydroxyphenyl)propyl formate	C10H12O3	M+H	181.0859	-2.3
HMDB0175294	3-(3-hydroxyphenyl)propyl formate	C10H12O3	M+H	181.0859	-2.3
HMDB0175291	2-hydroxy-3-phenylpropyl formate	C10H12O3	M+H	181.0859	-2.3
HMDB0170983	3-methoxy-5-[(1Z)-prop-1-en-1-yl]benzene-1,2-diol	C10H12O3	M+H	181.0859	-2.3
HMDB0177511	1-hydroxy-1-(4-methoxyphenyl)propan-2-one	C10H12O3	M+H	181.0859	-2.3
HMDB0179462	2-(hydroxymethyl)-5-(propan-2-yl)cyclohexa-2,5-diene-1,4-dione	C10H12O3	M+H	181.0859	-2.3
HMDB0182822	4-hydroxybenzyl propionate	C10H12O3	M+H	181.0859	-2.3
HMDB0179726	4-[(1E)-3-methoxyprop-1-en-1-yl]benzene-1,3-diol	C10H12O3	M+H	181.0859	-2.3
HMDB0179727	MolPort19-937-164	C10H12O3	M+H	181.0859	-2.3
HMDB0179728	4-[3-(methoxymethyl)oxiran-2-yl]phenol	C10H12O3	M+H	181.0859	-2.3
HMDB0179463	2-(2-hydroxypropan-2-yl)-5-methylcyclohexa-2,5-diene-1,4-dione	C10H12O3	M+H	181.0859	-2.3
HMDB0179465	1-methyl-4-(propan-2-yl)-7-oxabicyclo[4.1]hept-3-ene-2,5-dione	C10H12O3	M+H	181.0859	-2.3
HMDB0179466	2-(1-hydroxypropan-2-yl)-5-methylcyclohexa-2,5-diene-1,4-dione	C10H12O3	M+H	181.0859	-2.3
HMDB0179464	4-methyl-1-(propan-2-yl)-7-oxabicyclo[4.1]hept-3-ene-2,5-dione	C10H12O3	M+H	181.0859	-2.3
HMDB0170984	SCHEMBL12699	C10H12O3	M+H	181.0859	-2.3
HMDB0170981	2-methoxy-4-[(1Z)-prop-1-en-1-yl]benzene-1,3-diol	C10H12O3	M+H	181.0859	-2.3
HMDB0170982	4-methoxy-6-[(1Z)-prop-1-en-1-yl]benzene-1,3-diol	C10H12O3	M+H	181.0859	-2.3
HMDB0157132	a-methyltropic acid	C10H12O3	M+H	181.0859	-2.3
HMDB0157133	4-hydroxy-2-phenylbutanoic acid	C10H12O3	M+H	181.0859	-2.3
HMDB0147386	BRN 31128	C10H12O3	M+H	181.0859	-2.3
HMDB0146626	[3-(2-methoxyphenyl)oxiran-2-yl]methanol	C10H12O3	M+H	181.0859	-2.3
HMDB0146623	3-hydroxy-3-(2-methoxyphenyl)propanal	C10H12O3	M+H	181.0859	-2.3
HMDB0146625	4-(3-hydroxyprop-1-en-1-yl)-3-methoxyphenol	C10H12O3	M+H	181.0859	-2.3
HMDB0146624	2-(3-hydroxyprop-1-en-1-yl)-3-methoxyphenol	C10H12O3	M+H	181.0859	-2.3
HMDB0146622	2-hydroxy-3-(2-methoxyphenyl)propanal	C10H12O3	M+H	181.0859	-2.3
HMDB0157135	2-hydroxy-2-phenylbutanoic acid	C10H12O3	M+H	181.0859	-2.3
HMDB0160083	3-hydroxy-4-phenylbutanoic acid	C10H12O3	M+H	181.0859	-2.3
HMDB0168433	Acetic acid, hydroxy-, 2-phenylethyl ester	C10H12O3	M+H	181.0859	-2.3
HMDB0168430	beta-Hydroxyphenethyl acetate	C10H12O3	M+H	181.0859	-2.3
HMDB0168431	Benzeneethanol, 3-hydroxy-, 1-acetate	C10H12O3	M+H	181.0859	-2.3
HMDB0166637	638-48-8	C10H12O3	M+H	181.0859	-2.3
HMDB0166612	1,3-Benzodioxole-5-propanol	C10H12O3	M+H	181.0859	-2.3
HMDB0160086	4-(4-HYDROXYPHENYL)BUTANOIC ACID	C10H12O3	M+H	181.0859	-2.3
HMDB0160087	2-hydroxy-4-phenylbutanoic acid	C10H12O3	M+H	181.0859	-2.3
HMDB0160085	4-(3-Hydroxyphenyl)butanoic acid	C10H12O3	M+H	181.0859	-2.3
HMDB0157136	2-hydroxyphenylbutanoic acid	C10H12O3	M+H	181.0859	-2.3
HMDB0131174	3-(4-methoxyphenyl)propanoic acid	C10H12O3	M+H	181.0859	-2.3
HMDB0032640	Ethyl p-anisate	C10H12O3	M+H	181.0859	-2.3
HMDB0037733	Propyl 2-furanacrylate	C10H12O3	M+H	181.0859	-2.3
HMDB0032128	1-(2,4-Dihydroxyphenyl)-1-butanone	C10H12O3	M+H	181.0859	-2.3
HMDB0032574	Propylparaben	C10H12O3	M+H	181.0859	-2.3
HMDB0037602	4-Hydroxy-2,6,6-trimethyl-3-oxo-1,4-cyclohexadiene-1-carboxaldehyde	C10H12O3	M+H	181.0859	-2.3
HMDB0011751	3-Methoxybenzenepropanoic acid	C10H12O3	M+H	181.0859	-2.3
HMDB0029685	4-Ethoxy-3-methoxybenzaldehyde	C10H12O3	M+H	181.0859	-2.3
HMDB0033761	4-Methoxybenzyl acetate	C10H12O3	M+H	181.0859	-2.3
HMDB0060734	3-(3-Hydroxyphenyl)-2-methylpropionic acid	C10H12O3	M+H	181.0859	-2.3
HMDB0012915	Coniferyl alcohol	C10H12O3	M+H	181.0859	-2.3
HMDB0166652	Coniferyl alcohol	C10H12O3	M+H	181.0859	-2.3
HMDB0168432	p-HPEA-AC	C10H12O3	M+H	181.0859	-2.3

	HMDB0032174	Benzaldehyde glyceryl acetal	C10H12O3	M+H	181.0859	-2.3
	HMDB0031240	2-Phenyl-1,3-dioxolane-4-methanol	C10H12O3	M+H	181.0859	-2.3
	HMDB0129958	2-(4-methoxyphenyl)propanoic acid	C10H12O3	M+H	181.0859	-2.3
	HMDB0135240	3-methoxy-5-(prop-2-en-1-yl)benzene-1,2-diol	C10H12O3	M+H	181.0859	-2.3
	HMDB0127492	4-ethenyl-2,6-dimethoxyphenol	C10H12O3	M+H	181.0859	-2.3
	HMDB0146632	3-(2-methoxyphenyl)propanoic acid	C10H12O3	M+H	181.0859	-2.3
181.1219	HMDB0163240	(2E,5Z)-undeca-2,5,-trienoic acid	C11H16O2	M+H	181.1223	-2.2
	HMDB0151242	3-(4-methoxyphenyl)-2-methylpropan-1-ol	C11H16O2	M+H	181.1223	-2.2
	HMDB0164135	4-(4-methoxyphenyl)butan-2-ol	C11H16O2	M+H	181.1223	-2.2
	HMDB0163599	3-methyl-2-phenylbutane-1,3-diol	C11H16O2	M+H	181.1223	-2.2
	HMDB0163600	2-methyl-3-phenylbutane-1,4-diol	C11H16O2	M+H	181.1223	-2.2
	HMDB0176256	2-(3-hydroxy-3-methylbutyl)phenol	C11H16O2	M+H	181.1223	-2.2
	HMDB0176255	4-(3-hydroxy-3-methylbutyl)phenol	C11H16O2	M+H	181.1223	-2.2
	HMDB0176254	3-(3-hydroxy-3-methylbutyl)phenol	C11H16O2	M+H	181.1223	-2.2
	HMDB0176253	3-methyl-1-phenylbutane-1,3-diol	C11H16O2	M+H	181.1223	-2.2
	HMDB0176252	AKO231874	C11H16O2	M+H	181.1223	-2.2
	HMDB0163604	SCHEMBL12872219	C11H16O2	M+H	181.1223	-2.2
	HMDB0163603	SCHEMBL182446	C11H16O2	M+H	181.1223	-2.2
	HMDB0163602	3-methyl-2-phenylbutane-1,2-diol	C11H16O2	M+H	181.1223	-2.2
	HMDB0163605	2-(1-hydroxy-3-methylbutan-2-yl)phenol	C11H16O2	M+H	181.1223	-2.2
	HMDB0059926	2-tert-Butyl-4-hydroxyanisole	C11H16O2	M+H	181.1223	-2.2
	HMDB0059925	3-tert-Butyl-4-hydroxyanisole	C11H16O2	M+H	181.1223	-2.2
	HMDB0036669	(+)-Myrtenyl formate	C11H16O2	M+H	181.1223	-2.2
	HMDB0032468	2-Phenylpropionaldehyde dimethyl acetal	C11H16O2	M+H	181.1223	-2.2
	HMDB0030039	Jasmolone	C11H16O2	M+H	181.1223	-2.2
	HMDB0039957	4-(Butoxymethyl)phenol	C11H16O2	M+H	181.1223	-2.2
	HMDB0035240	Dihydroactinidiolide	C11H16O2	M+H	181.1223	-2.2
	HMDB0030007	2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]nona-3,8-diene	C11H16O2	M+H	181.1223	-2.2
	HMDB0039159	Bovolide	C11H16O2	M+H	181.1223	-2.2
	HMDB0036817	Norecasantalic acid	C11H16O2	M+H	181.1223	-2.2
181.1582	HMDB0038108	cis-Quinceoxepane	C12H20O	M+H	181.1587	-2.7
	HMDB0039590	(2E,4E)-2,4-Dodecadienal	C12H20O	M+H	181.1587	-2.7
	HMDB0039339	Tricycloekasantanol	C12H20O	M+H	181.1587	-2.7
	HMDB0031181	Homodihydrojasmone	C12H20O	M+H	181.1587	-2.7
	HMDB0032531	2-trans-6-cis-Dodecadienal	C12H20O	M+H	181.1587	-2.7
182.0807	HMDB0062774	3-(3-hydroxyphenyl)prop-2-enoic acid	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0125104	3-(3-hydroxyphenyl)prop-2-enoic acid	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0150717	hydroxychromanone	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0062605	methyl phenylglyoxalate	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0128076	3-(4-hydroxyphenyl)prop-2-enoic acid	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0166606	(2Z)-3-(3,4-dihydroxyphenyl)prop-2-enal	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0150720	4-hydroxychroman-2-one	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0150716	2669-94-5	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0150718	974-72-5	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0150719	5-hydroxychroman-2-one	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0150715	7-hydroxychroman-2-one	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0141767	(2E)-3-(3,4-dihydroxyphenyl)prop-2-enal	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0141768	3-(4-hydroxyphenyl)oxirane-2-carbaldehyde	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0134029	3-(2,3-dihydroxyphenyl)prop-2-enal	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0134031	3-(2-hydroxyphenyl)oxirane-2-carbaldehyde	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0134030	3-(2,5-dihydroxyphenyl)prop-2-enal	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0129375	4-methoxy-1-benzofuran-6-ol	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0126545	3-phenyloxirane-2-carboxylic acid	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0062655	Cis-2-coumarate	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0134028	Cis-2-coumarate	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0012225	Enol-phenylpyruvate	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0030677	cis-p-Coumaric acid	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0041592	Coumarinic acid	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0001713	m-Coumaric acid	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0163003	cis-3-coumaric acid	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0002035	4-Hydroxycinnamic acid	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0002641	2-Hydroxycinnamic acid	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0000205	Phenylpyruvic acid	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0031629	Phenylpyruvic acid	C9H8O3	M+NH4	182.0812	-2.6
	HMDB0062148	2-oxo-2-phenylethyl formate	C9H8O3	M+NH4	182.0812	-2.6

	HMDB0185178	4-(2-amino-1-hydroxyprop-2-en-1-yl)benzene-1,2-diol	C9H11NO3	M+H	182.0812	-2.6
	HMDB0164040	SCHEMBL62116	C9H11NO3	M+H	182.0812	-2.6
	HMDB0164039	ethyl 2-(hydroxyamino)benzoate	C9H11NO3	M+H	182.0812	-2.6
	HMDB0162086	8-methyl-1H,3H,4H-pyrano[3,4-c]pyridine-1,4-diol	C9H11NO3	M+H	182.0812	-2.6
	HMDB0162085	8-(hydroxymethyl)-1H,3H,4H-pyrano[3,4-c]pyridin-1-ol	C9H11NO3	M+H	182.0812	-2.6
	HMDB0059720	Meta-Tyrosine	C9H11NO3	M+H	182.0812	-2.6
	HMDB0001119	4-Hydroxy-4-(3-pyridyl)-butanoic acid	C9H11NO3	M+H	182.0812	-2.6
	HMDB0002184	L-Threo-3-Phenylserine	C9H11NO3	M+H	182.0812	-2.6
	HMDB0003831	Beta-Tyrosine	C9H11NO3	M+H	182.0812	-2.6
	HMDB0006050	o-Tyrosine	C9H11NO3	M+H	182.0812	-2.6
	HMDB0060280	4,6,7-Trihydroxy-1,2,3,4-tetrahydroisoquinoline	C9H11NO3	M+H	182.0812	-2.6
	HMDB0000158	L-Tyrosine	C9H11NO3	M+H	182.0812	-2.6
	HMDB0164171	L-Tyrosine	C9H11NO3	M+H	182.0812	-2.6
	HMDB0163595	3-methyl-2-phenylbut-3-enal	C11H12O	M+Na	183.0780	-2.4
	HMDB0038790	3-Phenyl-4-pentenal	C11H12O	M+Na	183.0780	-2.4
183.0776	HMDB0031567	3-Methyl-4-phenyl-3-buten-2-one	C11H12O	M+Na	183.0780	-2.4
	HMDB0035207	2-Phenyl-4-pentenal	C11H12O	M+Na	183.0780	-2.4
	HMDB0000765	Mannitol	C6H14O6	M+H	183.0863	0.5
	HMDB0000247	Sorbitol	C6H14O6	M+H	183.0863	0.5
183.0864	HMDB0000107	Galactitol	C6H14O6	M+H	183.0863	0.5
	HMDB0011632	L-Iditol	C6H14O6	M+H	183.0863	0.5
	HMDB0142086	4-ethyl-2,3-dimethoxyphenol	C10H14O3	M+H	183.1016	-2.6
	HMDB0145930	SCHEMBL83728	C10H14O3	M+H	183.1016	-2.6
183.1011	HMDB0163111	(2E,7Z)-9-hydroxydeca-2,4,7-trienoic acid	C10H14O3	M+H	183.1016	-2.6
	HMDB0163112	3-[(1Z,4Z)-hepta-1,4-dien-1-yl]oxirane-2-carboxylic acid	C10H14O3	M+H	183.1016	-2.6
	HMDB0163114	(2E,4Z)-6-(3-ethyloxiran-2-yl)hexa-2,4-dienoic acid	C10H14O3	M+H	183.1016	-2.6
	HMDB0163113	(2E)-3-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}prop-2-enoic acid	C10H14O3	M+H	183.1016	-2.6
	HMDB0163115	(2E,4Z,7Z)--hydroxydeca-2,4,7-trienoic acid	C10H14O3	M+H	183.1016	-2.6
	HMDB0179479	CTK8G51	C10H14O3	M+H	183.1016	-2.6
	HMDB0179483	2-(1-hydroxypropan-2-yl)-5-methylbenzene-1,4-diol	C10H14O3	M+H	183.1016	-2.6
	HMDB0179482	6-methyl-3-(propan-2-yl)benzene-1,2,4-triol	C10H14O3	M+H	183.1016	-2.6
	HMDB0181697	1-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M+H	183.1016	-2.6
	HMDB0181695	2-(hydroxymethyl)-3-methyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M+H	183.1016	-2.6
	HMDB0181694	3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M+H	183.1016	-2.6
	HMDB0181696	5-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M+H	183.1016	-2.6
	HMDB0179480	2,5-dihydroxy-4-isopropylbenzyl alcohol	C10H14O3	M+H	183.1016	-2.6
	HMDB0179477	6-hydroxy-2-methyl-5-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M+H	183.1016	-2.6
	HMDB0179478	2-hydroxy-2-isopropyl-5-methylcyclohex-5-ene-1,4-dione	C10H14O3	M+H	183.1016	-2.6
	HMDB0179470	4-methyl-1-(propan-2-yl)-7-oxabicyclo[4.1]heptane-2,5-dione	C10H14O3	M+H	183.1016	-2.6
	HMDB0179467	5-(hydroxymethyl)-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M+H	183.1016	-2.6
	HMDB0179469	2-(2-hydroxypropan-2-yl)-5-methylcyclohex-2-ene-1,4-dione	C10H14O3	M+H	183.1016	-2.6
	HMDB0179468	5-hydroxy-5-methyl-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M+H	183.1016	-2.6
	HMDB0179473	2-(hydroxymethyl)-5-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M+H	183.1016	-2.6
	HMDB0179471	2-(1-hydroxypropan-2-yl)-5-methylcyclohex-2-ene-1,4-dione	C10H14O3	M+H	183.1016	-2.6
	HMDB0179472	6-hydroxy-5-methyl-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M+H	183.1016	-2.6
	HMDB0179474	5-(2-hydroxypropan-2-yl)-2-methylcyclohex-2-ene-1,4-dione	C10H14O3	M+H	183.1016	-2.6
	HMDB0179475	1-methyl-4-(propan-2-yl)-7-oxabicyclo[4.1]heptane-2,5-dione	C10H14O3	M+H	183.1016	-2.6

	HMDB0179476	5-(1-hydroxypropan-2-yl)-2-methylcyclohex-2-ene-1,4-dione	C10H14O3	M+H	183.1016	-2.6
	HMDB0036522	Verimol J	C10H14O3	M+H	183.1016	-2.6
	HMDB0059891	Isoamyl 2-furoate	C10H14O3	M+H	183.1016	-2.6
	HMDB0033394	4-Ethyl-2,6-dimethoxyphenol	C10H14O3	M+H	183.1016	-2.6
	HMDB0037641	4-(Ethoxymethyl)-2-methoxyphenol	C10H14O3	M+H	183.1016	-2.6
	HMDB0037727	Furfuryl pentanoate	C10H14O3	M+H	183.1016	-2.6
	HMDB0038354	2-Ethoxy-4-(methoxymethyl)phenol	C10H14O3	M+H	183.1016	-2.6
	HMDB0032607	threo-Anethole glycol	C10H14O3	M+H	183.1016	-2.6
	HMDB0038181	Peperinic acid	C10H14O3	M+H	183.1016	-2.6
	HMDB0029456	Amyl 2-furoate	C10H14O3	M+H	183.1016	-2.6
	HMDB0039874	Furfuryl isovalerate	C10H14O3	M+H	183.1016	-2.6
	HMDB0179481	4427-54-7	C10H14O3	M+H	183.1016	-2.6
183.1375	HMDB0163226	(2E,5Z)-11-hydroxyundeca-2,5-dienal	C11H18O2	M+H	183.1380	-2.5
	HMDB0163225	(2E)-4-(3-pentylloxiran-2-yl)but-2-enal	C11H18O2	M+H	183.1380	-2.5
	HMDB0163224	3-[(2Z)-oct-2-en-1-yl]oxirane-2-carbaldehyde	C11H18O2	M+H	183.1380	-2.5
	HMDB0163223	(2E,5Z)--hydroxyundeca-2,5-dienal	C11H18O2	M+H	183.1380	-2.5
	HMDB0163222	(2E,5Z)-7-hydroxyundeca-2,5-dienal	C11H18O2	M+H	183.1380	-2.5
	HMDB0163221	(2E,5Z)-undeca-2,5-dienoic acid	C11H18O2	M+H	183.1380	-2.5
	HMDB0034708	Methyl 4,8-decadienoate	C11H18O2	M+H	183.1380	-2.5
	HMDB0030006	2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]non-3-ene	C11H18O2	M+H	183.1380	-2.5
	HMDB0036215	Ethyl octynecarboxylate	C11H18O2	M+H	183.1380	-2.5
	HMDB0038079	(2E,6Z)-2,6-Nonadien-1-yl acetate	C11H18O2	M+H	183.1380	-2.5
	HMDB0030424	Linalyl formate	C11H18O2	M+H	183.1380	-2.5
	HMDB0037388	Tsibulin 2	C11H18O2	M+H	183.1380	-2.5
	HMDB0034730	Methyl (2E,4Z)-decadienoate	C11H18O2	M+H	183.1380	-2.5
	HMDB0040595	Allyl cyclohexylacetate	C11H18O2	M+H	183.1380	-2.5
	HMDB0037829	6-(3-Hexenyl)tetrahydro-2H-pyran-2-one	C11H18O2	M+H	183.1380	-2.5
	HMDB0036191	4-Hydroxy-4-methyl-7-decenoic acid gamma-lactone	C11H18O2	M+H	183.1380	-2.5
	HMDB0035156	Neryl formate	C11H18O2	M+H	183.1380	-2.5
	HMDB0038068	(3E,6Z)-Nonadien-1-yl acetate	C11H18O2	M+H	183.1380	-2.5
	HMDB0038245	Bornyl formate	C11H18O2	M+H	183.1380	-2.5
	HMDB0038279	cis-3-Hexenyl tiglate	C11H18O2	M+H	183.1380	-2.5
	HMDB0059816	Methyl geranate	C11H18O2	M+H	183.1380	-2.5
	HMDB0032463	5-Pentyl-3h-furan-2-one	C11H18O2	M+H	183.1380	-2.5
	HMDB0032050	alpha-Terpineol formate	C11H18O2	M+H	183.1380	-2.5
	HMDB0038005	xi-2-Hexyl-5-methyl-3(2H)-furanone	C11H18O2	M+H	183.1380	-2.5
183.1739	HMDB0032279	2-Ethyl-1,3,3-trimethyl-2-norbornanol	C12H22O	M+H	183.1743	-2.4
	HMDB0038972	(E)-2-Butyl-2-octenal	C12H22O	M+H	183.1743	-2.4
	HMDB0031102	(Z,Z)-3,6-Dodecadien-1-ol	C12H22O	M+H	183.1743	-2.4
	HMDB0031020	2-Dodecenal	C12H22O	M+H	183.1743	-2.4
	HMDB0036461	Geosmin	C12H22O	M+H	183.1743	-2.4
	HMDB0031341	Cyclododecanone	C12H22O	M+H	183.1743	-2.4
184.0728	HMDB0032542	trans- and cis-2,4,8-Trimethyl-3,7-nona-dien-2-ol	C12H22O	M+H	183.1743	-2.4
	HMDB0040048	3,4-Dihydro-4-[(5-methyl-2-furanyl)methylene]-2H-pyrrole	C10H11NO	M+Na	184.0733	-2.6
	HMDB0003447	Tryptophol	C10H11NO	M+Na	184.0733	-2.6
	HMDB0030267	(R)-Boschniakine	C10H11NO	M+Na	184.0733	-2.6
	HMDB0040028	1-(2,3-Dihydro-1H-pyrrolizin-5-yl)-2-propen-1-one	C10H11NO	M+Na	184.0733	-2.6
	HMDB0040042	3-[(5-Methyl-2-furanyl)methyl]-1H-pyrrole	C10H11NO	M+Na	184.0733	-2.6
184.0813	HMDB0000539	Arabinonic acid	C5H10O6	M+NH4	184.0816	-1.4
	HMDB0060255	欽婁-欽婁yxonic acid	C5H10O6	M+NH4	184.0816	-1.4
	HMDB0060256	欽婁-Xylonic acid	C5H10O6	M+NH4	184.0816	-1.4
	HMDB0000867	Ribonic acid	C5H10O6	M+NH4	184.0816	-1.4
	HMDB0059750	欽婦-欽婦ylonic acid	C5H10O6	M+NH4	184.0816	-1.4
	HMDB0041584	3-Hydroxy-p-mentha-1,8-dien-7-al	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0163095	3-[(1Z,4Z)-hepta-1,4-dien-1-yl]oxirane-2-carbaldehyde	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0163098	(4Z,7Z)--hydroxydeca-2,4,7-trienal	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0163096	4,5-epoxy-(e,z)-2,7-decadienal	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0179460	NSC143559	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0179459	5-methyl-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0180472	2-(4-methylphenyl)propane-1,2-diol	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0180474	p-Cymene-9,-diol	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0180473	2-[4-(hydroxymethyl)phenyl]propan-1-ol	C10H14O2	M+NH4	184.1332	-2.7

184.1327	HMDB0181685	3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0181689	4-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0181688	1-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0181686	2-(hydroxymethyl)-3-methyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0181687	5-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0163097	(2E,4Z)-6-(3-ethyloxiran-2-yl)hexa-2,4-dienal	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0163094	(2E,7Z)-9-hydroxydeca-2,4,7-trienal	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0163093	SCHEMBL36924	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0062603	2-(4-methoxyphenyl)propan-2-ol	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0127496	1-ethyl-3,5-dimethoxybenzene	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0135742	3-(4-methoxyphenyl)propan-1-ol	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0146631	3-(2-methoxyphenyl)propan-1-ol	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0036878	1,4-Epidioxy-p-mentha-2,8-diene	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0032615	1,1-Dimethoxy-2-phenylethane	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0037044	Rotundifolone	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0037012	2-Hydroxy-p-mentha-1,8-dien-6-one	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0040176	4-Ethyl-1,2-dimethoxybenzene	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0032462	Pentyl 2-furyl ketone	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0035328	Perilla ketone	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0035063	Epinepetalactone	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0004586	Perillic acid	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0032135	2-Methoxy-4-propylphenol	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0036042	Marmelolactone A	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0034922	alpha-Teresantalic acid	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0039382	(1xi,4xi,6xi)-Carvone oxide	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0041000	Karahana lactone	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0032062	2-tert-Butyl-1,4-benzenediol	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0037011	5-Hydroxy-p-mentha-6,8-dien-2-one	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0031085	6-Pentyl-2H-pyran-2-one	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0029691	Wine lactone	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0036084	Isomintlactone	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0035235	2,4,7-Decatrienoic acid	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0036879	1,2:3,4-Diepoxyp-menth-8-ene	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0179461	2-methyl-5-(propan-2-yl)benzene-1,4-diol	C10H14O2	M+NH4	184.1332	-2.7
	HMDB0015239	Methyprylon	C10H17NO2	M+H	184.1332	-2.7
185.0318	HMDB0032927	Quinoxin	C8H6N2O2	M+Na	185.0321	-1.9
185.0682	HMDB0001297	Norcotinine	C9H10N2O	M+Na	185.0685	-1.8
185.0808	HMDB0240350	4-(2-Hydroxyethoxy)-2-methoxyphenol	C9H12O4	M+H	185.0808	-0.2
	HMDB0180894	4-(1-hydroxyethyl)-5-methoxybenzene-1,3-diol	C9H12O4	M+H	185.0808	-0.2
	HMDB0151525	4-(hydroxymethyl)-5-methoxy-6-methylbenzene-1,3-diol	C9H12O4	M+H	185.0808	-0.2
	HMDB0151526	5-methoxy-4,6-dimethylbenzene-1,2,3-triol	C9H12O4	M+H	185.0808	-0.2
	HMDB0131235	dimethoxy-methyl-hydroquinone	C9H12O4	M+H	185.0808	-0.2
	HMDB0131234	4,6-dimethoxy-3-methylbenzene-1,2-diol	C9H12O4	M+H	185.0808	-0.2
	HMDB0131233	2-(hydroxymethyl)-3,5-dimethoxyphenol	C9H12O4	M+H	185.0808	-0.2
	HMDB0126620	6-methoxy-3,5-dimethylbenzene-1,2,4-triol	C9H12O4	M+H	185.0808	-0.2
	HMDB0126619	4-(hydroxymethyl)-5-methoxy-2-methylbenzene-1,3-diol	C9H12O4	M+H	185.0808	-0.2
	HMDB0126618	2-(hydroxymethyl)-5-methoxy-4-methylbenzene-1,3-diol	C9H12O4	M+H	185.0808	-0.2
	HMDB0125597	5-ethyl-3-methoxybenzene-1,2,4-triol	C9H12O4	M+H	185.0808	-0.2
	HMDB0125593	4-ethyl-6-methoxybenzene-1,2,3-triol	C9H12O4	M+H	185.0808	-0.2
	HMDB0180032	syringyl alcohol	C9H12O4	M+H	185.0808	-0.2
	HMDB0059730	3,4-Methylenepimelic acid	C9H12O4	M+H	185.0808	-0.2
	HMDB0039650	4-Formyl-3-(formylmethyl)-4-hexenoic acid	C9H12O4	M+H	185.0808	-0.2
	HMDB0036072	Genipic acid	C9H12O4	M+H	185.0808	-0.2
	HMDB0035056	1-(3-Hydroxy-4-methoxyphenyl)-1,2-ethanediol	C9H12O4	M+H	185.0808	-0.2
	HMDB0040603	threo-1-(4-Hydroxyphenyl)-1,2,3-propanetriol	C9H12O4	M+H	185.0808	-0.2
	HMDB0001490	Vanylglycol	C9H12O4	M+H	185.0808	-0.2
	HMDB0040245	2-Methyl-3-(2-methylphenyl)propanal	C11H14O	M+Na	185.0937	-1.0

185.0935	HMDB0133676	3-methyl-4-phenylbutan-2-one	C11H14O	M+Na	185.0937	-1.0
	HMDB0163601	3-Methyl-2-phenyl-3-buten-1-ol	C11H14O	M+Na	185.0937	-1.0
	HMDB0032415	2-Methyl-4-phenylbutyraldehyde	C11H14O	M+Na	185.0937	-1.0
	HMDB0033562	3-Methyl-2-phenylbutanal	C11H14O	M+Na	185.0937	-1.0
	HMDB0039803	4,4alpha,5,6-Tetrahydro-7-methyl-2(3H)-naphthalenone	C11H14O	M+Na	185.0937	-1.0
	HMDB0031856	2-Methyl-3-(4-methylphenyl)propanal	C11H14O	M+Na	185.0937	-1.0
	HMDB0032025	4'-Isopropylacetophenone	C11H14O	M+Na	185.0937	-1.0
	HMDB0031208	1-Phenyl-1-pentanone	C11H14O	M+Na	185.0937	-1.0
	HMDB0036183	4-(4-Methylphenyl)-2-butanone	C11H14O	M+Na	185.0937	-1.0
	HMDB0041493	4-Isopropylphenylacetaldehyde	C11H14O	M+Na	185.0937	-1.0
185.1167	HMDB0131084	(5E)-2,2,5-trimethyl-7-oxohept-5-enoic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0176282	6-hydroxy-1-(hydroxymethyl)-7,7-dimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M+H	185.1172	-2.8
	HMDB0179401	(2E,4Z)-9-hydroxydeca-2,4-dienoic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0179402	3-[(1Z)-hept-1-en-1-yl]oxirane-2-carboxylic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0179404	(2E,4Z)--hydroxydeca-2,4-dienoic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0179403	SCHEMBL12833	C10H16O3	M+H	185.1172	-2.8
	HMDB0182627	2-[2-(hydroxymethyl)-2,3-dimethylcyclopent-3-en-1-yl]acetic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0182628	2-[3-(hydroxymethyl)-2,2-dimethylcyclopent-3-en-1-yl]acetic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0182629	SCHEMBL5986763	C10H16O3	M+H	185.1172	-2.8
	HMDB0182630	2-{1,2,2-trimethyl-6-oxabicyclo[3.1]hexan-3-yl}acetic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0182631	SCHEMBL59867	C10H16O3	M+H	185.1172	-2.8
	HMDB0179400	(4Z)-6-hydroxydeca-2,4-dienoic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0178775	(4Z,8Z)-2-hydroxydeca-4,8-dienoic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0178771	(4Z,8Z)-3-hydroxydeca-4,8-dienoic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0176283	1-Methyl-6-hydroxy-7-methyl-7-(hydroxymethyl)norbornane-2-one	C10H16O3	M+H	185.1172	-2.8
	HMDB0176284	6,6-dihydroxy-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M+H	185.1172	-2.8
	HMDB0176286	3,6-dihydroxy-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M+H	185.1172	-2.8
	HMDB0176285	5,6-dihydroxy-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M+H	185.1172	-2.8
	HMDB0178769	(4Z,8Z)-7-hydroxydeca-4,8-dienoic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0178770	(4Z,8Z)--hydroxydeca-4,8-dienoic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0178773	(4Z)-7-(3-methyloxiran-2-yl)hept-4-enoic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0178772	(4Z,8Z)-6-hydroxydeca-4,8-dienoic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0178774	3-{3-[(3Z)-pent-3-en-1-yl]oxiran-2-yl}propanoic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0039052	(4S,8R)-8,9-Dihydroxy-p-menth-1(6)-en-2-one	C10H16O3	M+H	185.1172	-2.8
	HMDB0040883	(E)-Oxo-8-decenoic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0036117	(1'R)-Nepetalic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0036998	(S)-Oleuropeic acid	C10H16O3	M+H	185.1172	-2.8
	HMDB0039710	1-Acetylcyclohexyl acetate	C10H16O3	M+H	185.1172	-2.8
	HMDB0163230	4-(3-pentyloxiran-2-yl)butanal	C11H20O2	M+H	185.1536	-2.7
	HMDB0163228	(5Z)-4-hydroxyundec-5-enal	C11H20O2	M+H	185.1536	-2.7
	HMDB0163854	6-hydroxyundec--en-2-one	C11H20O2	M+H	185.1536	-2.7
	HMDB0163855	5-hydroxyundec--en-2-one	C11H20O2	M+H	185.1536	-2.7
	HMDB0163860	1-hydroxyundec--en-2-one	C11H20O2	M+H	185.1536	-2.7
	HMDB0163857	SCHEMBL11481214	C11H20O2	M+H	185.1536	-2.7
	HMDB0163859	3-hydroxyundec--en-2-one	C11H20O2	M+H	185.1536	-2.7
	HMDB0163858	9-(oxiran-2-yl)nonan-2-one	C11H20O2	M+H	185.1536	-2.7
	HMDB0175165	SCHEMBL15641446	C11H20O2	M+H	185.1536	-2.7
	HMDB0180766	(2E)-11-hydroxyundec-2-enal	C11H20O2	M+H	185.1536	-2.7
	HMDB0180763	4-Hydroxy-2-undecenal	C11H20O2	M+H	185.1536	-2.7
	HMDB0180765	3-octyloxirane-2-carbaldehyde	C11H20O2	M+H	185.1536	-2.7
	HMDB0180764	(2E)--hydroxyundec-2-enal	C11H20O2	M+H	185.1536	-2.7
	HMDB0163853	7-hydroxyundec--en-2-one	C11H20O2	M+H	185.1536	-2.7
	HMDB0163856	4-hydroxyundec--en-2-one	C11H20O2	M+H	185.1536	-2.7
	HMDB0163227	(5Z)-7-hydroxyundec-5-enal	C11H20O2	M+H	185.1536	-2.7
	HMDB0163229	(5Z)--hydroxyundec-5-enal	C11H20O2	M+H	185.1536	-2.7
	HMDB0163234	(2E,5Z)-undeca-2,5-diene-1,-diol	C11H20O2	M+H	185.1536	-2.7

185.1531	HMDB0163231	(5Z)-11-hydroxyundec-5-enal	C11H20O2	M+H	185.1536	-2.7
	HMDB0163233	(2E,5Z)-undeca-2,5-diene-1,7-diol	C11H20O2	M+H	185.1536	-2.7
	HMDB0163232	(5Z)-2-hydroxyundec-5-enal	C11H20O2	M+H	185.1536	-2.7
	HMDB0163235	{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}methanol	C11H20O2	M+H	185.1536	-2.7
	HMDB0163237	(2E,5Z)-undeca-2,5-diene-1,11-diol	C11H20O2	M+H	185.1536	-2.7
	HMDB0163236	(2E)-4-(3-pentylloxiran-2-yl)but-2-en-1-ol	C11H20O2	M+H	185.1536	-2.7
	HMDB0163245	5Z-undecenoic acid	C11H20O2	M+H	185.1536	-2.7
	HMDB0163852	8-hydroxyundec--en-2-one	C11H20O2	M+H	185.1536	-2.7
	HMDB0038311	xi-gamma-Undecalactone	C11H20O2	M+H	185.1536	-2.7
	HMDB0038273	2-Hexenyl valerate	C11H20O2	M+H	185.1536	-2.7
	HMDB0038278	cis-3-Hexenyl 3-methylbutanoate	C11H20O2	M+H	185.1536	-2.7
	HMDB0032308	(E)-3-Heptenyl 2-methylpropanoate	C11H20O2	M+H	185.1536	-2.7
	HMDB0036784	6-Hexyltetrahydro-2H-pyran-2-one	C11H20O2	M+H	185.1536	-2.7
	HMDB0034428	Cyclohexyl 3-methylbutanoate	C11H20O2	M+H	185.1536	-2.7
	HMDB0034429	Cyclohexyl pentanoate	C11H20O2	M+H	185.1536	-2.7
	HMDB0037225	Methyl citronellate	C11H20O2	M+H	185.1536	-2.7
	HMDB0033724	Undecylenic acid	C11H20O2	M+H	185.1536	-2.7
	HMDB0038277	cis-3-Hexenyl 2-methylbutanoate	C11H20O2	M+H	185.1536	-2.7
	HMDB0040593	2-Propenyl octanoate	C11H20O2	M+H	185.1536	-2.7
	HMDB0037185	Rhodinyl formate	C11H20O2	M+H	185.1536	-2.7
	HMDB0038274	2-Hexenyl isovalerate	C11H20O2	M+H	185.1536	-2.7
	HMDB0031843	2,3-Undecanedione	C11H20O2	M+H	185.1536	-2.7
	HMDB0031062	(Z)-3-Methyl-3-decenoic acid	C11H20O2	M+H	185.1536	-2.7
	HMDB0031272	Ethyl (E)-2-nonenoate	C11H20O2	M+H	185.1536	-2.7
	HMDB0031063	(Z)-3-Methyl-4-decenoic acid	C11H20O2	M+H	185.1536	-2.7
	HMDB0031087	trans-2-Hexyl-1-cyclopropaneacetic acid	C11H20O2	M+H	185.1536	-2.7
	HMDB0033371	Citronellyl formate	C11H20O2	M+H	185.1536	-2.7
	HMDB0037106	(x)-1-Nonen-3-yl acetate	C11H20O2	M+H	185.1536	-2.7
	HMDB0036140	5-Hexyldihydro-5-methyl-2(3H)-furanone	C11H20O2	M+H	185.1536	-2.7
	HMDB0031691	cis-3-Hexenyl pentanoate	C11H20O2	M+H	185.1536	-2.7
	HMDB0031406	Ethyl 3-cyclohexylpropionate	C11H20O2	M+H	185.1536	-2.7
	HMDB0038906	5-Octenyl propanoate	C11H20O2	M+H	185.1536	-2.7
	HMDB0037309	5-Hexyldihydro-4-methyl-2(3H)-furanone	C11H20O2	M+H	185.1536	-2.7
	HMDB0032396	Methyl 2-decenoate	C11H20O2	M+H	185.1536	-2.7
	HMDB0032453	cis-3-Octenyl propionate	C11H20O2	M+H	185.1536	-2.7
	HMDB0032320	3-Hexenyl 2-methylbutyrate	C11H20O2	M+H	185.1536	-2.7
	HMDB0032534	trans-2-Hexenyl 2-methylbutyrate	C11H20O2	M+H	185.1536	-2.7
	HMDB0032461	Pent-2-enyl hexanoate	C11H20O2	M+H	185.1536	-2.7
	HMDB0032404	6-Methyl-5-hepten-2-one propyleneglycol acetal	C11H20O2	M+H	185.1536	-2.7
	HMDB0032489	Prenyl caproate	C11H20O2	M+H	185.1536	-2.7
	HMDB0062090	butyl cyclohexanecarboxylate	C11H20O2	M+H	185.1536	-2.7
186.0076	HMDB0174563	2-[(methylsulfanyl)disulfanyl]methyl}oxirane	C4H8OS3	M+NH4	186.0076	0.3
186.0158	HMDB0000263	Phosphoenolpyruvic acid	C3H5O6P	M+NH4	186.0162	-2.1
	HMDB0001721	DL-O-Phosphoserine	C3H8NO6P	M+H	186.0162	-2.2
186.0351	HMDB0000272	Phosphoserine	C3H8NO6P	M+H	186.0162	-2.2
	HMDB0015320	Desflurane	C3H2F6O	M+NH4	186.0348	1.6
	HMDB0060648	Hexafluoroisopropanol	C3H2F6O	M+NH4	186.0348	1.6
	HMDB0172360	benzyl(cyano)methylsulfanium	C9H10NS	M+Na	186.0348	1.7
	HMDB0040034	2-Ethylbenzothiazole	C9H9NS	M+Na	186.0348	1.7
186.1120	HMDB0038445	1-Isothiocyanato-2-phenylethane	C9H9NS	M+Na	186.0348	1.7
	HMDB0131223	3,5-dimethoxy-2-methylphenol	C9H12O3	M+NH4	186.1125	-2.5
	HMDB0168685	2-(4-(Hydroxymethyl)phenoxy)ethanol	C9H12O3	M+NH4	186.1125	-2.5
	HMDB0151518	SCHEMBL1954	C9H12O3	M+NH4	186.1125	-2.5
	HMDB0126600	5-methoxy-2,4-dimethylbenzene-1,3-diol	C9H12O3	M+NH4	186.1125	-2.5
	HMDB0125541	4-ethyl-2-methoxybenzene-1,3-diol	C9H12O3	M+NH4	186.1125	-2.5
	HMDB0125531	5-ethyl-3-methoxybenzene-1,2-diol	C9H12O3	M+NH4	186.1125	-2.5
	HMDB0125521	4-ethyl-6-methoxybenzene-1,3-diol	C9H12O3	M+NH4	186.1125	-2.5
	HMDB0059963	1,3,5-Trimethoxybenzene	C9H12O3	M+NH4	186.1125	-2.5
	HMDB0032252	Epoxyoxophorone	C9H12O3	M+NH4	186.1125	-2.5
	HMDB0030473	1-Ipomeanol	C9H12O3	M+NH4	186.1125	-2.5
	HMDB0038925	(4-Hydroxy-3-methoxyphenyl)ethanol	C9H12O3	M+NH4	186.1125	-2.5
	HMDB0030472	4-Ipomeanol	C9H12O3	M+NH4	186.1125	-2.5
	HMDB0029680	2,6-Dimethoxy-4-methylphenol	C9H12O3	M+NH4	186.1125	-2.5
	HMDB0037729	2-Furanylmethyl butanoate	C9H12O3	M+NH4	186.1125	-2.5
	HMDB0032921	Ethyl 2-furanpropionate	C9H12O3	M+NH4	186.1125	-2.5

	HMDB0006548	Ecgonine	C9H15NO3	M+H	186.1125	-2.5
	HMDB0006348	Pseudoecgonine	C9H15NO3	M+H	186.1125	-2.5
	HMDB0094730	2-[(1-hydroxyhept-4-en-1-ylidene)amino]acetic acid	C9H15NO3	M+H	186.1125	-2.5
	HMDB0094731	2-[(1-hydroxyhept-5-en-1-ylidene)amino]acetic acid	C9H15NO3	M+H	186.1125	-2.5
	HMDB0094728	2-amino-3-oxonon-4-enoic acid	C9H15NO3	M+H	186.1125	-2.5
186.1484	HMDB0094729	2-[(1-hydroxyhept-3-en-1-ylidene)amino]acetic acid	C9H15NO3	M+H	186.1125	-2.5
	HMDB0169534	geranic acid	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0176281	6-hydroxycamphor	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182618	2-hydroxy-2-(2,2,3-trimethylcyclopent-3-en-1-yl)acetaldehyde	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182617	25435-53-4	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0181690	[3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptan-3-yl]methanol	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0181692	7-(hydroxymethyl)-1,7-dimethyltricyclo[2.2.1,heptan-3-ol	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0181691	[7-(hydroxymethyl)-7-methyltricyclo[2.2.1,heptan-1-yl]methanol	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0181693	3-(hydroxymethyl)-2,3-dimethyltricyclo[2.2.1,heptan-1-ol	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0181639	5-(1-hydroxypropan-2-yl)-2-methylbicyclo[3.1]hex-3-en-2-ol	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0181638	2-methyl-5-(propan-2-yl)bicyclo[3.1]hex-3-ene-2,6-	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0181637	2-methyl-5-(propan-2-yl)bicyclo[3.1]hex-3-ene-1,2-	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0181636	5-methyl-1-(propan-2-yl)-3-oxatricyclo[4.1,heptan-5-ol	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182620	2-[3-(hydroxymethyl)-2,2-dimethylcyclopent-3-en-1-yl]acetaldehyde	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182621	SCHEMBL14359771	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182619	2-[2-(hydroxymethyl)-2,3-dimethylcyclopent-3-en-1-yl]acetaldehyde	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0240639	(1S,4R,6R)-1,3,3-Trimethyl-6-hydroxybicyclo[2.2.1]heptane-2-one	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182798	(1S,4R,6S)-1,3,3-Trimethyl-6-hydroxybicyclo[2.2.1]heptane-2-one	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182796	3-(hydroxymethyl)-1,3-dimethylbicyclo[2.2.1]heptan-2-one	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182797	7-hydroxy-1,3,3-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182799	5-hydroxy-1,3,3-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182685	6-Hydroxycarvotanacetone	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182684	SCHEMBL6689811	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182683	1-methyl-4-(propan-2-yl)-7-oxabicyclo[4.1]heptan-2-one	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182680	2-(hydroxymethyl)-5-(propan-2-yl)cyclohex-2-en-1-	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0181635	5-(2-hydroxypropan-2-yl)-2-methylbicyclo[3.1]hex-3-en-2-ol	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0181634	2-(hydroxymethyl)-5-(propan-2-yl)bicyclo[3.1]hex-3-en-2-ol	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0163102	(4Z)-6-(3-ethyloxiran-2-yl)hex-4-enal	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0163100	(7Z)-9-hydroxydeca-4,7-dienal	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182795	ACMC-mnp1	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0136694	6-hydroxy-3,7-dimethylocta-2,7-dienal	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0163099	(4Z,7Z)-3-hydroxydeca-4,7-dienal	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0163101	3-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}propanal	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0163103	(4Z,7Z)--hydroxydeca-4,7-dienal	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0179485	14-64-6	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0179394	2E,4Z-decadienoic acid	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0178761	SCHEMBL7756279	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0163117	(z,z)-4,7-decadienoic acid	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0163109	(2E)-3-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}prop-2-en-1-ol	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0163108	{3-[(1Z,4Z)-hepta-1,4-dien-1-yl]oxiran-2-yl}methanol	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0163110	(2E,4Z)-6-(3-ethyloxiran-2-yl)hexa-2,4-dien-1-ol	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0163104	(4Z,7Z)-2-hydroxydeca-4,7-dienal	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0163106	(4Z,7Z)-deca-2,4,7-triene-1,-diol	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0163105	(2E,7Z)-deca-2,4,7-triene-1,9-diol	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182681	8-Hydroxycarvotanacetone	C10H16O2	M+NH4	186.1489	-2.4

	HMDB0032313	2,4-Hexadienyl isobutyrate	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0033700	(-)-(Z)-Tetrahydro-6-(2-pentenyl)-2H-pyran-2-one	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0031273	Methyl octynecarboxylate	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0031156	Ethyl (4Z)-4,7-octadienoate	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0035714	Epoxypartemisia ketone	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0040639	(xi)-(Z)-5-(3-Hexenyl)dihydro-2(3H)-furanone	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0037175	4-Isopropyl-3-cyclohexene-1-carboxylic acid	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0036067	Epoxycampholenic aldehyde	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0037821	xi-1,8,8-Trimethyl-2-oxabicyclo[3.2.1]octan-3-one	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0034452	5,6-Dihydro-6-pentyl-2H-pyran-2-one	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0036103	Geranic acid	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0035766	Ascaridole	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0032312	2,4-Hexadienyl butyrate	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0032219	(+/-)-Dihydromintlactone	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0032319	cis-3-Hexenyl crotonate	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0032434	(+/-)-2-(5-Methyl-5-vinyltetrahydrofuran-2-yl)propionaldehyde	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0035829	Dihydronepetalactone	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0034670	6-Hydroxy-2,6-dimethyl-2,7-octadien-4-one	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0037014	gamma-Diosphenol	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0013105	trans-4,5-epoxy-2(E)-decenal	C10H16O2	M+NH4	186.1489	-2.4
	HMDB0182682	4-hydroxy-2-methyl-5-(propan-2-yl)cyclohex-2-en-1-one	C10H16O2	M+NH4	186.1489	-2.4
186.1848	HMDB0040247	2-Undecenal	C11H20O	M+NH4	186.1852	-2.4
	HMDB0163219	(Z)-5-Undecenal	C11H20O	M+NH4	186.1852	-2.4
	HMDB0163220	(2E,5Z)-2,5-undecadien-1-ol	C11H20O	M+NH4	186.1852	-2.4
	HMDB0035417	(1R,2R)-1,2,7,7-Tetramethylbicyclo[2.2.1]heptan-2-ol	C11H20O	M+NH4	186.1852	-2.4
	HMDB0033577	-Undecen-2-one	C11H20O	M+NH4	186.1852	-2.4
	HMDB0031128	-Undecenal	C11H20O	M+NH4	186.1852	-2.4
	HMDB0037807	9-Undecenal	C11H20O	M+NH4	186.1852	-2.4
	HMDB0032238	(+/-)-trans- and cis-4,8-Dimethyl-3,7-nonadien-2-ol	C11H20O	M+NH4	186.1852	-2.4
	HMDB0061995	2-Methyl-3-decen-5-one	C11H20O	M+NH4	186.1852	-2.4
187.0730	HMDB0041612	Phenyl butyrate	C10H12O2	M+Na	187.0729	0.3
	HMDB0133727	3-[(1E)-3-hydroxybut-1-en-1-yl]phenol	C10H12O2	M+Na	187.0729	0.3
	HMDB0133725	(3E)-4-phenylbut-3-ene-1,2-diol	C10H12O2	M+Na	187.0729	0.3
	HMDB0133728	4-(4-Hydroxyphenyl)-3-buten-2-ol	C10H12O2	M+Na	187.0729	0.3
	HMDB0133729	1-(3-phenyloxiran-2-yl)ethan-1-ol	C10H12O2	M+Na	187.0729	0.3
	HMDB0133753	1-hydroxy-4-phenylbutan-2-one	C10H12O2	M+Na	187.0729	0.3
	HMDB0133754	4-hydroxy-4-phenylbutan-2-one	C10H12O2	M+Na	187.0729	0.3
	HMDB0135737	3-(4-methoxyphenyl)propanal	C10H12O2	M+Na	187.0729	0.3
	HMDB0146615	3-(2-methoxyphenyl)propanal	C10H12O2	M+Na	187.0729	0.3
	HMDB0146616	2-Propen-1-ol, 3-(2-methoxyphenyl)-	C10H12O2	M+Na	187.0729	0.3
	HMDB0151234	AKO17888443	C10H12O2	M+Na	187.0729	0.3
	HMDB0170842	Estragole oxide	C10H12O2	M+Na	187.0729	0.3
	HMDB0179484	2-methyl-5-(prop-1-en-2-yl)benzene-1,4-diol	C10H12O2	M+Na	187.0729	0.3
	HMDB0179725	SCHEMBL1438714	C10H12O2	M+Na	187.0729	0.3
	HMDB0133617	2-methyl-3-phenylpropanoic acid	C10H12O2	M+Na	187.0729	0.3
	HMDB0133610	2-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]phenol	C10H12O2	M+Na	187.0729	0.3
	HMDB0133609	(2-methyl-3-phenyloxiran-2-yl)methanol	C10H12O2	M+Na	187.0729	0.3
	HMDB0127494	1-ethenyl-3,5-dimethoxybenzene	C10H12O2	M+Na	187.0729	0.3
	HMDB0133507	4-(3-hydroxyphenyl)butan-2-one	C10H12O2	M+Na	187.0729	0.3
	HMDB0133600	2-hydroxy-2-methyl-3-phenylpropanal	C10H12O2	M+Na	187.0729	0.3
	HMDB0133603	3-hydroxy-2-methyl-3-phenylpropanal	C10H12O2	M+Na	187.0729	0.3
	HMDB0133601	2-benzyl-3-hydroxypropanal	C10H12O2	M+Na	187.0729	0.3
	HMDB0133607	3-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]phenol	C10H12O2	M+Na	187.0729	0.3
	HMDB0133604	3-(3-hydroxyphenyl)-2-methylpropanal	C10H12O2	M+Na	187.0729	0.3
	HMDB0133605	3-(4-hydroxyphenyl)-2-methylpropanal	C10H12O2	M+Na	187.0729	0.3
	HMDB0133606	2-(phenylmethylidene)propane-1,3-diol	C10H12O2	M+Na	187.0729	0.3
	HMDB0133608	4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]phenol	C10H12O2	M+Na	187.0729	0.3
	HMDB0033945	2-Phenylethyl acetate	C10H12O2	M+Na	187.0729	0.3
	HMDB0035268	4-Isopropylbenzoic acid	C10H12O2	M+Na	187.0729	0.3
	HMDB0030060	Methyl 3-phenylpropanoate	C10H12O2	M+Na	187.0729	0.3
	HMDB0035414	Lepalone	C10H12O2	M+Na	187.0729	0.3
	HMDB0031761	Propyl benzoate	C10H12O2	M+Na	187.0729	0.3
	HMDB0037160	4-Methyl-2-phenyl-1,3-dioxolane	C10H12O2	M+Na	187.0729	0.3

	HMDB0038184	Egomaketone	C10H12O2	M+Na	187.0729	0.3
	HMDB0032618	Ethyl phenylacetate	C10H12O2	M+Na	187.0729	0.3
	HMDB0034471	3-Phenylpropyl formate	C10H12O2	M+Na	187.0729	0.3
	HMDB0032620	1-Phenylethyl acetate	C10H12O2	M+Na	187.0729	0.3
	HMDB0036098	Isoegomaketone	C10H12O2	M+Na	187.0729	0.3
	HMDB0032891	1-(4-Methoxyphenyl)-2-propanone	C10H12O2	M+Na	187.0729	0.3
	HMDB0040460	4-Methylbenzyl alcohol acetate	C10H12O2	M+Na	187.0729	0.3
	HMDB0170973	(Z)-Isoeugenol	C10H12O2	M+Na	187.0729	0.3
	HMDB0041473	(3-Methylphenyl)methyl acetate	C10H12O2	M+Na	187.0729	0.3
	HMDB0034615	Epoxyanethole	C10H12O2	M+Na	187.0729	0.3
	HMDB0034732	Thymoquinone	C10H12O2	M+Na	187.0729	0.3
	HMDB0000543	Benzenebutanoic acid	C10H12O2	M+Na	187.0729	0.3
	HMDB0000329	2-Phenylbutyric acid	C10H12O2	M+Na	187.0729	0.3
	HMDB0001955	3-Phenylbutyric acid	C10H12O2	M+Na	187.0729	0.3
	HMDB0005802	Isoeugenol	C10H12O2	M+Na	187.0729	0.3
	HMDB0005809	Eugenol	C10H12O2	M+Na	187.0729	0.3
	HMDB0037174	p-Mentha-2,4(8)-dien-9,3-olide	C10H12O2	M+Na	187.0729	0.3
	HMDB0030063	Benzyl propionate	C10H12O2	M+Na	187.0729	0.3
	HMDB0032038	Isopropyl benzoate	C10H12O2	M+Na	187.0729	0.3
	HMDB0035213	beta-Thujaplicin	C10H12O2	M+Na	187.0729	0.3
	HMDB0033723	4-(4-Hydroxyphenyl)-2-butanone	C10H12O2	M+Na	187.0729	0.3
	HMDB0041472	2-Methylbenzyl alcohol acetate	C10H12O2	M+Na	187.0729	0.3
	HMDB0032586	3-(4-Methoxyphenyl)-2-propen-1-ol	C10H12O2	M+Na	187.0729	0.3
	HMDB0040359	1,2-Dimethoxy-4-vinylbenzene	C10H12O2	M+Na	187.0729	0.3
	HMDB0032336	3-Hydroxy-4-phenylbutan-2-one	C10H12O2	M+Na	187.0729	0.3
	HMDB0135738	3-(4-methoxyphenyl)prop-2-en-1-ol	C10H12O2	M+Na	187.0729	0.3
187.0962	HMDB0030992	5-Butyltetrahydro-2-oxo-3-furancarboxylic acid	C9H14O4	M+H	187.0965	-1.5
	HMDB0030988	5-(2-Methylpropyl)tetrahydro-2-oxo-3-furancarboxylic acid	C9H14O4	M+H	187.0965	-1.5
187.1324	HMDB0180505	3-hydroxy-9-decenoic acid	C10H18O3	M+H	187.1329	-2.5
	HMDB0180507	5-hydroxydec-9-enoic acid	C10H18O3	M+H	187.1329	-2.5
	HMDB0180508	6-hydroxydec-9-enoic acid	C10H18O3	M+H	187.1329	-2.5
	HMDB0180506	4-hydroxydec-9-enoic acid	C10H18O3	M+H	187.1329	-2.5
	HMDB0180510	8-hydroxy-9-decenoic acid	C10H18O3	M+H	187.1329	-2.5
	HMDB0180511	Oxiraneoctanoic acid	C10H18O3	M+H	187.1329	-2.5
	HMDB0180509	7-hydroxydec-9-enoic acid	C10H18O3	M+H	187.1329	-2.5
	HMDB0180512	2-hydroxydec-9-enoic acid	C10H18O3	M+H	187.1329	-2.5
	HMDB0180148	1-(hydroxymethyl)-3,3-dimethyl-2-oxabicyclo[2.2.2]octan-6-ol	C10H18O3	M+H	187.1329	-2.5
	HMDB0180054	(6E)-9-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M+H	187.1329	-2.5
	HMDB0180055	(6E)-2-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M+H	187.1329	-2.5
	HMDB0164896	6,7-dihydroxy-7-methyl-3-methylideneoctanal	C10H18O3	M+H	187.1329	-2.5
	HMDB0164962	1-(2-hydroxypropan-2-yl)-4-methylbicyclo[3.1]hexane-2,4-diol	C10H18O3	M+H	187.1329	-2.5
	HMDB0180052	(6E)-5-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M+H	187.1329	-2.5
	HMDB0180051	(6E)-8-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M+H	187.1329	-2.5
	HMDB0180053	5-[3-(propan-2-yl)oxiran-2-yl]pentanoic acid	C10H18O3	M+H	187.1329	-2.5
	HMDB0038692	6-Methyl-2-methylene-6-octene-1,3,8-triol	C10H18O3	M+H	187.1329	-2.5
	HMDB0039582	6-Hexyl-1,4-dioxan-2-one	C10H18O3	M+H	187.1329	-2.5
	HMDB0163825	5-(1,2-dihydroxypropan-2-yl)-2-methylcyclohexan-1-one	C10H18O3	M+H	187.1329	-2.5
	HMDB0039587	5-Hexyl-1,4-dioxan-2-one	C10H18O3	M+H	187.1329	-2.5
	HMDB0041545	(1R,2R,4R)-1,8-Epoxy-p-menthane-2,4-diol	C10H18O3	M+H	187.1329	-2.5
	HMDB0038978	(1beta,2beta,5beta)-p-Menth-3-ene-1,2,5-triol	C10H18O3	M+H	187.1329	-2.5
	HMDB0010724	3-Oxodecanoic acid	C10H18O3	M+H	187.1329	-2.5
	HMDB0033010	(1S,2S,4S,5R)-1,8-Epoxy-p-menthane-2,5-diol	C10H18O3	M+H	187.1329	-2.5
	HMDB0039533	(E)--Hydroxy-8-decenoic acid	C10H18O3	M+H	187.1329	-2.5
	HMDB0041376	exo,exo-1,8-Epoxy-p-menthane-2,6-diol	C10H18O3	M+H	187.1329	-2.5
	HMDB0030369	3-Hydroxy-5Z-octenyl acetate	C10H18O3	M+H	187.1329	-2.5
	HMDB0040204	2-Methylbutyl 3-hydroxy-2-methylidenebutanoate	C10H18O3	M+H	187.1329	-2.5
	HMDB0040205	3-Methylbutyl 3-hydroxy-2-methylidenebutanoate	C10H18O3	M+H	187.1329	-2.5
	HMDB0030367	Ethyl (3R,5Z)-3-hydroxy-5-octenoate	C10H18O3	M+H	187.1329	-2.5
	HMDB0180761	3-octyloxiranemethanol	C11H22O2	M+H	187.1693	-2.4
	HMDB0180760	(2E)-undec-2-ene-1,-diol	C11H22O2	M+H	187.1693	-2.4
	HMDB0180762	(2E)-undec-2-ene-1,11-diol	C11H22O2	M+H	187.1693	-2.4

187.1688	HMDB0180759	(2E)-undec-2-ene-1,4-diol	C11H22O2	M+H	187.1693	-2.4
	HMDB0165571	3-Hydroxy-2-undecanone	C11H22O2	M+H	187.1693	-2.4
	HMDB0165570	1-HYDROXYUNDECAN-2-ONE	C11H22O2	M+H	187.1693	-2.4
	HMDB0165569	11-hydroxy-2-undecanone	C11H22O2	M+H	187.1693	-2.4
	HMDB0165568	SCHEMBL117411	C11H22O2	M+H	187.1693	-2.4
	HMDB0094659	tert-butyl heptanoate	C11H22O2	M+H	187.1693	-2.4
	HMDB0034458	Isobutyl enanthate	C11H22O2	M+H	187.1693	-2.4
	HMDB0040171	Heptyl 2-methylpropanoate	C11H22O2	M+H	187.1693	-2.4
	HMDB0040266	Nonyl acetate	C11H22O2	M+H	187.1693	-2.4
	HMDB0041559	Butyl heptanoate	C11H22O2	M+H	187.1693	-2.4
	HMDB0034460	Heptyl butanoate	C11H22O2	M+H	187.1693	-2.4
	HMDB0034134	Octyl propanoate	C11H22O2	M+H	187.1693	-2.4
	HMDB0039215	Hexyl 2-methylbutanoate	C11H22O2	M+H	187.1693	-2.4
	HMDB0034456	9-Methyldecanoic acid	C11H22O2	M+H	187.1693	-2.4
	HMDB0033618	3-Methylbutyl hexanoate	C11H22O2	M+H	187.1693	-2.4
	HMDB0038237	xi-8-Methyldecanoic acid	C11H22O2	M+H	187.1693	-2.4
	HMDB0002373	4,6-Dimethylnonanoic acid	C11H22O2	M+H	187.1693	-2.4
	HMDB0000947	Undecanoic acid	C11H22O2	M+H	187.1693	-2.4
	HMDB0033848	Methyl decanoate	C11H22O2	M+H	187.1693	-2.4
	HMDB0036034	6,6-Dimethoxy-2,5,5-trimethyl-2-hexene	C11H22O2	M+H	187.1693	-2.4
	HMDB0032044	Hexyl 3-methylbutanoate	C11H22O2	M+H	187.1693	-2.4
	HMDB0062119	Hexyl valerate	C11H22O2	M+H	187.1693	-2.4
	HMDB0059860	2-Methylbutyl hexanoate	C11H22O2	M+H	187.1693	-2.4
	HMDB0059831	Propyl octanoate	C11H22O2	M+H	187.1693	-2.4
	HMDB0032325	2-Hexyl-4,5-dimethyl-1,3-dioxolane	C11H22O2	M+H	187.1693	-2.4
	HMDB0032448	Octanal propyleneglycol acetal	C11H22O2	M+H	187.1693	-2.4
	HMDB0036229	Pentyl hexanoate	C11H22O2	M+H	187.1693	-2.4
	HMDB0040193	Ethyl nonanoate	C11H22O2	M+H	187.1693	-2.4
	HMDB0038267	7,7-Diethoxy-3-heptene	C11H22O2	M+H	187.1693	-2.4
188.0138	HMDB0032580	4-Hydroxybenzyl isothiocyanate	C8H7NOS	M+Na	188.0141	-1.3
	HMDB0168670	3-hydroxybenzyl isothiocyanate	C8H7NOS	M+Na	188.0141	-1.3
	HMDB0168669	SCHEMBL418	C8H7NOS	M+Na	188.0141	-1.3
	HMDB0172358	{[(3-hydroxyphenyl)methyl]sulfanyl}carbonitrile	C8H7NOS	M+Na	188.0141	-1.3
	HMDB0172357	{[(2-hydroxyphenyl)methyl]sulfanyl}carbonitrile	C8H7NOS	M+Na	188.0141	-1.3
	HMDB0172359	4-Hydroxybenzyl thiocyanate	C8H7NOS	M+Na	188.0141	-1.3
188.0682	HMDB0062407	5-(3-Pyridyl)-2-hydroxytetrahydrofuran	C9H11NO2	M+Na	188.0682	0.0
	HMDB0062402	4-Hydroxy-1-(3-pyridinyl)-1-butanone	C9H11NO2	M+Na	188.0682	0.0
	HMDB0006044	Norsalsolinol	C9H11NO2	M+Na	188.0682	0.0
	HMDB0001007	3-Pyridinebutanoic acid	C9H11NO2	M+Na	188.0682	0.0
	HMDB0004992	Benzocaine	C9H11NO2	M+Na	188.0682	0.0
	HMDB0034169	Methyl N-methylantranilate	C9H11NO2	M+Na	188.0682	0.0
	HMDB0033485	Gentiatibetine	C9H11NO2	M+Na	188.0682	0.0
	HMDB0059934	Benzyl glycinate	C9H11NO2	M+Na	188.0682	0.0
	HMDB0033589	Ethyl 2-aminobenzoate	C9H11NO2	M+Na	188.0682	0.0
	HMDB0000159	L-Phenylalanine	C9H11NO2	M+Na	188.0682	0.0
188.0912	HMDB0159744	L-Phenylalanine	C9H11NO2	M+Na	188.0682	0.0
	HMDB0132906	3,5-dimethoxybenzene-1,2-diol	C8H10O4	M+NH4	188.0917	-2.8
	HMDB0133971	3,4-dimethoxybenzene-1,2-diol	C8H10O4	M+NH4	188.0917	-2.8
	HMDB0133972	2,3-dimethoxybenzene-1,4-diol	C8H10O4	M+NH4	188.0917	-2.8
	HMDB0133982	4,5-dimethoxybenzene-1,3-diol	C8H10O4	M+NH4	188.0917	-2.8
	HMDB0153684	2-(hydroxymethyl)-5-methoxybenzene-1,3-diol	C8H10O4	M+NH4	188.0917	-2.8
	HMDB0173106	2,5-dimethoxycyclohex-2-ene-1,4-dione	C8H10O4	M+NH4	188.0917	-2.8
	HMDB0179996	SCHEMBL285344	C8H10O4	M+NH4	188.0917	-2.8
	HMDB0132907	2,6-dimethoxybenzene-1,4-diol	C8H10O4	M+NH4	188.0917	-2.8
	HMDB0059756	3,4-Methyleneadipic acid	C8H10O4	M+NH4	188.0917	-2.8
	HMDB0038760	Herierin III	C8H10O4	M+NH4	188.0917	-2.8
	HMDB0038761	Herierin IV	C8H10O4	M+NH4	188.0917	-2.8
	HMDB0032966	Furaneol acetate	C8H10O4	M+NH4	188.0917	-2.8
	HMDB0000318	3,4-Dihydroxyphenylglycol	C8H10O4	M+NH4	188.0917	-2.8
	HMDB0153685	6-methoxy-3-methylbenzene-1,2,4-triol	C8H10O4	M+NH4	188.0917	-2.8
	HMDB0012150	2-Keto-6-acetamidocaproate	C8H13NO4	M+H	188.0917	-2.8
	HMDB0167056	(2E,6Z)-9-hydroxynona-2,6-dienoic acid	C9H14O3	M+NH4	188.1281	-2.7
	HMDB0167055	(2E)-5-(3-ethyloxiran-2-yl)pent-2-enoic acid	C9H14O3	M+NH4	188.1281	-2.7
	HMDB0167054	3-[(3Z)-hex-3-en-1-yl]oxirane-2-carboxylic acid	C9H14O3	M+NH4	188.1281	-2.7
	HMDB0167052	(2E,6Z)-8-hydroxynona-2,6-dienoic acid	C9H14O3	M+NH4	188.1281	-2.7

188.1276	HMDB0167053	(2E,6Z)-5-hydroxynona-2,6-dienoic acid	C9H14O3	M+NH4	188.1281	-2.7
	HMDB0167051	(2E,6Z)-4-hydroxynona-2,6-dienoic acid	C9H14O3	M+NH4	188.1281	-2.7
	HMDB0164924	7-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M+NH4	188.1281	-2.7
	HMDB0164925	6-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M+NH4	188.1281	-2.7
	HMDB0164926	5-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M+NH4	188.1281	-2.7
	HMDB0164922	1,3-bis(hydroxymethyl)bicyclo[2.2.1]heptan-2-one	C9H14O3	M+NH4	188.1281	-2.7
	HMDB0164923	3-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M+NH4	188.1281	-2.7
	HMDB0038276	cis-3-Hexenyl pyruvate	C9H14O3	M+NH4	188.1281	-2.7
	HMDB0030471	1,4-Ipomeadiol	C9H14O3	M+NH4	188.1281	-2.7
	HMDB0240687	7-Keto-8-Aminopelargonic Acid	C9H17NO3	M+H	188.1281	-2.8
	HMDB0013010	N-Heptanoylglycine	C9H17NO3	M+H	188.1281	-2.8
	HMDB0182601	4-Hydroxypiperitone	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182595	8-hydroxy-p-menthan-3-one	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182600	5-(hydroxymethyl)-2-(propan-2-yl)cyclohexan-1-one	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182598	2-hydroxy-p-menthanone-(3)	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182599	(+)-4-hydroxy-p-menth-3-one	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182596	2-(2-Hydroxy-1-methylethyl)-5-methylcyclohexanone	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182594	5-Hydroxy-2-isopropyl-5-methylcyclohexanone	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182528	SCHEMBL12683693	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182525	2-(hydroxymethyl)-5-(propan-2-yl)cyclohexan-1-one	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182524	2-hydroxy-6-methyl-3-(propan-2-yl)cyclohexan-1-one	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182526	Oxytetrahydrocarvon	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182527	4-hydroxy-2-methyl-5-(propan-2-yl)cyclohexan-1-one	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182522	AC1LCBYF	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182521	5-(2-hydroxypropan-2-yl)-2-methylcyclohexan-1-one	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182602	SCHEMBL16581455	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182622	2-[2-(hydroxymethyl)-2,3-dimethylcyclopent-3-en-1-yl]ethan-1-ol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182701	(1S)-1,7,7-trimethylbicyclo[2.2.1]heptane-2,5-diol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182700	1,7,7-trimethylbicyclo[2.2.1]heptane-2,6-diol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182698	(1S)-1,7,7-trimethylbicyclo[2.2.1]heptane-2,3-diol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182699	(1S)-1,7,7-trimethylbicyclo[2.2.1]heptane-2,2-diol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182697	(1S)-7-(hydroxymethyl)-1,7-dimethylbicyclo[2.2.1]heptan-2-ol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182696	SCHEMBL15462834	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182626	2-{1,2,2-trimethyl-6-oxabicyclo[3.1]hexan-3-yl}ethan-1-ol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182623	2-[3-(hydroxymethyl)-2,2-dimethylcyclopent-3-en-1-yl]ethan-1-ol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182624	SCHEMBL5398	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182625	5-(2-hydroxyethyl)-3,4,4-trimethylcyclopent-2-en-1-ol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0182520	SCHEMBL12683689	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0181920	AC1MS2IY	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0181921	1,3,3-trimethylbicyclo[2.2.1]heptane-2,5-diol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0180107	8-METHYL-8-NONENOIC ACID	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0161935	(2Z)-3,7-dimethylocta-2,6-diene-1,5-diol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0161937	(2Z)-3,7-Dimethyl-6,7-epoxy-2-octene-1-ol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0161936	2,3-Epoxy-3,7-dimethyloct-6-enol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0161933	SCHEMBL15361567	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0161934	8-hydroxyneryl	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0161932	SCHEMBL9863268	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0161931	(2Z)-3,7-dimethylocta-2,6-diene-1,4-diol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0179965	3-exo-hydroxy-1,8-cineole	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0131081	(2E)-7-hydroxy-3,6,6-trimethylhept-2-enal	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0180489	3-hydroxydec-9-enal	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0180492	6-hydroxydec-9-enal	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0181919	1,3,3-trimethylbicyclo[2.2.1]heptane-2,7-diol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0181916	62853-86-5	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0181918	1,3,3-trimethylbicyclo[2.2.1]heptane-2,2-diol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0181917	3-(hydroxymethyl)-1,3-dimethylbicyclo[2.2.1]heptan-2-ol	C10H18O2	M+NH4	188.1645	-2.7

188.1640	HMDB0180591	4-methylnon-8-enoic acid	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0180590	4-methylidenenonanoic acid	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0180494	SCHEMBL186654	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0180496	2-hydroxydec-9-enal	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0180493	7-hydroxydec-9-enal	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0180495	SCHEMBL58664	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0180491	5-hydroxydec-9-enal	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0180490	4-hydroxydec-9-enal	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0039768	5-Decenoic acid	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0030031	6-Methyl-5-hepten-2-yl acetate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0040213	cis-3-Hexenyl isobutyrate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0036990	2,6-Dimethyl-3,7-octadiene-2,6-diol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0031362	Cyclohexylethyl acetate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0036211	Hexyl crotonate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0035365	Cnidiol C	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0040330	Menthone lactone	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0040530	Isopentyl 3-methyl-2-butenate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0031003	9-Decenoic acid	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0040194	Methyl 2-nonenate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0033377	cis-3-Hexenyl butyrate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0035907	Linalyl oxide	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0035837	Citronelllic acid	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0029859	Methyl (xi)-3-nonenate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0059610	2-Exo-hydroxy-1,8-cineole	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0031441	Linalool oxide III	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0041630	Linalool oxide III	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0031440	Linalool oxide (trans-pyranoid)	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0032393	2-Methylbutyl 3-methyl-2-butenate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0032452	1-Octen-3-yl acetate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0032275	Ethyl 3-octenoate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0031297	2-Octenyl acetate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0040208	2-Propenyl heptanoate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0036992	1-Cyclopropyl-4-methyl-1,3-cyclohexanediol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0061293	1-p-Menthene-8,9-diol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0035122	(S,E)-2,6-Dimethyl-5,7-octadiene-2,3-diol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0037632	xi-Tetrahydro-3-pentyl-2H-pyran-2-one	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0037217	xi-5-Hexyldihydro-2(3H)-furanone	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0035839	(E)-3-(Tetrahydro-5,5-dimethyl-2-furanyl)-2-buten-1-ol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0038744	9-Hydroxygeraniol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0039149	(+)-6-Hydroxy-2,6-dimethyl-7-octen-4-one	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0012183	8-Methylnonenate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0010726	trans-Dec-2-enoic acid	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0037116	delta-Decalactone	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0037497	Ethyl (E)-2-octenoate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0039795	Ethyl 4Z-octenoate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0034581	2-Hexenyl butanoate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0034427	Cyclohexyl butanoate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0037021	trans-p-Menth-2-ene-1,4-diol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0032119	4-Hydroxy-2,6-dimethyl-7-octen-3-one	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0029358	5Z-Octenyl acetate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0041012	6-Decenoic acid	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0036099	Lilac alcohol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0040726	cis-Linalyl oxide	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0031002	3-Decenoic acid	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0033203	6-Decanolide	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0040727	trans-Linalyl oxide	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0004980	cis-4-Decenoic acid	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0164952	4-methyl-1-(propan-2-yl)bicyclo[3.1]hexane-2,4-diol	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0034880	3-Methyl-2,4-nonanedione	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0062152	Propyl cyclohexanecarboxylate	C10H18O2	M+NH4	188.1645	-2.7
	HMDB0059852	2-Hydroxycineol	C10H18O2	M+NH4	188.1645	-2.7
188.1752	HMDB0001276	N1-Acetylspermidine	C9H21N3O	M+H	188.1757	-2.9
	HMDB0002189	N8-Acetylspermidine	C9H21N3O	M+H	188.1757	-2.9
	HMDB0060288	N8-Acetylspermidine	C9H21N3O	M+H	188.1757	-2.9
	HMDB0002107	Phthalic acid	C8H6O4	M+Na	189.0158	-2.3

189.0154	HMDB0032613	3,4-Methylenedioxybenzoic acid	C8H6O4	M+Na	189.0158	-2.3
	HMDB0002428	Terephthalic acid	C8H6O4	M+Na	189.0158	-2.3
	HMDB0061917	Terephthalic acid	C8H6O4	M+Na	189.0158	-2.3
	HMDB0002334	Benzoquinoneacetic acid	C8H6O4	M+Na	189.0158	-2.3
189.0376	HMDB0034394	S-Propyl 1-propanesulfinothioate	C6H14OS2	M+Na	189.0378	-1.2
189.0658	HMDB0038633	(-)-3-Cyanomethyl-3-hydroxy-1H-indol-2(3H)-one	C10H8N2O2	M+H	189.0659	-0.3
	HMDB0182037	2-(4,5-dihydroxy-1H-indol-3-yl)acetonitrile	C10H8N2O2	M+H	189.0659	-0.3
	HMDB0182036	2-(4,6-dihydroxy-1H-indol-3-yl)acetonitrile	C10H8N2O2	M+H	189.0659	-0.3
189.0910	HMDB0032061	3-Butylidene-1(3H)-isobenzofuranone	C12H12O2	M+H	189.0910	0.0
	HMDB0032028	(E)-3-(2-Methylpropylidene)-1(3H)-isobenzofuranone	C12H12O2	M+H	189.0910	0.0
	HMDB0029495	Trigoforin	C12H12O2	M+H	189.0910	0.0
	HMDB0041219	Allyl cinnamate	C12H12O2	M+H	189.0910	0.0
	HMDB0132978	(4E)-5-(4-methoxyphenyl)penta-1,4-dien-3-one	C12H12O2	M+H	189.0910	0.0
189.1117	HMDB0179176	3-hydroxy-4-oxononanoic acid	C9H16O4	M+H	189.1121	-2.3
	HMDB0179175	2-hydroxy-4-oxononanoic acid	C9H16O4	M+H	189.1121	-2.3
	HMDB0179177	5-hydroxy-4-oxononanoic acid	C9H16O4	M+H	189.1121	-2.3
	HMDB0179174	9-hydroxy-4-oxononanoic acid	C9H16O4	M+H	189.1121	-2.3
	HMDB0179173	8-hydroxy-4-oxononanoic acid	C9H16O4	M+H	189.1121	-2.3
	HMDB0059783	3-Methylsuberic acid	C9H16O4	M+H	189.1121	-2.3
	HMDB0059760	2,4-Dimethylpimelic acid	C9H16O4	M+H	189.1121	-2.3
	HMDB0059879	Diethyl glutarate	C9H16O4	M+H	189.1121	-2.3
	HMDB0032387	(+/-)-Methyl 5-acetoxyhexanoate	C9H16O4	M+H	189.1121	-2.3
	HMDB0032200	cis- and trans-Ethyl 2,4-dimethyl-1,3-dioxolane-2-acetate	C9H16O4	M+H	189.1121	-2.3
	HMDB0032258	(+/-)-Ethyl 3-acetoxy-2-methylbutyrate	C9H16O4	M+H	189.1121	-2.3
	HMDB0036233	Butyl ethyl malonate	C9H16O4	M+H	189.1121	-2.3
	HMDB0011717	Nonate	C9H16O4	M+H	189.1121	-2.3
	HMDB0059814	Diethyl methylsuccinate	C9H16O4	M+H	189.1121	-2.3
	HMDB0000784	Azelaic acid	C9H16O4	M+H	189.1121	-2.3
189.1254	HMDB0036815	Norecasantalol	C11H18O	M+Na	189.1250	2.2
	HMDB0036190	2-Heptylfuran	C11H18O	M+Na	189.1250	2.2
	HMDB0031728	2-Hexylidenecyclopentanone	C11H18O	M+Na	189.1250	2.2
	HMDB0031359	2,4-Undecadienal	C11H18O	M+Na	189.1250	2.2
	HMDB0030002	(-)-Nopol	C11H18O	M+Na	189.1250	2.2
	HMDB0030252	Limonene aldehyde	C11H18O	M+Na	189.1250	2.2
	HMDB0031565	Dihydrojasmane	C11H18O	M+Na	189.1250	2.2
	HMDB0032540	2,6,6-Trimethyl-1-cyclohexen-1-acetaldehyde	C11H18O	M+Na	189.1250	2.2
	HMDB0033546	2,5-Undecadienal	C11H18O	M+Na	189.1250	2.2
189.1484	HMDB0002203	3-Hydroxycapric acid	C10H20O3	M+H	189.1485	-0.6
	HMDB0179929	(5E)-3,7-dimethyloct-5-ene-1,4,7-triol	C10H20O3	M+H	189.1485	-0.6
	HMDB0179928	(5E)-3,7-dimethyloct-5-ene-1,3,7-triol	C10H20O3	M+H	189.1485	-0.6
	HMDB0041600	Ethyl 3-hydroxyoctanoate	C10H20O3	M+H	189.1485	-0.6
	HMDB0179930	4-[3-(2-hydroxypropan-2-yl)oxiran-2-yl]-3-methylbutan-1-ol	C10H20O3	M+H	189.1485	-0.6
	HMDB0179931	(3E)-2,6-dimethyloct-3-ene-1,2,8-triol	C10H20O3	M+H	189.1485	-0.6
	HMDB0179932	(5E)-3-(hydroxymethyl)-7-methyloct-5-ene-1,7-diol	C10H20O3	M+H	189.1485	-0.6
	HMDB0094656	2s-hydroxy-decanoic acid	C10H20O3	M+H	189.1485	-0.6
	HMDB0180589	SCHEMBL45681	C10H20O3	M+H	189.1485	-0.6
	HMDB0180587	4-(hydroxymethyl)nonanoic acid	C10H20O3	M+H	189.1485	-0.6
	HMDB0180585	AKO19123491	C10H20O3	M+H	189.1485	-0.6
	HMDB0180586	8-hydroxy-4-methylnonanoic acid	C10H20O3	M+H	189.1485	-0.6
	HMDB0180588	9-hydroxy-4-methylnonanoic acid	C10H20O3	M+H	189.1485	-0.6
	HMDB0180106	SCHEMBL4626344	C10H20O3	M+H	189.1485	-0.6
	HMDB0180104	8-Hydroxy-8-methylnonanoic acid	C10H20O3	M+H	189.1485	-0.6
	HMDB0180105	9-hydroxy-8-methylnonanoic acid	C10H20O3	M+H	189.1485	-0.6
	HMDB0039669	2-Hexyl-1,3-dioxolane-4-methanol	C10H20O3	M+H	189.1485	-0.6
	HMDB0033640	7-Methyl-3-methylene-1,6,7-octanetriol	C10H20O3	M+H	189.1485	-0.6
	HMDB0038186	2,6-Dimethyl-7-octene-2,3,6-triol	C10H20O3	M+H	189.1485	-0.6
	HMDB0033201	9-Hydroxydecanoic acid	C10H20O3	M+H	189.1485	-0.6
	HMDB0039668	2-Hexyl-1,3-dioxan-5-ol	C10H20O3	M+H	189.1485	-0.6
	HMDB0039470	(1S,2S,4R,8R)-p-Menthane-1,2,9-triol	C10H20O3	M+H	189.1485	-0.6
	HMDB0039893	(1R,2R,4S)-p-Menthane-1,2,8-triol	C10H20O3	M+H	189.1485	-0.6
	HMDB0033574	(1R,2R,4R,8R)-p-Menthane-2,8,9-triol	C10H20O3	M+H	189.1485	-0.6
	HMDB0040329	xi-5-Hydroxydecanoic acid	C10H20O3	M+H	189.1485	-0.6
	HMDB0010725	(R)-3-Hydroxydecanoic acid	C10H20O3	M+H	189.1485	-0.6

	HMDB0034783	cis-p-Menthane-1,7,8-triol	C10H20O3	M+H	189.1485	-0.6
189.1601	HMDB0163441	3-[(3-methylbutyl)(nitroso)amino]butan-2-ol	C9H20N2O2	M+H	189.1598	1.8
	HMDB0001325	N6,N6,N6-Trimethyl-L-lysine	C9H20N2O2	M+H	189.1598	1.8
	HMDB0005015	Gabapentin	C9H17NO2	M+NH4	189.1598	1.8
190.0198	HMDB0172083	[(1-sulfanyloxypropan-2-yl)oxy]sulfonic acid	C3H8O4S2	M+NH4	190.0202	-2.2
	HMDB0172087	SCHEMBL171809	C3H8O4S2	M+NH4	190.0202	-2.2
190.0827	HMDB0029419	Glycylglycylglycine	C6H11N3O4	M+H	190.0822	2.5
	HMDB0028731	Asparaginyglycine	C6H11N3O4	M+H	190.0822	2.5
	HMDB0028836	Glycyl-Asparagine	C6H11N3O4	M+H	190.0822	2.5
	HMDB0034322	L-alpha-Amino-5-oxo-2(5H)-isoxazolepropanoic acid	C6H8N2O4	M+NH4	190.0822	2.5
	HMDB0001212	Hydantoin-5-propionic acid	C6H8N2O4	M+NH4	190.0822	2.5
	HMDB0160104	bis(hydroxymethyl)pyrimidine-2,4-diol	C6H8N2O4	M+NH4	190.0822	2.5
190.1069	HMDB0159134	2-(3-hydroxy-4-oxocyclohexyl)acetic acid	C8H12O4	M+NH4	190.1074	-2.5
	HMDB0038601	Diethyl fumarate	C8H12O4	M+NH4	190.1074	-2.5
	HMDB0000341	2-Octenedioic acid	C8H12O4	M+NH4	190.1074	-2.5
	HMDB0004982	cis-4-Octenedioic acid	C8H12O4	M+NH4	190.1074	-2.5
	HMDB0034851	Ethyl 2,4-dioxohexanoate	C8H12O4	M+NH4	190.1074	-2.5
	HMDB0032352	3-Isopropenylpentanedioic acid	C8H12O4	M+NH4	190.1074	-2.5
	HMDB0173107	2,5-dimethoxycyclohexane-1,4-dione	C8H12O4	M+NH4	190.1074	-2.5
	HMDB0159135	2-hydroxy-2-(4-oxocyclohexyl)acetic acid	C8H12O4	M+NH4	190.1074	-2.5
	HMDB0013312	trans-3-Octenedioic acid	C8H12O4	M+NH4	190.1074	-2.5
	HMDB0094722	2-[(1,5-dihydroxyhexylidene)amino]acetic acid	C8H15NO4	M+H	190.1074	-2.5
	HMDB0094721	2-[(1,4-dihydroxyhexylidene)amino]acetic acid	C8H15NO4	M+H	190.1074	-2.5
	HMDB0240627	1-Carboxyethylvaline	C8H15NO4	M+H	190.1074	-2.5
	HMDB0094719	2-[(1,2-dihydroxyhexylidene)amino]acetic acid	C8H15NO4	M+H	190.1074	-2.5
	HMDB0094720	2-[(1,3-dihydroxyhexylidene)amino]acetic acid	C8H15NO4	M+H	190.1074	-2.5
	HMDB0094718	1-hydroxyhexanoylglycine	C8H15NO4	M+H	190.1074	-2.5
	HMDB0036604	N-Methylcalystegine B2	C8H15NO4	M+H	190.1074	-2.5
	HMDB0062181	N-lactoyl-Valine	C8H15NO4	M+H	190.1074	-2.5
190.1433	HMDB0040202	Butyl 3-hydroxy-2-methylidenebutanoate	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0179168	3-caproyl propionic acid	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0094711	9-oxononanoic acid	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0163466	(2Z)-8-hydroxy-2-methyloct-2-enoic acid	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0163465	(2Z)-7-hydroxy-2-methyloct-2-enoic acid	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0163469	(2Z)-4-hydroxy-2-methyloct-2-enoic acid	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0163470	2-methyl-3-pentyloxirane-2-carboxylic acid	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0163468	SCHEMBL7173369	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0169421	2-ethenyl-4,6-diethyl-1,3,5-trioxane	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0040203	2-Methylpropyl 3-hydroxy-2-methylidenebutanoate	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0036213	cis-3-Hexenyl lactate	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0036188	Tetrahydrofurfuryl butyrate	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0040165	Butyl levulinate	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0036396	3-Methylbutyl 3-oxobutanoate	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0059937	6-Pentyl-1,4-dioxan-2-one	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0059936	5-Pentyl-1,4-dioxan-2-one	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0060287	4-Hydroperoxy-2-nonenal	C9H16O3	M+NH4	190.1438	-2.5
	HMDB0062081	9-oxononanoate	C9H15O3	M+NH4	190.1438	-2.5
	HMDB0169534	geranic acid	C10H16O2	M+Na	191.1042	-0.8
	HMDB0176281	6-hydroxycamphor	C10H16O2	M+Na	191.1042	-0.8
	HMDB0182620	2-[3-(hydroxymethyl)-2,2-dimethylcyclopent-3-en-1-yl]acetaldehyde	C10H16O2	M+Na	191.1042	-0.8
	HMDB0182618	2-hydroxy-2-(2,2,3-trimethylcyclopent-3-en-1-yl)acetaldehyde	C10H16O2	M+Na	191.1042	-0.8
	HMDB0182617	25435-53-4	C10H16O2	M+Na	191.1042	-0.8
	HMDB0181690	[3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptan-3-yl]methanol	C10H16O2	M+Na	191.1042	-0.8
	HMDB0181692	7-(hydroxymethyl)-1,7-dimethyltricyclo[2.2.1,heptan-3-ol	C10H16O2	M+Na	191.1042	-0.8
	HMDB0181691	[7-(hydroxymethyl)-7-methyltricyclo[2.2.1,heptan-1-yl]methanol	C10H16O2	M+Na	191.1042	-0.8
	HMDB0181693	3-(hydroxymethyl)-2,3-dimethyltricyclo[2.2.1,heptan-1-ol	C10H16O2	M+Na	191.1042	-0.8
	HMDB0181639	5-(1-hydroxypropan-2-yl)-2-methylbicyclo[3.1]hex-3-en-2-ol	C10H16O2	M+Na	191.1042	-0.8
	HMDB0181638	2-methyl-5-(propan-2-yl)bicyclo[3.1]hex-3-ene-2,6-	C10H16O2	M+Na	191.1042	-0.8

191.1041

HMDB0181635	5-(2-hydroxypropan-2-yl)-2-methylbicyclo[3.1]hex-3-en-2-ol	C10H16O2	M+Na	191.1042	-0.8
HMDB0182621	SCHEMBL14359771	C10H16O2	M+Na	191.1042	-0.8
HMDB0182619	2-[2-(hydroxymethyl)-2,3-dimethylcyclopent-3-en-1-yl]acetaldehyde	C10H16O2	M+Na	191.1042	-0.8
HMDB0240639	(1S,4R,6R)-1,3,3-Trimethyl-6-hydroxybicyclo[2.2.1]heptane-2-one	C10H16O2	M+Na	191.1042	-0.8
HMDB0182798	(1S,4R,6S)-1,3,3-Trimethyl-6-hydroxybicyclo[2.2.1]heptane-2-one	C10H16O2	M+Na	191.1042	-0.8
HMDB0182796	3-(hydroxymethyl)-1,3-dimethylbicyclo[2.2.1]heptan-2-one	C10H16O2	M+Na	191.1042	-0.8
HMDB0182797	7-hydroxy-1,3,3-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O2	M+Na	191.1042	-0.8
HMDB0182799	5-hydroxy-1,3,3-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O2	M+Na	191.1042	-0.8
HMDB0182685	6-Hydroxycarvotanacetone	C10H16O2	M+Na	191.1042	-0.8
HMDB0182684	SCHEMBL6689811	C10H16O2	M+Na	191.1042	-0.8
HMDB0182683	1-methyl-4-(propan-2-yl)-7-oxabicyclo[4.1]heptan-2-one	C10H16O2	M+Na	191.1042	-0.8
HMDB0182680	2-(hydroxymethyl)-5-(propan-2-yl)cyclohex-2-en-1-	C10H16O2	M+Na	191.1042	-0.8
HMDB0181637	2-methyl-5-(propan-2-yl)bicyclo[3.1]hex-3-ene-1,2-	C10H16O2	M+Na	191.1042	-0.8
HMDB0181636	5-methyl-1-(propan-2-yl)-3-oxatricyclo[4.1,heptan-5-ol	C10H16O2	M+Na	191.1042	-0.8
HMDB0181634	2-(hydroxymethyl)-5-(propan-2-yl)bicyclo[3.1]hex-3-en-2-ol	C10H16O2	M+Na	191.1042	-0.8
HMDB0163099	(4Z,7Z)-3-hydroxydeca-4,7-dienal	C10H16O2	M+Na	191.1042	-0.8
HMDB0163102	(4Z)-6-(3-ethyloxiran-2-yl)hex-4-enal	C10H16O2	M+Na	191.1042	-0.8
HMDB0163100	(7Z)-9-hydroxydeca-4,7-dienal	C10H16O2	M+Na	191.1042	-0.8
HMDB0182795	ACMC-mnpl	C10H16O2	M+Na	191.1042	-0.8
HMDB0136694	6-hydroxy-3,7-dimethylocta-2,7-dienal	C10H16O2	M+Na	191.1042	-0.8
HMDB0163101	3-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}propanal	C10H16O2	M+Na	191.1042	-0.8
HMDB0163103	(4Z,7Z)--hydroxydeca-4,7-dienal	C10H16O2	M+Na	191.1042	-0.8
HMDB0179485	14-64-6	C10H16O2	M+Na	191.1042	-0.8
HMDB0179394	2E,4Z-decadienoic acid	C10H16O2	M+Na	191.1042	-0.8
HMDB0178761	SCHEMBL7756279	C10H16O2	M+Na	191.1042	-0.8
HMDB0163117	(z,z)-4,7-decadienoic acid	C10H16O2	M+Na	191.1042	-0.8
HMDB0163109	(2E)-3-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}prop-2-en-1-ol	C10H16O2	M+Na	191.1042	-0.8
HMDB0163108	{3-[(1Z,4Z)-hepta-1,4-dien-1-yl]oxiran-2-yl}methanol	C10H16O2	M+Na	191.1042	-0.8
HMDB0163110	(2E,4Z)-6-(3-ethyloxiran-2-yl)hexa-2,4-dien-1-ol	C10H16O2	M+Na	191.1042	-0.8
HMDB0163104	(4Z,7Z)-2-hydroxydeca-4,7-dienal	C10H16O2	M+Na	191.1042	-0.8
HMDB0163106	(4Z,7Z)-deca-2,4,7-triene-1,1-diol	C10H16O2	M+Na	191.1042	-0.8
HMDB0163105	(2E,7Z)-deca-2,4,7-triene-1,9-diol	C10H16O2	M+Na	191.1042	-0.8
HMDB0182681	8-Hydroxycarvotanacetone	C10H16O2	M+Na	191.1042	-0.8
HMDB0032313	2,4-Hexadienyl isobutyrate	C10H16O2	M+Na	191.1042	-0.8
HMDB0032312	2,4-Hexadienyl butyrate	C10H16O2	M+Na	191.1042	-0.8
HMDB0033700	(-)-(Z)-Tetrahydro-6-(2-pentenyl)-2H-pyran-2-one	C10H16O2	M+Na	191.1042	-0.8
HMDB0031273	Methyl octylenecarboxylate	C10H16O2	M+Na	191.1042	-0.8
HMDB0031156	Ethyl (4Z)-4,7-octadienoate	C10H16O2	M+Na	191.1042	-0.8
HMDB0035714	Epoxycarvotanacetone	C10H16O2	M+Na	191.1042	-0.8
HMDB0040639	(xi)-(Z)-5-(3-Hexenyl)dihydro-2(3H)-furanone	C10H16O2	M+Na	191.1042	-0.8
HMDB0037175	4-Isopropyl-3-cyclohexene-1-carboxylic acid	C10H16O2	M+Na	191.1042	-0.8
HMDB0036067	Epoxycampholenic aldehyde	C10H16O2	M+Na	191.1042	-0.8
HMDB0037821	xi-1,8,8-Trimethyl-2-oxabicyclo[3.2.1]octan-3-one	C10H16O2	M+Na	191.1042	-0.8
HMDB0034452	5,6-Dihydro-6-pentyl-2H-pyran-2-one	C10H16O2	M+Na	191.1042	-0.8
HMDB0036103	Geranic acid	C10H16O2	M+Na	191.1042	-0.8
HMDB0032219	(+/-)-Dihydromintlactone	C10H16O2	M+Na	191.1042	-0.8
HMDB0032319	cis-3-Hexenyl crotonate	C10H16O2	M+Na	191.1042	-0.8
HMDB0032434	(+/-)-2-(5-Methyl-5-vinyltetrahydrofuran-2-yl)propionaldehyde	C10H16O2	M+Na	191.1042	-0.8
HMDB0035829	Dihydronepetalactone	C10H16O2	M+Na	191.1042	-0.8
HMDB0034670	6-Hydroxy-2,6-dimethyl-2,7-octadien-4-one	C10H16O2	M+Na	191.1042	-0.8
HMDB0037014	gamma-Diosphenol	C10H16O2	M+Na	191.1042	-0.8
HMDB0013105	trans-4,5-epoxy-2(E)-decenal	C10H16O2	M+Na	191.1042	-0.8
HMDB0035766	Ascaridole	C10H16O2	M+Na	191.1042	-0.8
HMDB0182682	4-hydroxy-2-methyl-5-(propan-2-yl)cyclohex-2-en-1-one	C10H16O2	M+Na	191.1042	-0.8
HMDB0163757	3,5-dihydroxy-6-methyloctanoic acid	C9H18O4	M+H	191.1278	-2.0

191.1274	HMDB0169419	1-(4,6-diethyl-1,3,5-trioxan-2-yl)ethan-1-ol	C9H18O4	M+H	191.1278	-2.0
	HMDB0169420	2-(4,6-diethyl-1,3,5-trioxan-2-yl)ethan-1-ol	C9H18O4	M+H	191.1278	-2.0
191.1389	HMDB0000701	Hexanoylglycine	C8H15NO3	M+NH4	191.1390	-0.6
	HMDB0000747	Isovalerylalanine	C8H15NO3	M+NH4	191.1390	-0.6
	HMDB0002087	Isovalerylsarcosine	C8H15NO3	M+NH4	191.1390	-0.6
	HMDB0011756	N-Acetyl-leucine	C8H15NO3	M+NH4	191.1390	-0.6
	HMDB0061684	N-Acetyl-isoleucine	C8H15NO3	M+NH4	191.1390	-0.6
191.1789	HMDB0013820	2-Methyl-2-phenyl-undecane	C14H22	M+H	191.1794	-2.8
	HMDB0059739	1-Ethyl-3,5-diisopropyl-benzene	C14H22	M+H	191.1794	-2.8
	HMDB0061923	1,3-Di-tert-butylbenzene	C14H22	M+H	191.1794	-2.8
	HMDB0094670	1,4-Di-tert-butylbenzene	C14H22	M+H	191.1794	-2.8
192.0394	HMDB0060244	Phosphodimethylethanolamine	C4H12NO4P	M+Na	192.0396	-1.1
192.0508	HMDB0015155	Isosorbide Mononitrate	C6H9NO6	M+H	192.0503	2.8
	HMDB0041900	gamma-Carboxyglutamic acid	C6H9NO6	M+H	192.0503	2.8
	HMDB0001264	Dehydroascorbic acid	C6H6O6	M+NH4	192.0503	2.8
	HMDB0000072	cis-Aconitic acid	C6H6O6	M+NH4	192.0503	2.8
	HMDB0000958	trans-Aconitic acid	C6H6O6	M+NH4	192.0503	2.8
	HMDB0062706	dehydroascorbide(1-)	C6H6O6	M+NH4	192.0503	2.8
	HMDB0040200	2,5-Dimethyl-3-(methylthio)furan	C7H10OS2	M+NH4	192.0511	-1.7
	HMDB0166093	(2-hydroxy-4-isothiocyanatobutyl)dimethylsulfonium	C7H14NOS2	M+H	192.0511	-1.7
192.1225	HMDB0166089	(3-hydroxy-4-isothiocyanatobutyl)dimethylsulfonium	C7H14NOS2	M+H	192.0511	-1.7
	HMDB0159133	2-hydroxy-2-(4-hydroxycyclohexyl)acetic acid	C8H14O4	M+NH4	192.1230	-2.8
	HMDB0041606	Dimethyl adipate	C8H14O4	M+NH4	192.1230	-2.8
	HMDB0060684	2-Propylglutaric acid	C8H14O4	M+NH4	192.1230	-2.8
	HMDB0059757	3-Methylpimelic acid	C8H14O4	M+NH4	192.1230	-2.8
	HMDB0059727	2,4-Dimethyladipic acid	C8H14O4	M+NH4	192.1230	-2.8
	HMDB0033838	Diethyl succinate	C8H14O4	M+NH4	192.1230	-2.8
	HMDB0002023	Ethyladipic acid	C8H14O4	M+NH4	192.1230	-2.8
192.1378	HMDB0000893	Suberic acid	C8H14O4	M+NH4	192.1230	-2.8
	HMDB0171339	4-(4-methylphenyl)pent-4-en-2-one	C12H14O	M+NH4	192.1383	-2.5
	HMDB0040823	(S)-11,12,13-Trinor-7-calamenone	C12H14O	M+NH4	192.1383	-2.5
	HMDB0039153	(R)-11,12,13-Trinor-1(5),6,9-guaiatrien-8-one	C12H14O	M+NH4	192.1383	-2.5
	HMDB0037281	4-Methyl-2-phenyl-2-pentenal	C12H14O	M+NH4	192.1383	-2.5
	HMDB0031622	6-Phenyl-3-hexen-2-one	C12H14O	M+NH4	192.1383	-2.5
	HMDB0032854	N-Acetyl-2,6-diethylaniline	C12H17NO	M+H	192.1383	-2.6
	HMDB0032635	N,N-Diethylbenzeneacetamide	C12H17NO	M+H	192.1383	-2.6
192.1590	HMDB0015519	Phendimetrazine	C12H17NO	M+H	192.1383	-2.6
	HMDB0170940	2-hydroxynonanoic acid	C9H18O3	M+NH4	192.1594	-2.2
	HMDB0179169	1,8-dihydroxynonan-4-one	C9H18O3	M+NH4	192.1594	-2.2
	HMDB0179172	1,5-dihydroxynonan-4-one	C9H18O3	M+NH4	192.1594	-2.2
	HMDB0179170	SCHEMBL1635	C9H18O3	M+NH4	192.1594	-2.2
	HMDB0179171	1,3-dihydroxynonan-4-one	C9H18O3	M+NH4	192.1594	-2.2
	HMDB0179999	2-hydroxy-7-methyloctanoic acid	C9H18O3	M+NH4	192.1594	-2.2
	HMDB0179998	SCHEMBL9379	C9H18O3	M+NH4	192.1594	-2.2
	HMDB0179997	SCHEMBL3537	C9H18O3	M+NH4	192.1594	-2.2
	HMDB0034040	2,4,6-Triethyl-1,3,5-trioxane	C9H18O3	M+NH4	192.1594	-2.2
	HMDB0031513	3-Hydroxynonanoic acid	C9H18O3	M+NH4	192.1594	-2.2
	HMDB0170939	9-Hydroxynonanoic acid	C9H18O3	M+NH4	192.1594	-2.2
	HMDB0170938	8-hydroxy-nonanoic acid	C9H18O3	M+NH4	192.1594	-2.2
193.0621	HMDB0032582	2-Biphenylol	C12H10O	M+Na	193.0624	-1.5
	HMDB0182512	2-(hex-2,4-diynyl)phenol	C12H10O	M+Na	193.0624	-1.5
	HMDB0182513	3-(hexa-2,4-diyn-1-yl)phenol	C12H10O	M+Na	193.0624	-1.5
	HMDB0174873	biphenyl-3-ol	C12H10O	M+Na	193.0624	-1.5
	HMDB0174872	4-Phenylphenol	C12H10O	M+Na	193.0624	-1.5
	HMDB0032412	Methyl beta-naphthyl ketone	C12H10O	M+Na	193.0624	-1.5
	HMDB0034446	Diphenyl ether	C12H10O	M+Na	193.0624	-1.5
	HMDB0182514	4-(hexa-2,4-diyn-1-yl)phenol	C12H10O	M+Na	193.0624	-1.5
193.0992	HMDB0040464	Dowicide A	C12H9NaO	M+H	193.0624	-1.5
	HMDB0059701	1,6,7-Trimethylnaphthalene	C13H14	M+Na	193.0988	2.2
193.1183	HMDB0059733	1,4,5-Trimethyl-naphtalene	C13H14	M+Na	193.0988	2.2
	HMDB0094717	hydroxyvaleryl-glycine	C7H13NO4	M+NH4	193.1183	0.1
	HMDB0002201	N-Carboxyethyl-g-aminobutyric acid	C7H13NO4	M+NH4	193.1183	0.1
	HMDB0036383	Calystegine B5	C7H13NO4	M+NH4	193.1183	0.1
	HMDB0034252	2-Aminoheptanedioic acid	C7H13NO4	M+NH4	193.1183	0.1

	HMDB0038594	Calystegine B2	C7H13NO4	M+NH4	193.1183	0.1
193.1582	HMDB0151804	2-benzylhexan-1-ol	C13H20O	M+H	193.1587	-2.5
	HMDB0041615	Phenethyl isoamyl ether	C13H20O	M+H	193.1587	-2.5
	HMDB0032498	Pseudoionone	C13H20O	M+H	193.1587	-2.5
	HMDB0037139	4-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-butanone	C13H20O	M+H	193.1587	-2.5
	HMDB0035682	delta-Damascone	C13H20O	M+H	193.1587	-2.5
	HMDB0033545	(2E,4Z,7Z)-2,4,7-Tridecatrienal	C13H20O	M+H	193.1587	-2.5
	HMDB0036565	beta-Ionone	C13H20O	M+H	193.1587	-2.5
	HMDB0036144	Cycloionone	C13H20O	M+H	193.1587	-2.5
	HMDB0029821	2,5-Diisopropyl-4-methylphenol	C13H20O	M+H	193.1587	-2.5
	HMDB0032541	4-(2,6,6-Trimethylcyclohex-1-enyl)but-2-en-4-one	C13H20O	M+H	193.1587	-2.5
	HMDB0029824	2,4-Diisopropyl-3-methylphenol	C13H20O	M+H	193.1587	-2.5
	HMDB0029822	2,5-Diisopropyl-3-methylphenol	C13H20O	M+H	193.1587	-2.5
	HMDB0034979	gamma-Ionone	C13H20O	M+H	193.1587	-2.5
	HMDB0035753	(R)-(E)-4,7-Megastigmadien-9-one	C13H20O	M+H	193.1587	-2.5
	HMDB0034959	Edulan I	C13H20O	M+H	193.1587	-2.5
	HMDB0036818	Vitispirane	C13H20O	M+H	193.1587	-2.5
	HMDB0036022	Isospiroene	C13H20O	M+H	193.1587	-2.5
	HMDB0031733	4-(4-Methyl-3-pentenyl)-3-cyclohexene-1-carboxaldehyde	C13H20O	M+H	193.1587	-2.5
	HMDB0029823	2,4-Diisopropyl-5-methylphenol	C13H20O	M+H	193.1587	-2.5
	HMDB0029820	2,6-Diisopropyl-3-methylphenol	C13H20O	M+H	193.1587	-2.5
	HMDB0059883	alpha-Ionone	C13H20O	M+H	193.1587	-2.5
	HMDB0029825	2,3-Diisopropyl-5-methylphenol	C13H20O	M+H	193.1587	-2.5
	HMDB0036684	2,4,5,7alpha-Tetrahydro-1,4,4,7a-tetramethyl-1H-inden-2-ol	C13H20O	M+H	193.1587	-2.5
	HMDB0036027	alpha-Damascone	C13H20O	M+H	193.1587	-2.5
	HMDB0034671	(E)-5,8-Megastigmadien-4-one	C13H20O	M+H	193.1587	-2.5
194.0322	HMDB0041624	Phosphocreatinine	C4H8N3O4P	M+H	194.0325	-1.6
194.1535	HMDB0034177	(S)-4-(4-Methylphenyl)-2-pentanone	C12H16O	M+NH4	194.1539	-2.3
	HMDB0036171	3-(4-Isopropylphenyl)propanal	C12H16O	M+NH4	194.1539	-2.3
	HMDB0094661	1-phenylhexan-2-one	C12H16O	M+NH4	194.1539	-2.3
	HMDB0031569	4-Methyl-1-phenyl-2-pentanone	C12H16O	M+NH4	194.1539	-2.3
	HMDB0036021	Rhubafuran	C12H16O	M+NH4	194.1539	-2.3
	HMDB0032210	N-Cyclopropyl-trans-2-cis-6-nonadienamide	C12H19NO	M+H	194.1539	-2.3
195.0647	HMDB0146628	ZINC2222827	C10H10O4	M+H	195.0652	-2.5
	HMDB0146629	CTK4057	C10H10O4	M+H	195.0652	-2.5
	HMDB0146630	3-(2-methoxyphenyl)oxirane-2-carboxylic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0154365	3-(3-hydroxy-2-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0166608	3-(6-hydroxy-2H-1,3-benzodioxol-5-yl)propanal	C10H10O4	M+H	195.0652	-2.5
	HMDB0166607	3-(2H-1,3-benzodioxol-5-yl)-3-hydroxypropanal	C10H10O4	M+H	195.0652	-2.5
	HMDB0166609	2815-95-4	C10H10O4	M+H	195.0652	-2.5
	HMDB0166611	3-(2H-1,3-benzodioxol-5-yl)-2-hydroxypropanal	C10H10O4	M+H	195.0652	-2.5
	HMDB0166614	[3-(2H-1,3-benzodioxol-5-yl)oxiran-2-yl]methanol	C10H10O4	M+H	195.0652	-2.5
	HMDB0166613	6-[(1Z)-3-hydroxyprop-1-en-1-yl]-2H-1,3-benzodioxol-5-ol	C10H10O4	M+H	195.0652	-2.5
	HMDB0178262	(2Z)-3-(3-hydroxy-5-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0146403	SCHEMBL2535852	C10H10O4	M+H	195.0652	-2.5
	HMDB0142175	2-benzylpropanedioic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0141263	(2Z)-2-hydroxy-3-(3-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0125096	3-(4-hydroxy-3-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0125524	(2E)-3-(3-hydroxy-5-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0125588	3-(3-hydroxy-5-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0127500	3-(4-methoxyphenyl)-2-oxopropanoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0131137	3-(3-hydroxy-4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0131173	3-(4-methoxyphenyl)oxirane-2-carboxylic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0131171	(2Z)-2-hydroxy-3-(4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0131172	(2E)-3-(2-hydroxy-4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0137510	3-(4-hydroxy-2-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0140957	(2E)-3-(3-hydroxy-2-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0141265	3-(3-methoxyphenyl)-2-oxopropanoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0000954	Ferulic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0135741	3-(2-hydroxy-4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0000955	Isoferulic acid	C10H10O4	M+H	195.0652	-2.5

	HMDB0002120	Monoethyl phthalate	C10H10O4	M+H	195.0652	-2.5
	HMDB0030765	(-)-trans-3,4-Dihydro-4,8-dihydroxy-3-methyl-1H-2-benzopyran-1-one	C10H10O4	M+H	195.0652	-2.5
	HMDB0039606	Repandiol	C10H10O4	M+H	195.0652	-2.5
	HMDB0032652	Meconine	C10H10O4	M+H	195.0652	-2.5
	HMDB0037644	3-(2-Hydroxy-3-methoxyphenyl)-2-propenoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0029663	Vanillin acetate	C10H10O4	M+H	195.0652	-2.5
	HMDB0032614	Piperonyl acetate	C10H10O4	M+H	195.0652	-2.5
	HMDB0165533	Ferulic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0240705	Ferulic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0059721	mono-Benzyl malonate	C10H10O4	M+H	195.0652	-2.5
	HMDB0061686	2,5-Dihydroxycinnamic acid methyl ester	C10H10O4	M+H	195.0652	-2.5
	HMDB0134088	3-(2-hydroxy-3-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+H	195.0652	-2.5
	HMDB0124918	2-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C11H14O3	M+H	195.1016	-2.9
	HMDB0126162	3-(3-methylbut-2-en-1-yl)benzene-1,2,4-triol	C11H14O3	M+H	195.1016	-2.9
	HMDB0126161	2-(4-hydroxy-3-methylbut-2-en-1-yl)benzene-1,3-diol	C11H14O3	M+H	195.1016	-2.9
	HMDB0126163	2-[(3,3-dimethyloxiran-2-yl)methyl]benzene-1,3-diol	C11H14O3	M+H	195.1016	-2.9
	HMDB0126262	2-[(2E)-4-hydroxy-3-methylbut-2-en-1-yl]benzene-1,3-diol	C11H14O3	M+H	195.1016	-2.9
	HMDB0126462	2-[(1E)-3-hydroxy-3-methylbut-1-en-1-yl]benzene-1,3-diol	C11H14O3	M+H	195.1016	-2.9
	HMDB0126463	3-[(1E)-3-methylbut-1-en-1-yl]benzene-1,2,4-triol	C11H14O3	M+H	195.1016	-2.9
	HMDB0126466	2-[(1E)-4-hydroxy-3-methylbut-1-en-1-yl]benzene-1,3-diol	C11H14O3	M+H	195.1016	-2.9
	HMDB0126464	2-[(1E)-3-methylbut-1-en-1-yl]benzene-1,3,5-triol	C11H14O3	M+H	195.1016	-2.9
	HMDB0126465	2-[3-(propan-2-yl)oxiran-2-yl]benzene-1,3-diol	C11H14O3	M+H	195.1016	-2.9
	HMDB0166268	76773-99-4	C11H14O3	M+H	195.1016	-2.9
	HMDB0132270	5-(4-hydroxyphenyl)pentanoic acid	C11H14O3	M+H	195.1016	-2.9
	HMDB0133190	4-[(2E)-4-hydroxy-3-methylbut-2-en-1-yl]benzene-1,3-diol	C11H14O3	M+H	195.1016	-2.9
	HMDB0163609	2-hydroxy-3-methyl-2-phenylbutanoic acid	C11H14O3	M+H	195.1016	-2.9
	HMDB0163606	3-hydroxy-3-methyl-2-phenylbutanoic acid	C11H14O3	M+H	195.1016	-2.9
	HMDB0163607	4-hydroxy-3-methyl-2-phenylbutanoic acid	C11H14O3	M+H	195.1016	-2.9
	HMDB0163611	2-(4-hydroxyphenyl)-3-methylbutanoic acid	C11H14O3	M+H	195.1016	-2.9
	HMDB0163610	SCHEMBL8733687	C11H14O3	M+H	195.1016	-2.9
	HMDB0163612	AKO229142	C11H14O3	M+H	195.1016	-2.9
	HMDB0164132	(4r)-hydroxy-4-(4'-methoxyphenyl)-butan-2-one	C11H14O3	M+H	195.1016	-2.9
	HMDB0164133	SCHEMBL13742814	C11H14O3	M+H	195.1016	-2.9
	HMDB0164134	2-Butanone, 4-hydroxy-4-(4-methoxyphenyl)-	C11H14O3	M+H	195.1016	-2.9
	HMDB0171010	cis-4-Propenylsyringol	C11H14O3	M+H	195.1016	-2.9
	HMDB0182834	4-hydroxybenzyl butyrate	C11H14O3	M+H	195.1016	-2.9
	HMDB0151236	[3-(4-methoxyphenyl)-2-methyloxiran-2-yl]methanol	C11H14O3	M+H	195.1016	-2.9
	HMDB0151235	2-(3-hydroxy-2-methylprop-1-en-1-yl)-5-methoxyphenol	C11H14O3	M+H	195.1016	-2.9
	HMDB0133193	5-(3-methylbut-2-en-1-yl)benzene-1,2,4-triol	C11H14O3	M+H	195.1016	-2.9
	HMDB0133192	4-(3-methylbut-2-en-1-yl)benzene-1,2,3-triol	C11H14O3	M+H	195.1016	-2.9
	HMDB0133191	4-(4-hydroxy-3-methylbut-2-en-1-yl)benzene-1,3-diol	C11H14O3	M+H	195.1016	-2.9
	HMDB0133194	4-[(3,3-dimethyloxiran-2-yl)methyl]benzene-1,3-diol	C11H14O3	M+H	195.1016	-2.9
	HMDB0133463	4-(3-hydroxybut-1-en-1-yl)-2-methoxyphenol	C11H14O3	M+H	195.1016	-2.9
	HMDB0133484	3-hydroxy-4-(3-methoxyphenyl)butan-2-one	C11H14O3	M+H	195.1016	-2.9
	HMDB0133515	4-(3-hydroxy-5-methoxyphenyl)butan-2-one	C11H14O3	M+H	195.1016	-2.9
	HMDB0133538	1-hydroxy-4-(3-methoxyphenyl)butan-2-one	C11H14O3	M+H	195.1016	-2.9
	HMDB0141323	4-hydroxy-4-(3-methoxyphenyl)butan-2-one	C11H14O3	M+H	195.1016	-2.9
	HMDB0146411	3-(3-Methoxyphenyl)-2-methylpropanoic acid	C11H14O3	M+H	195.1016	-2.9
	HMDB0151230	3-hydroxy-2-[(4-methoxyphenyl)methyl]propanal	C11H14O3	M+H	195.1016	-2.9
	HMDB0151229	3-(4-methoxyphenyl)-2-methylpropanoic acid	C11H14O3	M+H	195.1016	-2.9
	HMDB0151228	3-hydroxy-3-(4-methoxyphenyl)-2-methylpropanal	C11H14O3	M+H	195.1016	-2.9
	HMDB0151232	2-hydroxy-3-(4-methoxyphenyl)-2-methylpropanal	C11H14O3	M+H	195.1016	-2.9
	HMDB0151233	2-(4-methoxybenzylidene)propane-1,3-diol	C11H14O3	M+H	195.1016	-2.9
	HMDB0031517	(R)-3-Hydroxy-5-phenylpentanoic acid	C11H14O3	M+H	195.1016	-2.9
	HMDB0059943	2-(2-Methylphenyl)-1,3-dioxan-5-ol	C11H14O3	M+H	195.1016	-2.9
	HMDB0179740	gamma-Methoxyisoeugenol	C11H14O3	M+H	195.1016	-2.9
	HMDB0062055	4-hydroxy-5-phenylpentanoic acid	C11H14O3	M+H	195.1016	-2.9
	HMDB0059944	2-(3-Methylphenyl)-1,3-dioxan-5-ol	C11H14O3	M+H	195.1016	-2.9
	HMDB0059942	[2-(4-Methylphenyl)-1,3-dioxolan-4-yl]methanol	C11H14O3	M+H	195.1016	-2.9

	HMDB0059945	2-(4-Methylphenyl)-1,3-dioxan-5-ol	C11H14O3	M+H	195.1016	-2.9
	HMDB0032575	Butylparaben	C11H14O3	M+H	195.1016	-2.9
	HMDB0034990	4-Methoxybenzyl propanoate	C11H14O3	M+H	195.1016	-2.9
	HMDB0041505	5-Hydroxy-2-benzyl-1,3-dioxane	C11H14O3	M+H	195.1016	-2.9
	HMDB0040730	Butyl salicylate	C11H14O3	M+H	195.1016	-2.9
	HMDB0037271	2,6-Dimethoxy-4-(1-propenyl)phenol	C11H14O3	M+H	195.1016	-2.9
	HMDB0032590	Zingerone	C11H14O3	M+H	195.1016	-2.9
	HMDB0041506	2-Benzyl-5-hydroxymethyl-1,3-dioxolane	C11H14O3	M+H	195.1016	-2.9
	HMDB0036432	Isobutyl salicylate	C11H14O3	M+H	195.1016	-2.9
	HMDB0034206	Ethyl 4-methylphenoxyacetate	C11H14O3	M+H	195.1016	-2.9
	HMDB0041194	Methoxyeugenol	C11H14O3	M+H	195.1016	-2.9
	HMDB0031984	2,5-Dimethoxy-4-(2-propenyl)phenol	C11H14O3	M+H	195.1016	-2.9
	HMDB0041666	3-Hydroxyphenyl-valeric acid	C11H14O3	M+H	195.1016	-2.9
	HMDB0059898	Ethyl 4-ethoxybenzoate	C11H14O3	M+H	195.1016	-2.9
	HMDB0059941	[2-(3-Methylphenyl)-1,3-dioxolan-4-yl]methanol	C11H14O3	M+H	195.1016	-2.9
	HMDB0059940	[2-(2-Methylphenyl)-1,3-dioxolan-4-yl]methanol	C11H14O3	M+H	195.1016	-2.9
195.1225	HMDB0094708	Tetraethylene glycol	C8H18O5	M+H	195.1227	-1.0
195.1375	HMDB0132986	1-(4-methoxyphenyl)pentan-3-ol	C12H18O2	M+H	195.1380	-2.3
	HMDB0041610	(2,2-Diethoxyethyl)benzene	C12H18O2	M+H	195.1380	-2.3
	HMDB0032567	Hexylresorcinol	C12H18O2	M+H	195.1380	-2.3
	HMDB0034450	Neocnidilide	C12H18O2	M+H	195.1380	-2.3
	HMDB0035126	Myrtenyl acetate	C12H18O2	M+H	195.1380	-2.3
	HMDB0037231	Perillyl acetate	C12H18O2	M+H	195.1380	-2.3
	HMDB0037018	(S)-p-Mentha-1,8-dien--yl acetate	C12H18O2	M+H	195.1380	-2.3
	HMDB0038046	Carvyl acetate	C12H18O2	M+H	195.1380	-2.3
	HMDB0040439	1-(2-Furanyl)-1-octanone	C12H18O2	M+H	195.1380	-2.3
	HMDB0038292	Menthadienyl acetate	C12H18O2	M+H	195.1380	-2.3
	HMDB0037389	(R)-2-Acetoxy-p-mentha-1,8-diene	C12H18O2	M+H	195.1380	-2.3
	HMDB0039685	8-Ocimenyl acetate	C12H18O2	M+H	195.1380	-2.3
	HMDB0041497	(S)-Neolylratyl acetate	C12H18O2	M+H	195.1380	-2.3
	HMDB0031840	(S,Z)-Lyratol acetate	C12H18O2	M+H	195.1380	-2.3
	HMDB0035376	Ethyl (2E,4Z,7Z)-Decatrienoate	C12H18O2	M+H	195.1380	-2.3
	HMDB0035375	Ethyl (2E,4E,7Z)-Decatrienoate	C12H18O2	M+H	195.1380	-2.3
	HMDB0014018	4-Hydroxypropofol	C12H18O2	M+H	195.1380	-2.3
	HMDB0035801	(2S,4R)-p-Mentha-1(7),5-dien-2-ol acetate	C12H18O2	M+H	195.1380	-2.3
195.1738	HMDB0038897	(E)-2-(2-Octenyl)cyclopentanone	C13H22O	M+H	195.1743	-2.8
	HMDB0182746	4-(2,2-Dimethyl-6-methylenecyclohexyl)butan-2-one	C13H22O	M+H	195.1743	-2.8
	HMDB0163188	SCHEMBL15656566	C13H22O	M+H	195.1743	-2.8
	HMDB0163189	(2E,4E,7Z)-trideca-2,4,7-trien-1-ol	C13H22O	M+H	195.1743	-2.8
	HMDB0178134	3-[(2Z)-but-2-en-1-yl]-2,4,4-trimethylcyclohexan-1-one	C13H22O	M+H	195.1743	-2.8
	HMDB0038731	4,7-Megastigmadien-9-ol	C13H22O	M+H	195.1743	-2.8
	HMDB0038026	Dihydro-alpha-ionone	C13H22O	M+H	195.1743	-2.8
	HMDB0038216	5-Isopropyl-2-(2-methylpropyl)-2-cyclohexen-1-one	C13H22O	M+H	195.1743	-2.8
	HMDB0032913	4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-butanone	C13H22O	M+H	195.1743	-2.8
	HMDB0036823	Theaspirane	C13H22O	M+H	195.1743	-2.8
	HMDB0036026	Octahydro-6-isopropyl-2(1H)-naphthalenone	C13H22O	M+H	195.1743	-2.8
	HMDB0031846	Geranylacetone	C13H22O	M+H	195.1743	-2.8
	HMDB0036184	7,8-Dehydro-3,4-dihydro-beta-ionol	C13H22O	M+H	195.1743	-2.8
	HMDB0036820	beta-Ionol	C13H22O	M+H	195.1743	-2.8
	HMDB0032355	(+/-)-[R-(E)]-5-Isopropyl-8-methylnona-6,8-dien-2-one	C13H22O	M+H	195.1743	-2.8
195.9768	HMDB0000250	Pyrophosphate	H4O7P2	M+NH4	195.9770	-1.3
	HMDB0155221	Pyrophosphate	H4O7P2	M+NH4	195.9770	-1.3
196.1192	HMDB0029569	Dibutyl disulfide	C8H18S2	M+NH4	196.1188	2.0
	HMDB0040348	1,8-Octanedithiol	C8H18S2	M+NH4	196.1188	2.0
	HMDB0126149	2-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0151221	3-(4-methoxyphenyl)-2-methylpropanal	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0151222	3-(4-methoxyphenyl)-2-methylprop-2-en-1-ol	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0163593	SCHEMBL11476137	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0163592	38-94-9	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0163594	4-hydroxy-3-methyl-2-phenylbutanal	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0163597	SCHEMBL9714781	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0163596	2-hydroxy-3-methyl-2-phenylbutanal	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0163598	SCHEMBL9714564	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0133687	1-hydroxy-3-methyl-4-phenylbutan-2-one	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0133686	3-benzyl-4-hydroxybutan-2-one	C11H14O2	M+NH4	196.1332	-2.6

196.1327	HMDB0126449	2-[(1E)-3-methylbut-1-en-1-yl]benzene-1,3-diol	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0132981	1-(4-hydroxyphenyl)pentan-3-one	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0133181	4-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0133469	4-(3-methoxyphenyl)butan-2-one	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0133683	4-hydroxy-3-methyl-4-phenylbutan-2-one	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0133682	3-hydroxy-3-methyl-4-phenylbutan-2-one	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0133684	4-(3-hydroxyphenyl)-3-methylbutan-2-one	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0133685	4-(4-hydroxyphenyl)-3-methylbutan-2-one	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0040583	2-Methylpropyl benzoate	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0031864	Methyleugenol	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0036235	alpha, alpha-Dimethylphenethyl formate	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0040356	Osmorhizole	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0037708	p-Tolyl isobutyrate	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0040287	1-Phenylethyl propanoate	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0031250	Phenylmethyl 2-methylpropanoate	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0033376	Phenylmethyl butanoate	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0033386	3-Phenylpropyl acetate	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0033597	4-(4-Methoxyphenyl)-2-butanone	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0036385	Methyl 4-phenylbutanoate	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0002043	5-Phenylvaleric acid	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0040425	Propyl phenylacetate	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0041553	Methylisoeugenol	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0035013	2-Phenylethyl propanoate	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0037680	2-Methylphenyl 2-methylpropanoate	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0038179	3-(2-Hydroxy-4-methylphenyl)-2-butanone	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0040426	Isopropyl phenylacetate	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0040800	2-Ethoxy-5-(1-propenyl)phenol	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0040411	Ethyl 3-phenylpropanoate	C11H14O2	M+NH4	196.1332	-2.6
	HMDB0060954	p-hydroxymexiletine	C11H17NO2	M+H	196.1332	-2.6
	HMDB0060953	2-hydroxymexiletine	C11H17NO2	M+H	196.1332	-2.6
196.1693	HMDB0032579	2,5-Diisopropylphenol	C12H18O	M+NH4	196.1696	-1.5
	HMDB0038107	Quinceoxepine	C12H18O	M+NH4	196.1696	-1.5
	HMDB0031731	3-Methyl-1-phenyl-3-pentanol	C12H18O	M+NH4	196.1696	-1.5
	HMDB0035055	Photocitral A	C12H18O	M+NH4	196.1696	-1.5
	HMDB0036681	7-Isopropyl-5-methylbicyclo[2.2.2]oct-5-en-2-one	C12H18O	M+NH4	196.1696	-1.5
	HMDB0037272	2-Ethoxy-1-methyl-4-(1-methylethyl)benzene	C12H18O	M+NH4	196.1696	-1.5
	HMDB0031194	Tricycloekasantal	C12H18O	M+NH4	196.1696	-1.5
	HMDB0031568	4-Methyl-1-phenyl-2-pentanol	C12H18O	M+NH4	196.1696	-1.5
	HMDB0038194	Geijerone	C12H18O	M+NH4	196.1696	-1.5
	HMDB0014956	Propofol	C12H18O	M+NH4	196.1696	-1.5
	HMDB0037898	2,5-Dibutyl-4-methyloxazole	C12H21NO	M+H	196.1696	-1.5
	HMDB0037902	4,5-Dimethyl-2-heptyloxazole	C12H21NO	M+H	196.1696	-1.5
	HMDB0037899	5-Ethyl-2-hexyl-4-methyloxazole	C12H21NO	M+H	196.1696	-1.5
	HMDB0037901	4-Ethyl-2-hexyl-5-methyloxazole	C12H21NO	M+H	196.1696	-1.5
	HMDB0037900	4-Methyl-2-pentyl-5-propyloxazole	C12H21NO	M+H	196.1696	-1.5
	HMDB0060703	1-Amino-3-hydroxymethyl-5-methyl-adamantane	C12H21NO	M+H	196.1696	-1.5
	HMDB0060738	3-Amino-1-hydroxy-5,7-dimethyl-adamantane	C12H21NO	M+H	196.1696	-1.5
197.0568	HMDB0031845	3-Propylidene-1(3H)-isobenzofuranone	C11H10O2	M+Na	197.0573	-2.5
	HMDB0032727	4-Methoxy-1-naphthol	C11H10O2	M+Na	197.0573	-2.5
	HMDB0166920	Menadiol	C11H10O2	M+Na	197.0573	-2.5
197.0684	HMDB0006240	Demethylated antipyrine	C10H10N2O	M+Na	197.0685	-0.7
	HMDB0029739	1H-Indole-3-acetamide	C10H10N2O	M+Na	197.0685	-0.7
197.0951	HMDB0029442	(R)C(R)S-S-Propylcysteine sulfoxide	C6H13NO3S	M+NH4	197.0954	-1.7
	HMDB0172921	NSC6266	C6H13NO3S	M+NH4	197.0954	-1.7
	HMDB0031340	Cyclamic acid	C6H13NO3S	M+NH4	197.0954	-1.7
	HMDB0172920	2-amino-3-(2-hydroxypropylsulfanyl)propanoic acid	C6H13NO3S	M+NH4	197.0954	-1.7
197.1047	HMDB0004370	N-Methyltryptamine	C11H14N2	M+Na	197.1049	-1.1
	HMDB0033755	2-Butyl-1H-benzimidazole	C11H14N2	M+Na	197.1049	-1.1
	HMDB0035762	3-(Dimethylaminomethyl)indole	C11H14N2	M+Na	197.1049	-1.1
197.1168	HMDB0135672	4-(3-hydroxybutyl)-2-methoxyphenol	C11H16O3	M+H	197.1172	-2.1
	HMDB0179541	3-methoxy-2-methyl-5-(propan-2-yl)benzene-1,4-diol	C11H16O3	M+H	197.1172	-2.1
	HMDB0036226	2,6-Dimethoxy-4-propylphenol	C11H16O3	M+H	197.1172	-2.1
	HMDB0037734	Isobutyl 2-furanpropionate	C11H16O3	M+H	197.1172	-2.1
	HMDB0037725	Hexyl 2-furoate	C11H16O3	M+H	197.1172	-2.1
	HMDB0179545	3-methoxy-5-methyl-2-(propan-2-yl)benzene-1,4-diol	C11H16O3	M+H	197.1172	-2.1

197.1284	HMDB0040021	2,3-Dihydro-5-(3-hydroxypropanoyl)-1H-pyrrolizine	C10H13NO2	M+NH4	197.1285	-0.3
	HMDB0033763	Ethyl N-methylanthranilate	C10H13NO2	M+NH4	197.1285	-0.3
	HMDB0039655	1,2,3,4,5,6-Hexahydro-5-(1-hydroxyethylidene)-7H-cyclopenta[b]pyridin-7-one	C10H13NO2	M+NH4	197.1285	-0.3
	HMDB0031811	3,5-Dimethylphenyl methylcarbamate	C10H13NO2	M+NH4	197.1285	-0.3
	HMDB0005199	(R)-Salsolinol	C10H13NO2	M+NH4	197.1285	-0.3
	HMDB0001189	2(N)-Methyl-norsalsolinol	C10H13NO2	M+NH4	197.1285	-0.3
	HMDB0041931	3,4-Methylenedioxyamphetamine	C10H13NO2	M+NH4	197.1285	-0.3
	HMDB0030372	Maltoxazine	C10H13NO2	M+NH4	197.1285	-0.3
	HMDB0042012	Salsolinol	C10H13NO2	M+NH4	197.1285	-0.3
	HMDB0029224	N-methylphenylalanine	C10H13NO2	M+NH4	197.1285	-0.3
	HMDB0029223	alpha-Methylphenylalanine	C10H13NO2	M+NH4	197.1285	-0.3
	HMDB0029741	2-Isopropyl-3,5-dimethoxy-6-methylpyrazine	C10H16N2O2	M+H	197.1285	-0.3
	HMDB0040551	L-alpha-Amino-1H-pyrrole-1-hexanoic acid	C10H16N2O2	M+H	197.1285	-0.3
197.1531	HMDB0240493	Cyclo(L-prolyl-L-valyl)	C10H16N2O2	M+H	197.1285	-0.3
	HMDB0031692	cis-3-Hexenyl trans-4-hexenoate	C12H20O2	M+H	197.1536	-2.6
	HMDB0030867	Dihydro-5-(2-octenyl)-2(3H)-furanone	C12H20O2	M+H	197.1536	-2.6
	HMDB0038270	cis-3-Hexenyl cis-3-hexenoate	C12H20O2	M+H	197.1536	-2.6
	HMDB0030945	Methyl 2-undecynoate	C12H20O2	M+H	197.1536	-2.6
	HMDB0039522	Linalyl acetate	C12H20O2	M+H	197.1536	-2.6
	HMDB0040725	Fenchyl acetate	C12H20O2	M+H	197.1536	-2.6
	HMDB0036048	Artemisia alcohol acetate	C12H20O2	M+H	197.1536	-2.6
	HMDB0040397	(-)-Bornyl acetate	C12H20O2	M+H	197.1536	-2.6
	HMDB0040206	Allyl 3-cyclohexylpropionate	C12H20O2	M+H	197.1536	-2.6
	HMDB0031030	6-Heptyl-5,6-dihydro-2H-pyran-2-one	C12H20O2	M+H	197.1536	-2.6
	HMDB0036599	Ethyl 2Z,4E-decadienoic acid	C12H20O2	M+H	197.1536	-2.6
	HMDB0034903	(3R,3aR,7aS)-3-Butylhexahydro-1(3H)-isobenzofuranone	C12H20O2	M+H	197.1536	-2.6
	HMDB0032901	Yuzu lactone	C12H20O2	M+H	197.1536	-2.6
	HMDB0038280	cis-3-Hexenyl trans-2-hexenoate	C12H20O2	M+H	197.1536	-2.6
	HMDB0041469	Dihydrocarveol acetate	C12H20O2	M+H	197.1536	-2.6
	HMDB0032193	alpha-Campholene acetate	C12H20O2	M+H	197.1536	-2.6
	HMDB0032051	alpha-Terpineol acetate	C12H20O2	M+H	197.1536	-2.6
	HMDB0041494	(S)-Santolina acetate	C12H20O2	M+H	197.1536	-2.6
	HMDB0061816	3,7-Dimethyl-2,6-octadien-1-ylacetate	C12H20O2	M+H	197.1536	-2.6
	HMDB0040227	Isopulegol acetate	C12H20O2	M+H	197.1536	-2.6
	HMDB0037301	p-Menth-1-en-9-ol acetate	C12H20O2	M+H	197.1536	-2.6
	HMDB0032331	(Z)-4-Hydroxy-6-dodecenoic acid lactone	C12H20O2	M+H	197.1536	-2.6
	HMDB0062144	p-Menth-1-en-4-yl acetate	C12H20O2	M+H	197.1536	-2.6
197.1897	HMDB0035157	geranyl acetate	C12H20O2	M+H	197.1536	-2.6
	HMDB0032247	(Z)-4-Dodecenal	C13H24O	M+H	197.1900	-1.5
	HMDB0036172	4-(2,6,6-Trimethyl-1-cyclohexenyl)-2-butanol	C13H24O	M+H	197.1900	-1.5
	HMDB0041404	2-Methylcyclododecanone	C13H24O	M+H	197.1900	-1.5
	HMDB0037275	2-Tridecenal	C13H24O	M+H	197.1900	-1.5
	HMDB0041490	Dihydrogeranylacetone	C13H24O	M+H	197.1900	-1.5
	HMDB0163217	57981-61	C13H24O	M+H	197.1900	-1.5
	HMDB0062100	(3R,4R,5S)-5-[(1R)-1,2-dihydroxyethyl]oxolane-2,3,4-triol	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0062113	(3R,4R,5S)-5-[(1R)-1,2-dihydroxyethyl]-3,4-dihydroxyoxolan-2-olate	C6H11O6	M+NH4	198.0972	-2.6
	HMDB0062138	muco-Inositol	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0062473	Glycoprotein-phospho-D-mannose	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0033704	alpha-L-galactose	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0166371	SCHEMBL14339418	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0240208	neo-inositol	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0240210	cis-inositol	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0003418	D-Tagatose	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0125599	2,5-bis(hydroxymethyl)oxolane-2,3,4-triol	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0000660	D-Fructose	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0001151	Allose	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0001266	L-Sorbose	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0003345	alpha-D-Glucose	C6H12O6	M+NH4	198.0972	-2.6

198.0967	HMDB0061922	alpha-D-Glucose	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0003449	Beta-D-Galactose	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0240207	epi-Inositol	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0012326	L-Gulose	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0155830	Inositol	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0000122	Beta-D-Glucose	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0062170	Beta-D-Glucose	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0000516	Beta-D-Glucose	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0000346	3-Deoxyarabinohexonic acid	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0000211	myo-Inositol	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0006088	scyllo-Inositol	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0000143	D-Galactose	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0240209	D-chiro-Inositol	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0240211	allo-Inositol	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0034220	Levoinositol	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0155309	keto-D-fructose	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0032222	Dihydroxyacetone (dimer)	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0062538	Fructose-1P	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0000169	Alpha-D-Mannose	C6H12O6	M+NH4	198.0972	-2.6
	HMDB0062086	beta-D-galactofuranose	C6H12O6	M+NH4	198.0972	-2.6
198.1272	HMDB0036173	2-(3-Phenylpropyl)pyridine	C14H15N	M+H	198.1277	-2.6
198.1484	HMDB0151242	3-(4-methoxyphenyl)-2-methylpropan-1-ol	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0164135	4-(4-methoxyphenyl)butan-2-ol	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0163240	(2E,5Z)-undeca-2,5,-trienoic acid	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0163599	3-methyl-2-phenylbutane-1,3-diol	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0176254	3-(3-hydroxy-3-methylbutyl)phenol	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0176256	2-(3-hydroxy-3-methylbutyl)phenol	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0176255	4-(3-hydroxy-3-methylbutyl)phenol	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0176253	3-methyl-1-phenylbutane-1,3-diol	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0176252	AKO231874	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0163603	SCHEMBL182446	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0163602	3-methyl-2-phenylbutane-1,2-diol	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0163605	2-(1-hydroxy-3-methylbutan-2-yl)phenol	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0163604	SCHEMBL12872219	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0163600	2-methyl-3-phenylbutane-1,4-diol	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0059926	2-tert-Butyl-4-hydroxyanisole	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0059925	3-tert-Butyl-4-hydroxyanisole	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0036669	(+)-Myrtenyl formate	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0032468	2-Phenylpropionaldehyde dimethyl acetal	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0030039	Jasmolone	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0039957	4-(Butoxymethyl)phenol	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0035240	Dihydroactinidiolide	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0030007	2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]nona-3,8-diene	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0039159	Bovolid	C11H16O2	M+NH4	198.1489	-2.3
	HMDB0036817	Norecasantic acid	C11H16O2	M+NH4	198.1489	-2.3
198.1848	HMDB0038108	cis-Quinceoxepane	C12H20O	M+NH4	198.1852	-2.2
	HMDB0032531	2-trans-6-cis-Dodecadienal	C12H20O	M+NH4	198.1852	-2.2
	HMDB0031181	Homodihydrojasmone	C12H20O	M+NH4	198.1852	-2.2
	HMDB0039339	Tricycloekasantanol	C12H20O	M+NH4	198.1852	-2.2
	HMDB0039590	(2E,4E)-2,4-Dodecadienal	C12H20O	M+NH4	198.1852	-2.2
199.0321	HMDB0000828	Ureidosuccinic acid	C5H8N2O5	M+Na	199.0325	-2.2
	HMDB0038668	L-3-Amino-2-(oxalylamino)propanoic acid	C5H8N2O5	M+Na	199.0325	-2.2
	HMDB0029402	L-2-Amino-3-(oxalylamino)propanoic acid	C5H8N2O5	M+Na	199.0325	-2.2
	HMDB0159928	N-carbamoylaspartic acid	C5H8N2O5	M+Na	199.0325	-2.2
199.0726	HMDB0126379	2,2-dimethyl-2H-chromen-5-ol	C11H12O2	M+Na	199.0729	-1.7
	HMDB0126467	2-[(1E)-3-methylbuta-1,3-dien-1-yl]benzene-1,3-diol	C11H12O2	M+Na	199.0729	-1.7
	HMDB0163608	alpha-Isopropenylbenzeneacetic acid	C11H12O2	M+Na	199.0729	-1.7
	HMDB0151237	119711-59	C11H12O2	M+Na	199.0729	-1.7
	HMDB0151231	2-(4-methoxybenzyl)acrylaldehyde	C11H12O2	M+Na	199.0729	-1.7
	HMDB0133680	4-(4-hydroxyphenyl)-3-methylbut-3-en-2-one	C11H12O2	M+Na	199.0729	-1.7
	HMDB0133681	1-(2-methyl-3-phenyloxiran-2-yl)ethan-1-one	C11H12O2	M+Na	199.0729	-1.7
	HMDB0133679	4-(3-hydroxyphenyl)-3-methylbut-3-en-2-one	C11H12O2	M+Na	199.0729	-1.7
	HMDB0133677	1-hydroxy-3-methyl-4-phenylbut-3-en-2-one	C11H12O2	M+Na	199.0729	-1.7
	HMDB0133678	3-(hydroxymethyl)-4-phenylbut-3-en-2-one	C11H12O2	M+Na	199.0729	-1.7
	HMDB0133466	4-(3-methoxyphenyl)but-3-en-2-one	C11H12O2	M+Na	199.0729	-1.7

	HMDB0132973	(1E)-1-(4-hydroxyphenyl)pent-1-en-3-one	C11H12O2	M+Na	199.0729	-1.7
	HMDB0033834	Ethyl cinnamate	C11H12O2	M+Na	199.0729	-1.7
	HMDB0037145	3-(4-Methoxyphenyl)-2-methyl-2-propenal	C11H12O2	M+Na	199.0729	-1.7
	HMDB0037142	2-(Phenylethenyl)-1,3-dioxolane	C11H12O2	M+Na	199.0729	-1.7
	HMDB0029699	Cinnamyl acetate	C11H12O2	M+Na	199.0729	-1.7
	HMDB0036905	2-Propenyl phenylacetate	C11H12O2	M+Na	199.0729	-1.7
	HMDB0132267	5-benzylloxolan-2-one	C11H12O2	M+Na	199.0729	-1.7
199.0961	HMDB0135755	4-ethyl-2,6-dimethoxybenzene-1,3-diol	C10H14O4	M+H	199.0965	-1.9
	HMDB0131265	2,3,5-trimethoxy-6-methylphenol	C10H14O4	M+H	199.0965	-1.9
	HMDB0059779	2,3-Methylene suberic acid	C10H14O4	M+H	199.0965	-1.9
	HMDB0059768	3,4-Methylene suberic acid	C10H14O4	M+H	199.0965	-1.9
	HMDB0030991	5-(3E-Pentenyl)tetrahydro-2-oxo-3-furancarboxylic acid	C10H14O4	M+H	199.0965	-1.9
	HMDB0033093	3-(4-Hydroxy-3-methoxyphenyl)-1,2-propanediol	C10H14O4	M+H	199.0965	-1.9
	HMDB0034099	(2E,4E)-2,7-Dimethyl-2,4-octadienedioic acid	C10H14O4	M+H	199.0965	-1.9
	HMDB0177594	1-(3,4-dimethoxyphenyl)ethane-1,2-diol	C10H14O4	M+H	199.0965	-1.9
199.1325	HMDB0004998	Guaiifenesin	C10H14O4	M+H	199.0965	-1.9
	HMDB0163241	(2E,5Z)-7-hydroxyundeca-2,5-dienoic acid	C11H18O3	M+H	199.1329	-1.9
	HMDB0163242	3-[(2Z)-oct-2-en-1-yl]oxirane-2-carboxylic acid	C11H18O3	M+H	199.1329	-1.9
	HMDB0163243	(2E)-4-(3-pentylloxiran-2-yl)but-2-enoic acid	C11H18O3	M+H	199.1329	-1.9
	HMDB0178762	methyl (4Z,8Z)-7-hydroxydeca-4,8-dienoate	C11H18O3	M+H	199.1329	-1.9
	HMDB0178763	methyl (4Z,8Z)--hydroxydeca-4,8-dienoate	C11H18O3	M+H	199.1329	-1.9
	HMDB0178764	methyl (4Z,8Z)-3-hydroxydeca-4,8-dienoate	C11H18O3	M+H	199.1329	-1.9
	HMDB0178766	methyl (4Z)-7-(3-methylloxiran-2-yl)hept-4-enoate	C11H18O3	M+H	199.1329	-1.9
	HMDB0178765	methyl (4Z,8Z)-6-hydroxydeca-4,8-dienoate	C11H18O3	M+H	199.1329	-1.9
	HMDB0178767	methyl 3-{3-[(3Z)-pent-3-en-1-yl]oxiran-2-yl}propanoate	C11H18O3	M+H	199.1329	-1.9
	HMDB0178768	methyl (4Z,8Z)-2-hydroxydeca-4,8-dienoate	C11H18O3	M+H	199.1329	-1.9
	HMDB0179397	methyl 3-[(1Z)-hept-1-en-1-yl]oxirane-2-carboxylate	C11H18O3	M+H	199.1329	-1.9
	HMDB0179396	methyl (2E,4Z)-9-hydroxydeca-2,4-dienoate	C11H18O3	M+H	199.1329	-1.9
	HMDB0179395	methyl (4Z)-6-hydroxydeca-2,4-dienoate	C11H18O3	M+H	199.1329	-1.9
	HMDB0179398	methyl (2E)-3-(3-pentylloxiran-2-yl)prop-2-enoate	C11H18O3	M+H	199.1329	-1.9
	HMDB0163239	(2E,5Z)-11-hydroxyundeca-2,5-dienoic acid	C11H18O3	M+H	199.1329	-1.9
	HMDB0163238	(2E,5Z)--hydroxyundeca-2,5-dienoic acid	C11H18O3	M+H	199.1329	-1.9
	HMDB0179399	methyl (2E,4Z)--hydroxydeca-2,4-dienoate	C11H18O3	M+H	199.1329	-1.9
199.1687	HMDB0000529	5Z-Dodecenoic acid	C12H22O2	M+H	199.1693	-2.8
	HMDB0038081	2-Octenyl butyrate	C12H22O2	M+H	199.1693	-2.8
	HMDB0029763	Allyl nonanoate	C12H22O2	M+H	199.1693	-2.8
	HMDB0040158	Hexyl 2-methyl-3-pentenoate	C12H22O2	M+H	199.1693	-2.8
	HMDB0033378	cis-3-Hexenyl hexanoate	C12H22O2	M+H	199.1693	-2.8
	HMDB0037498	1-Ethenylhexyl butanoate	C12H22O2	M+H	199.1693	-2.8
	HMDB0039220	Ethyl 4-decenoate	C12H22O2	M+H	199.1693	-2.8
	HMDB0029585	Methyl -undecenoate	C12H22O2	M+H	199.1693	-2.8
	HMDB0037186	Rhodinyl acetate	C12H22O2	M+H	199.1693	-2.8
	HMDB0040361	1,1-Dimethoxy-3,7-dimethyl-2,6-octadiene	C12H22O2	M+H	199.1693	-2.8
	HMDB0036182	5,5-Dibutyl-4,5-dihydro-2(3H)furanone	C12H22O2	M+H	199.1693	-2.8
	HMDB0038895	7-Hexyl-2-oxepanone	C12H22O2	M+H	199.1693	-2.8
	HMDB0010729	trans-Dodec-2-enoic acid	C12H22O2	M+H	199.1693	-2.8
	HMDB0037742	xi-5-Dodecanolide	C12H22O2	M+H	199.1693	-2.8
	HMDB0031683	xi-Dihydro-5-octyl-2(3H)-furanone	C12H22O2	M+H	199.1693	-2.8
	HMDB0037305	Methyl 9-undecenoate	C12H22O2	M+H	199.1693	-2.8
	HMDB0041264	Menthyl acetate	C12H22O2	M+H	199.1693	-2.8
	HMDB0037813	3-Heptyldihydro-5-methyl-2(3H)-furanone	C12H22O2	M+H	199.1693	-2.8
	HMDB0038269	Hexyl 2E-hexenoate	C12H22O2	M+H	199.1693	-2.8
	HMDB0034844	Citronellyl acetate	C12H22O2	M+H	199.1693	-2.8
	HMDB0037329	Ethyl 2-decenoate	C12H22O2	M+H	199.1693	-2.8
	HMDB0041449	[(3,7-Dimethyl-6-octenyl)oxy]acetaldehyde	C12H22O2	M+H	199.1693	-2.8
	HMDB0040163	Hexyl 2-methyl-4-pentenoate	C12H22O2	M+H	199.1693	-2.8
	HMDB0038924	2-Hexenyl hexanoate	C12H22O2	M+H	199.1693	-2.8
	HMDB0034160	Citronellyl acetate	C12H22O2	M+H	199.1693	-2.8
	HMDB0032214	cis-4-Decenyl acetate	C12H22O2	M+H	199.1693	-2.8
	HMDB0032248	11-Dodecenoic acid	C12H22O2	M+H	199.1693	-2.8
	HMDB0032235	2,6-Dimethyl-5-heptenal propyleneglycol acetal	C12H22O2	M+H	199.1693	-2.8
199.2060	HMDB0034148	2-Tridecanone	C13H26O	M+H	199.2056	1.8
	HMDB0062117	6,-Dimethylundecan-2-one	C13H26O	M+H	199.2056	1.8

200.1124	HMDB0030928	Tridecanal	C13H26O	M+H	199.2056	1.8
	HMDB0000765	Mannitol	C6H14O6	M+NH4	200.1129	-2.3
	HMDB0000247	Sorbitol	C6H14O6	M+NH4	200.1129	-2.3
	HMDB0000107	Galactitol	C6H14O6	M+NH4	200.1129	-2.3
200.1276	HMDB0011632	L-Iditol	C6H14O6	M+NH4	200.1129	-2.3
	HMDB0142086	4-ethyl-2,3-dimethoxyphenol	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179477	6-hydroxy-2-methyl-5-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0145930	SCHEMBL83728	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0163112	3-[(1Z,4Z)-hepta-1,4-dien-1-yl]oxirane-2-carboxylic acid	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179475	1-methyl-4-(propan-2-yl)-7-oxabicyclo[4.1]heptane-2,5-dione	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179480	2,5-dihydroxy-4-isopropylbenzyl alcohol	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179483	2-(1-hydroxypropan-2-yl)-5-methylbenzene-1,4-diol	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179479	CTK8G51	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179482	6-methyl-3-(propan-2-yl)benzene-1,2,4-triol	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0181695	2-(hydroxymethyl)-3-methyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0181694	3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0181696	5-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0181697	1-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179478	2-hydroxy-2-isopropyl-5-methylcyclohex-5-ene-1,4-dione	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179476	5-(1-hydroxypropan-2-yl)-2-methylcyclohex-2-ene-1,4-dione	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0163114	(2E,4Z)-6-(3-ethyloxiran-2-yl)hexa-2,4-dienoic acid	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0163111	(2E,7Z)-9-hydroxydeca-2,4,7-trienoic acid	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0163113	(2E)-3-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}prop-2-enoic acid	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0163115	(2E,4Z,7Z)--hydroxydeca-2,4,7-trienoic acid	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179467	5-(hydroxymethyl)-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179468	5-hydroxy-5-methyl-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179470	4-methyl-1-(propan-2-yl)-7-oxabicyclo[4.1]heptane-2,5-dione	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179469	2-(2-hydroxypropan-2-yl)-5-methylcyclohex-2-ene-1,4-dione	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179473	2-(hydroxymethyl)-5-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179474	5-(2-hydroxypropan-2-yl)-2-methylcyclohex-2-ene-1,4-dione	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179471	2-(1-hydroxypropan-2-yl)-5-methylcyclohex-2-ene-1,4-dione	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179472	6-hydroxy-5-methyl-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0037641	4-(Ethoxymethyl)-2-methoxyphenol	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0059891	Isoamyl 2-furoate	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0036522	Verimol J	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0033394	4-Ethyl-2,6-dimethoxyphenol	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0037727	Furfuryl pentanoate	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0038354	2-Ethoxy-4-(methoxymethyl)phenol	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0032607	threo-Anethole glycol	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0038181	Peperinic acid	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0029456	Amyl 2-furoate	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0039874	Furfuryl isovalerate	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0179481	4427-54-7	C10H14O3	M+NH4	200.1281	-2.6
	HMDB0094803	2-[(1-hydroxyoct-4-en-1-ylidene)amino]acetic acid	C10H17NO3	M+H	200.1281	-2.6
	HMDB0006406	Ecgonine methyl ester	C10H17NO3	M+H	200.1281	-2.6
	HMDB0031820	Neotussilagine	C10H17NO3	M+H	200.1281	-2.6
	HMDB0094802	2-[(1-hydroxyoct-3-en-1-ylidene)amino]acetic acid	C10H17NO3	M+H	200.1281	-2.6

	HMDB0094804	2-[(1-hydroxyoct-5-en-1-ylidene)amino]acetic acid	C10H17NO3	M+H	200.1281	-2.6
	HMDB0094805	2-[(1-hydroxyoct-6-en-1-ylidene)amino]acetic acid	C10H17NO3	M+H	200.1281	-2.6
	HMDB0094806	7-octenoylglycine	C10H17NO3	M+H	200.1281	-2.6
	HMDB0094801	2-amino-3-oxodec-4-enoic acid	C10H17NO3	M+H	200.1281	-2.6
	HMDB0062751	ecgoninium methyl ester(1+)	C10H18NO3	M+H	200.1281	-2.6
200.1640	HMDB0163226	(2E,5Z)-11-hydroxyundeca-2,5-dienal	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0163223	(2E,5Z)--hydroxyundeca-2,5-dienal	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0163225	(2E)-4-(3-pentylloxiran-2-yl)but-2-enal	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0163224	3-[(2Z)-oct-2-en-1-yl]oxirane-2-carbaldehyde	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0163221	(2E,5Z)-undeca-2,5-dienoic acid	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0163222	(2E,5Z)-7-hydroxyundeca-2,5-dienal	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0038245	Bornyl formate	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0036191	4-Hydroxy-4-methyl-7-decenoic acid gamma-lactone	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0038068	(3E,6Z)-Nonadien-1-yl acetate	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0034708	Methyl 4,8-decadienoate	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0030006	2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]non-3-ene	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0036215	Ethyl octynecarboxylate	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0038079	(2E,6Z)-2,6-Nonadien-1-Yl acetate	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0030424	Linalyl formate	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0037388	Tsibulin 2	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0034730	Methyl (2E,4Z)-decadienoate	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0040595	Allyl cyclohexylacetate	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0038279	cis-3-Hexenyl tiglate	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0032050	alpha-Terpineol formate	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0032463	5-Pentyl-3h-furan-2-one	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0038005	xi-2-Hexyl-5-methyl-3(2H)-furanone	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0035156	Neryl formate	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0059816	Methyl geranate	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0037829	6-(3-Hexenyl)tetrahydro-2H-pyran-2-one	C11H18O2	M+NH4	200.1645	-2.5
	HMDB0062669	11-nitro-1-undecene	C11H21NO2	M+H	200.1645	-2.5
200.2005	HMDB0031341	Cyclododecanone	C12H22O	M+NH4	200.2009	-1.9
	HMDB0036461	Geosmin	C12H22O	M+NH4	200.2009	-1.9
	HMDB0031020	2-Dodecenal	C12H22O	M+NH4	200.2009	-1.9
	HMDB0031102	(Z,Z)-3,6-Dodecadien-1-ol	C12H22O	M+NH4	200.2009	-1.9
	HMDB0038972	(E)-2-Butyl-2-octenal	C12H22O	M+NH4	200.2009	-1.9
	HMDB0032542	trans- and cis-2,4,8-Trimethyl-3,7-nona-dien-2-ol	C12H22O	M+NH4	200.2009	-1.9
	HMDB0032279	2-Ethyl-1,3,3-trimethyl-2-norbornanol	C12H22O	M+NH4	200.2009	-1.9
201.0378	HMDB0029684	Melizame	C7H6N4O2	M+Na	201.0383	-2.5
	HMDB0031714	Methylthiomethyl 2-methylbutanethiolate	C7H14OS2	M+Na	201.0378	-0.1
	HMDB0174739	3-[(1E)-prop-1-en-1-yl]disulfanylbutan-1-ol	C7H14OS2	M+Na	201.0378	-0.1
	HMDB0174737	3-[(1E)-prop-1-en-1-yl]disulfanylbutan-2-ol	C7H14OS2	M+Na	201.0378	-0.1
	HMDB0174738	2-[(1E)-prop-1-en-1-yl]disulfanylbutan-1-ol	C7H14OS2	M+Na	201.0378	-0.1
201.0483	HMDB0038631	Camalexin	C11H8N2S	M+H	201.0481	1.0
201.0882	HMDB0126149	2-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C11H14O2	M+Na	201.0886	-2.0
	HMDB0126449	2-[(1E)-3-methylbut-1-en-1-yl]benzene-1,3-diol	C11H14O2	M+Na	201.0886	-2.0
	HMDB0132981	1-(4-hydroxyphenyl)pentan-3-one	C11H14O2	M+Na	201.0886	-2.0
	HMDB0163598	SCHEMBL9714564	C11H14O2	M+Na	201.0886	-2.0
	HMDB0163596	2-hydroxy-3-methyl-2-phenylbutanal	C11H14O2	M+Na	201.0886	-2.0
	HMDB0163597	SCHEMBL9714781	C11H14O2	M+Na	201.0886	-2.0
	HMDB0163594	4-hydroxy-3-methyl-2-phenylbutanal	C11H14O2	M+Na	201.0886	-2.0
	HMDB0163592	38-94-9	C11H14O2	M+Na	201.0886	-2.0
	HMDB0163593	SCHEMBL11476137	C11H14O2	M+Na	201.0886	-2.0
	HMDB0151222	3-(4-methoxyphenyl)-2-methylprop-2-en-1-ol	C11H14O2	M+Na	201.0886	-2.0
	HMDB0151221	3-(4-methoxyphenyl)-2-methylpropanal	C11H14O2	M+Na	201.0886	-2.0
	HMDB0133687	1-hydroxy-3-methyl-4-phenylbutan-2-one	C11H14O2	M+Na	201.0886	-2.0
	HMDB0133686	3-benzyl-4-hydroxybutan-2-one	C11H14O2	M+Na	201.0886	-2.0
	HMDB0133685	4-(4-hydroxyphenyl)-3-methylbutan-2-one	C11H14O2	M+Na	201.0886	-2.0
	HMDB0133684	4-(3-hydroxyphenyl)-3-methylbutan-2-one	C11H14O2	M+Na	201.0886	-2.0
	HMDB0133682	3-hydroxy-3-methyl-4-phenylbutan-2-one	C11H14O2	M+Na	201.0886	-2.0
	HMDB0133683	4-hydroxy-3-methyl-4-phenylbutan-2-one	C11H14O2	M+Na	201.0886	-2.0
	HMDB0133469	4-(3-methoxyphenyl)butan-2-one	C11H14O2	M+Na	201.0886	-2.0
	HMDB0133181	4-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C11H14O2	M+Na	201.0886	-2.0
	HMDB0040287	1-Phenylethyl propanoate	C11H14O2	M+Na	201.0886	-2.0
	HMDB0037708	p-Tolyl isobutyrate	C11H14O2	M+Na	201.0886	-2.0
	HMDB0040356	Osmorhizole	C11H14O2	M+Na	201.0886	-2.0

	HMDB0036235	alpha, alpha-Dimethylphenethyl formate	C11H14O2	M+Na	201.0886	-2.0
	HMDB0031864	Methyleugenol	C11H14O2	M+Na	201.0886	-2.0
	HMDB0033597	4-(4-Methoxyphenyl)-2-butanone	C11H14O2	M+Na	201.0886	-2.0
	HMDB0036385	Methyl 4-phenylbutanoate	C11H14O2	M+Na	201.0886	-2.0
	HMDB0040800	2-Ethoxy-5-(1-propenyl)phenol	C11H14O2	M+Na	201.0886	-2.0
	HMDB0040426	Isopropyl phenylacetate	C11H14O2	M+Na	201.0886	-2.0
	HMDB0038179	3-(2-Hydroxy-4-methylphenyl)-2-butanone	C11H14O2	M+Na	201.0886	-2.0
	HMDB0037680	2-Methylphenyl 2-methylpropanoate	C11H14O2	M+Na	201.0886	-2.0
	HMDB0040411	Ethyl 3-phenylpropanoate	C11H14O2	M+Na	201.0886	-2.0
	HMDB0035013	2-Phenylethyl propanoate	C11H14O2	M+Na	201.0886	-2.0
	HMDB0041553	Methylisoeugenol	C11H14O2	M+Na	201.0886	-2.0
	HMDB0040425	Propyl phenylacetate	C11H14O2	M+Na	201.0886	-2.0
	HMDB0031250	Phenylmethyl 2-methylpropanoate	C11H14O2	M+Na	201.0886	-2.0
	HMDB0033376	Phenylmethyl butanoate	C11H14O2	M+Na	201.0886	-2.0
	HMDB0033386	3-Phenylpropyl acetate	C11H14O2	M+Na	201.0886	-2.0
	HMDB0040583	2-Methylpropyl benzoate	C11H14O2	M+Na	201.0886	-2.0
	HMDB0002043	5-Phenylvaleric acid	C11H14O2	M+Na	201.0886	-2.0
201.1117	HMDB0170504	SCHEMBL4585236	C10H16O4	M+H	201.1121	-2.2
	HMDB0061295	526-51-6	C10H16O4	M+H	201.1121	-2.2
	HMDB0013227	cis-5-Decenedioic acid	C10H16O4	M+H	201.1121	-2.2
	HMDB0034491	Camphoric acid	C10H16O4	M+H	201.1121	-2.2
	HMDB0030989	5-Pentyltetrahydro-2-oxo-3-furancarboxylic acid	C10H16O4	M+H	201.1121	-2.2
	HMDB0030990	alpha-Carboxy-delta-nonalactone	C10H16O4	M+H	201.1121	-2.2
	HMDB0036715	Matsutakic acid A	C10H16O4	M+H	201.1121	-2.2
	HMDB0034971	(1R,2R,3S,1'R)-Nepetalinic acid	C10H16O4	M+H	201.1121	-2.2
	HMDB0000603	cis-4-Decenedioic acid	C10H16O4	M+H	201.1121	-2.2
201.1480	HMDB0037179	3-Nonanon-1-yl acetate	C11H20O3	M+H	201.1485	-2.6
	HMDB0165686	6-hydroxyundec--enoic acid	C11H20O3	M+H	201.1485	-2.6
	HMDB0165685	7-hydroxyundec--enoic acid	C11H20O3	M+H	201.1485	-2.6
	HMDB0165684	8-hydroxyundec--enoic acid	C11H20O3	M+H	201.1485	-2.6
	HMDB0165690	9-(oxiran-2-yl)nonanoic Acid	C11H20O3	M+H	201.1485	-2.6
	HMDB0165689	3-hydroxy--undecenoic acid	C11H20O3	M+H	201.1485	-2.6
	HMDB0165688	4-hydroxyundec--enoic acid	C11H20O3	M+H	201.1485	-2.6
	HMDB0165687	5-hydroxyundec--enoic acid	C11H20O3	M+H	201.1485	-2.6
	HMDB0032662	(S)-9-Hydroxy--undecenoic acid	C11H20O3	M+H	201.1485	-2.6
	HMDB0036029	Clarycet	C11H20O3	M+H	201.1485	-2.6
201.1635	HMDB0165691	2-hydroxy--undecenoic acid	C11H20O3	M+H	201.1485	-2.6
	HMDB0036451	(S)-gamma-Calacorene	C15H20	M+H	201.1638	-1.4
	HMDB0038204	alpha-Corocalene	C15H20	M+H	201.1638	-1.4
	HMDB0036453	3,4-Dihydrocadalene	C15H20	M+H	201.1638	-1.4
	HMDB0059829	Isolongifolene, 4,5,9,-dehydro-	C15H20	M+H	201.1638	-1.4
201.1845	HMDB0059858	beta-Calacorene	C15H20	M+H	201.1638	-1.4
	HMDB0168121	2-hydroxydodecanal	C12H24O2	M+H	201.1849	-2.0
	HMDB0168119	11-hydroxydodecanal	C12H24O2	M+H	201.1849	-2.0
	HMDB0168120	12-hydroxydodecanal	C12H24O2	M+H	201.1849	-2.0
	HMDB0034128	Isopropyl nonanoate	C12H24O2	M+H	201.1849	-2.0
	HMDB0034136	Octyl butanoate	C12H24O2	M+H	201.1849	-2.0
	HMDB0036225	Pentyl heptanoate	C12H24O2	M+H	201.1849	-2.0
	HMDB0034137	Octyl 2-methylpropanoate	C12H24O2	M+H	201.1849	-2.0
	HMDB0030998	Ethyl decanoate	C12H24O2	M+H	201.1849	-2.0
	HMDB0040166	Decyl acetate	C12H24O2	M+H	201.1849	-2.0
	HMDB0033619	Hexyl hexanoate	C12H24O2	M+H	201.1849	-2.0
	HMDB0035410	(R)-Dihydrocitronellol acetate	C12H24O2	M+H	201.1849	-2.0
	HMDB0032310	2-Heptyl butyrate	C12H24O2	M+H	201.1849	-2.0
	HMDB0032440	Nonanal propyleneglycol acetal	C12H24O2	M+H	201.1849	-2.0
	HMDB0061988	2-ethylhexyl butanoate	C12H24O2	M+H	201.1849	-2.0
	HMDB0059868	Isobutyl octanoate	C12H24O2	M+H	201.1849	-2.0
	HMDB0000638	Dodecanoic acid	C12H24O2	M+H	201.1849	-2.0
	HMDB0240350	4-(2-Hydroxyethoxy)-2-methoxyphenol	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0125593	4-ethyl-6-methoxybenzene-1,2,3-triol	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0180894	4-(1-hydroxyethyl)-5-methoxybenzene-1,3-diol	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0151526	5-methoxy-4,6-dimethylbenzene-1,2,3-triol	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0151525	4-(hydroxymethyl)-5-methoxy-6-methylbenzene-1,3-diol	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0131235	dimethoxy-methyl-hydroquinone	C9H12O4	M+NH4	202.1074	-2.4

202.1069	HMDB0131234	4,6-dimethoxy-3-methylbenzene-1,2-diol	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0131233	2-(hydroxymethyl)-3,5-dimethoxyphenol	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0126620	6-methoxy-3,5-dimethylbenzene-1,2,4-triol	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0126619	4-(hydroxymethyl)-5-methoxy-2-methylbenzene-1,3-diol	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0126618	2-(hydroxymethyl)-5-methoxy-4-methylbenzene-1,3-diol	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0125597	5-ethyl-3-methoxybenzene-1,2,4-triol	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0180032	syringyl alcohol	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0059730	3,4-Methylenepimelic acid	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0039650	4-Formyl-3-(formylmethyl)-4-hexenoic acid	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0036072	Genipic acid	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0035056	1-(3-Hydroxy-4-methoxyphenyl)-1,2-ethanediol	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0040603	threo-1-(4-Hydroxyphenyl)-1,2,3-propanetriol	C9H12O4	M+NH4	202.1074	-2.4
	HMDB0001490	Vanylglycol	C9H12O4	M+NH4	202.1074	-2.4
202.1432	HMDB0131084	(5E)-2,2,5-trimethyl-7-oxohept-5-enoic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0179401	(2E,4Z)-9-hydroxydeca-2,4-dienoic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0179400	(4Z)-6-hydroxydeca-2,4-dienoic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0179402	3-[(1Z)-hept-1-en-1-yl]oxirane-2-carboxylic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0179404	(2E,4Z)--hydroxydeca-2,4-dienoic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0179403	SCHEMBL12833	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0182629	SCHEMBL5986763	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0182628	2-[3-(hydroxymethyl)-2,2-dimethylcyclopent-3-en-1-yl]acetic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0182627	2-[2-(hydroxymethyl)-2,3-dimethylcyclopent-3-en-1-yl]acetic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0182630	2-{1,2,2-trimethyl-6-oxabicyclo[3.1]hexan-3-yl}acetic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0182631	SCHEMBL59867	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0178775	(4Z,8Z)-2-hydroxydeca-4,8-dienoic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0178774	3-{3-[(3Z)-pent-3-en-1-yl]oxiran-2-yl}propanoic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0178771	(4Z,8Z)-3-hydroxydeca-4,8-dienoic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0176282	6-hydroxy-1-(hydroxymethyl)-7,7-dimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0176286	3,6-dihydroxy-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0176285	5,6-dihydroxy-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0176283	1-Methyl-6-hydroxy-7-methyl-7-(hydroxymethyl)norbornane-2-one	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0176284	6,6-dihydroxy-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0178769	(4Z,8Z)-7-hydroxydeca-4,8-dienoic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0178770	(4Z,8Z)--hydroxydeca-4,8-dienoic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0178772	(4Z,8Z)-6-hydroxydeca-4,8-dienoic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0178773	(4Z)-7-(3-methyloxiran-2-yl)hept-4-enoic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0036998	(S)-Oleuropeic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0039052	(4S,8R)-8,9-Dihydroxy-p-menth-1(6)-en-2-one	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0040883	(E)--Oxo-8-decenoic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0036117	(1'R)-Nepetalic acid	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0039710	1-Acetylcyclohexyl acetate	C10H16O3	M+NH4	202.1438	-2.8
	HMDB0059745	N-Acetylaminooctanoic acid	C10H19NO3	M+H	202.1438	-2.8
	HMDB0041540	N-(5-Methyl-3-oxohexyl)alanine	C10H19NO3	M+H	202.1438	-2.8
	HMDB0000832	Capryloylglycine	C10H19NO3	M+H	202.1438	-2.8
	HMDB0013116	Valproylglycine	C10H19NO3	M+H	202.1438	-2.8
	HMDB0163228	(5Z)-4-hydroxyundec-5-enal	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163229	(5Z)--hydroxyundec-5-enal	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163854	6-hydroxyundec--en-2-one	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163853	7-hydroxyundec--en-2-one	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163857	SCHEMBL11481214	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163859	3-hydroxyundec--en-2-one	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163858	9-(oxiran-2-yl)nonan-2-one	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163860	1-hydroxyundec--en-2-one	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0175165	SCHEMBL15641446	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0180766	(2E)-11-hydroxyundec-2-enal	C11H20O2	M+NH4	202.1802	-2.2

202.1797	HMDB0180763	4-Hydroxy-2-undecenal	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0180765	3-octyloxirane-2-carbaldehyde	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0180764	(2E)--hydroxyundec-2-enal	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163856	4-hydroxyundec--en-2-one	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163855	5-hydroxyundec--en-2-one	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163227	(5Z)-7-hydroxyundec-5-enal	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163230	4-(3-pentyloxiran-2-yl)butanal	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163232	(5Z)-2-hydroxyundec-5-enal	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163234	(2E,5Z)-undeca-2,5-diene-1,-diol	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163233	(2E,5Z)-undeca-2,5-diene-1,7-diol	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163231	(5Z)-11-hydroxyundec-5-enal	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163235	{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}methanol	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163237	(2E,5Z)-undeca-2,5-diene-1,11-diol	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163236	(2E)-4-(3-pentyloxiran-2-yl)but-2-en-1-ol	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163245	5Z-undecenoic acid	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0163852	8-hydroxyundec--en-2-one	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0038311	xi-gamma-Undecalactone	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0038278	cis-3-Hexenyl 3-methylbutanoate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0032308	(E)-3-Heptenyl 2-methylpropanoate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0036784	6-Hexyltetrahydro-2H-pyran-2-one	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0034428	Cyclohexyl 3-methylbutanoate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0034429	Cyclohexyl pentanoate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0037225	Methyl citronellate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0033724	Undecylenic acid	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0038277	cis-3-Hexenyl 2-methylbutanoate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0040593	2-Propenyl octanoate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0037185	Rhodinyl formate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0032396	Methyl 2-decenoate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0032453	cis-3-Octenyl propionate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0038273	2-Hexenyl valerate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0038274	2-Hexenyl isovalerate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0031062	(Z)-3-Methyl-3-decenoic acid	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0031272	Ethyl (E)-2-nonenoate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0031063	(Z)-3-Methyl-4-decenoic acid	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0031087	trans-2-Hexyl-1-cyclopropaneacetic acid	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0033371	Citronellyl formate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0037106	(x)-1-Nonen-3-yl acetate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0036140	5-Hexyldihydro-5-methyl-2(3H)-furanone	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0031691	cis-3-Hexenyl pentanoate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0031406	Ethyl 3-cyclohexylpropionate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0038906	5-Octenyl propanoate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0037309	5-Hexyldihydro-4-methyl-2(3H)-furanone	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0031843	2,3-Undecanedione	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0032320	3-Hexenyl 2-methylbutyrate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0032534	trans-2-Hexenyl 2-methylbutyrate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0032461	Pent-2-enyl hexanoate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0062090	butyl cyclohexanecarboxylate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0032489	Prenyl caproate	C11H20O2	M+NH4	202.1802	-2.2
	HMDB0032404	6-Methyl-5-hepten-2-one propyleneglycol acetal	C11H20O2	M+NH4	202.1802	-2.2
202.2162	HMDB0033933	Lauric aldehyde	C12H24O	M+NH4	202.2165	-1.7
	HMDB0031019	2-Dodecanone	C12H24O	M+NH4	202.2165	-1.7
	HMDB0031734	2-Methylundecanal	C12H24O	M+NH4	202.2165	-1.7
	HMDB0032543	(+/-)-2,4,8-Trimethyl-7-nonen-2-ol	C12H24O	M+NH4	202.2165	-1.7
	HMDB0062100	(3R,4R,5S)-5-[(1R)-1,2-dihydroxyethyl]oxolane-2,3,4-triol	C6H12O6	M+Na	203.0526	1.9
	HMDB0062113	(3R,4R,5S)-5-[(1R)-1,2-dihydroxyethyl]-3,4-dihydroxyoxolan-2-olate	C6H11O6	M+Na	203.0526	1.9
	HMDB0062138	muco-Inositol	C6H12O6	M+Na	203.0526	1.9
	HMDB0062473	Glycoprotein-phospho-D-mannose	C6H12O6	M+Na	203.0526	1.9
	HMDB0033704	alpha-L-galactose	C6H12O6	M+Na	203.0526	1.9
	HMDB0166371	SCHEMBL14339418	C6H12O6	M+Na	203.0526	1.9
	HMDB0240208	neo-inositol	C6H12O6	M+Na	203.0526	1.9
	HMDB0240210	cis-inositol	C6H12O6	M+Na	203.0526	1.9
	HMDB0003418	D-Tagatose	C6H12O6	M+Na	203.0526	1.9
	HMDB0125599	2,5-bis(hydroxymethyl)oxolane-2,3,4-triol	C6H12O6	M+Na	203.0526	1.9

203.0530	HMDB0000660	D-Fructose	C6H12O6	M+Na	203.0526	1.9
	HMDB0001151	Allose	C6H12O6	M+Na	203.0526	1.9
	HMDB0001266	L-Sorbose	C6H12O6	M+Na	203.0526	1.9
	HMDB0003345	alpha-D-Glucose	C6H12O6	M+Na	203.0526	1.9
	HMDB0061922	alpha-D-Glucose	C6H12O6	M+Na	203.0526	1.9
	HMDB0003449	Beta-D-Galactose	C6H12O6	M+Na	203.0526	1.9
	HMDB0240207	epi-Inositol	C6H12O6	M+Na	203.0526	1.9
	HMDB0012326	L-Gulose	C6H12O6	M+Na	203.0526	1.9
	HMDB0155830	Inositol	C6H12O6	M+Na	203.0526	1.9
	HMDB0000122	Beta-D-Glucose	C6H12O6	M+Na	203.0526	1.9
	HMDB0062170	Beta-D-Glucose	C6H12O6	M+Na	203.0526	1.9
	HMDB0000516	Beta-D-Glucose	C6H12O6	M+Na	203.0526	1.9
	HMDB0000346	3-Deoxyarabinohexonic acid	C6H12O6	M+Na	203.0526	1.9
	HMDB0000211	myo-Inositol	C6H12O6	M+Na	203.0526	1.9
	HMDB0006088	scyllo-Inositol	C6H12O6	M+Na	203.0526	1.9
	HMDB0000143	D-Galactose	C6H12O6	M+Na	203.0526	1.9
	HMDB0155309	keto-D-fructose	C6H12O6	M+Na	203.0526	1.9
	HMDB0240211	allo-Inositol	C6H12O6	M+Na	203.0526	1.9
	HMDB0062086	beta-D-galactofuranose	C6H12O6	M+Na	203.0526	1.9
	HMDB0240209	D-chiro-Inositol	C6H12O6	M+Na	203.0526	1.9
	HMDB0032222	Dihydroxyacetone (dimer)	C6H12O6	M+Na	203.0526	1.9
	HMDB0062538	Fructose-1P	C6H12O6	M+Na	203.0526	1.9
	HMDB0000169	Alpha-D-Mannose	C6H12O6	M+Na	203.0526	1.9
	HMDB0034220	Levoinositol	C6H12O6	M+Na	203.0526	1.9
203.1024	HMDB0155838	4-(2-amino-1-hydroxyethyl)benzene-1,2,3-triol	C8H11NO4	M+NH4	203.1026	-1.1
	HMDB0155837	5-(2-amino-1-hydroxyethyl)benzene-1,2,3-triol	C8H11NO4	M+NH4	203.1026	-1.1
	HMDB0155839	2623-77	C8H11NO4	M+NH4	203.1026	-1.1
	HMDB0029047	Serylproline	C8H14N2O4	M+H	203.1026	-1.1
	HMDB0034266	L-Coprine	C8H14N2O4	M+H	203.1026	-1.1
	HMDB0029026	Prolyl-Serine	C8H14N2O4	M+H	203.1026	-1.1
	HMDB0028856	Hydroxyprolyl-Alanine	C8H14N2O4	M+H	203.1026	-1.1
203.1275	HMDB0028688	Alanylhydroxyproline	C8H14N2O4	M+H	203.1026	-1.1
	HMDB0062180	(2S,5S)-2-[(2R)-butan-2-yl]-5-hydroxy-4-oxohexanoic acid	C10H18O4	M+H	203.1278	-1.4
	HMDB0031510	R-2-Hydroxy-3-methylbutanoic acid 3-Methylbutanoyl	C10H18O4	M+H	203.1278	-1.4
	HMDB0040196	Oxalic acid dibutyl ester	C10H18O4	M+H	203.1278	-1.4
	HMDB0059708	2-Ethylsuberic acid	C10H18O4	M+H	203.1278	-1.4
	HMDB0059719	Heptylmalonic acid	C10H18O4	M+H	203.1278	-1.4
	HMDB0059754	3-Methylazelaic acid	C10H18O4	M+H	203.1278	-1.4
203.1425	HMDB0000792	Sebacic acid	C10H18O4	M+H	203.1278	-1.4
	HMDB0039274	Dictagymnin	C14H18O	M+H	203.1430	-2.7
	HMDB0030838	Feniculin	C14H18O	M+H	203.1430	-2.7
	HMDB0030572	Anisoxide	C14H18O	M+H	203.1430	-2.7
	HMDB0039356	Panaquinquecol 5	C14H18O	M+H	203.1430	-2.7
	HMDB0031313	2-Pentyl-3-phenyl-2-propenal	C14H18O	M+H	203.1430	-2.7
	HMDB0061830	2-Pentyl-3-phenyl-2-propenal	C14H18O	M+H	203.1430	-2.7
203.1499	HMDB0001539	Asymmetric dimethylarginine	C8H18N4O2	M+H	203.1503	-1.7
	HMDB0003334	Symmetric dimethylarginine	C8H18N4O2	M+H	203.1503	-1.7
203.1637	HMDB0032443	3-Hydroxynonyl acetate	C11H22O3	M+H	203.1642	-2.3
	HMDB0166976	Methyl 9-hydroxydecanoate	C11H22O3	M+H	203.1642	-2.3
	HMDB0166977	Methyl -hydroxydecanoate	C11H22O3	M+H	203.1642	-2.3
	HMDB0175164	2-hydroxy-9-methyldecanoic acid	C11H22O3	M+H	203.1642	-2.3
	HMDB0175162	SCHEMBL9794217	C11H22O3	M+H	203.1642	-2.3
	HMDB0175163	SCHEMBL8984439	C11H22O3	M+H	203.1642	-2.3
	HMDB0183924	4-hydroxy-4,8-dimethylnonanoic acid	C11H22O3	M+H	203.1642	-2.3
	HMDB0183925	8-hydroxy-4,8-dimethylnonanoic acid	C11H22O3	M+H	203.1642	-2.3
	HMDB0183926	4-(hydroxymethyl)-8-methylnonanoic acid	C11H22O3	M+H	203.1642	-2.3
	HMDB0183927	9-hydroxy-4,8-dimethylnonanoic acid	C11H22O3	M+H	203.1642	-2.3
	HMDB0061654	3-hydroxyundecanoic acid	C11H22O3	M+H	203.1642	-2.3
	HMDB0059736	2-Hydroxyundecanoate	C11H22O3	M+H	203.1642	-2.3
	HMDB0183928	2-hydroxy-4,8-dimethylnonanoic acid	C11H22O3	M+H	203.1642	-2.3
203.2225	HMDB0001256	Spermine	C10H26N4	M+H	203.2230	-2.6
	HMDB0185178	4-(2-amino-1-hydroxyprop-2-en-1-yl)benzene-1,2-diol	C9H11NO3	M+Na	204.0631	-2.5
	HMDB0164040	SCHEMBL62116	C9H11NO3	M+Na	204.0631	-2.5
	HMDB0164039	ethyl 2-(hydroxyamino)benzoate	C9H11NO3	M+Na	204.0631	-2.5

204.0626	HMDB0162086	8-methyl-1H,3H,4H-pyrano[3,4-c]pyridine-1,4-diol	C9H11NO3	M+Na	204.0631	-2.5
	HMDB0162085	8-(hydroxymethyl)-1H,3H,4H-pyrano[3,4-c]pyridin-1-ol	C9H11NO3	M+Na	204.0631	-2.5
	HMDB0060280	4,6,7-Trihydroxy-1,2,3,4-tetrahydroisoquinoline	C9H11NO3	M+Na	204.0631	-2.5
	HMDB0006050	o-Tyrosine	C9H11NO3	M+Na	204.0631	-2.5
	HMDB0003831	Beta-Tyrosine	C9H11NO3	M+Na	204.0631	-2.5
	HMDB0002184	L-Threo-3-Phenylserine	C9H11NO3	M+Na	204.0631	-2.5
	HMDB0001119	4-Hydroxy-4-(3-pyridyl)-butanoic acid	C9H11NO3	M+Na	204.0631	-2.5
	HMDB0059720	Meta-Tyrosine	C9H11NO3	M+Na	204.0631	-2.5
	HMDB0000158	L-Tyrosine	C9H11NO3	M+Na	204.0631	-2.5
204.0862	HMDB0164171	L-Tyrosine	C9H11NO3	M+Na	204.0631	-2.5
	HMDB0041026	Erinapyrone C	C8H10O5	M+NH4	204.0866	-2.2
	HMDB0132202	2,4-dimethoxyphloroglucinol	C8H10O5	M+NH4	204.0866	-2.2
	HMDB0062715	2-[(1-hydroxyethylidene)amino]hexanedioic acid	C8H13NO5	M+H	204.0866	-2.2
204.1226	HMDB0240731	6-81-9	C8H13NO5	M+H	204.0866	-2.2
	HMDB0030988	5-(2-Methylpropyl)tetrahydro-2-oxo-3-furancarboxylic acid	C9H14O4	M+NH4	204.1230	-2.1
	HMDB0030992	5-Butyltetrahydro-2-oxo-3-furancarboxylic acid	C9H14O4	M+NH4	204.1230	-2.1
	HMDB0062176	(2S)-2-{[(2S)-1,2-dihydroxypropylidene]amino}-4-methylpentanoic acid	C9H17NO4	M+H	204.1230	-2.1
204.1589	HMDB0240626	1-Carboxyethylleucine	C9H17NO4	M+H	204.1230	-2.1
	HMDB0180508	6-hydroxydec-9-enoic acid	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0180506	4-hydroxydec-9-enoic acid	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0180505	3-hydroxy-9-decenoic acid	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0180507	5-hydroxydec-9-enoic acid	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0180509	7-hydroxydec-9-enoic acid	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0180510	8-hydroxy-9-decenoic acid	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0180512	2-hydroxydec-9-enoic acid	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0180511	Oxiraneoctanoic acid	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0180148	1-(hydroxymethyl)-3,3-dimethyl-2-oxabicyclo[2.2.2]octan-6-ol	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0180055	(6E)-2-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0180053	5-[3-(propan-2-yl)oxiran-2-yl]pentanoic acid	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0164896	6,7-dihydroxy-7-methyl-3-methylideneoctanal	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0164962	1-(2-hydroxypropan-2-yl)-4-methylbicyclo[3.1]hexane-2,4-diol	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0180051	(6E)-8-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0180052	(6E)-5-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0180054	(6E)-9-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0039587	5-Hexyl-1,4-dioxan-2-one	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0038692	6-Methyl-2-methylene-6-octene-1,3,8-triol	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0039582	6-Hexyl-1,4-dioxan-2-one	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0041545	(1R,2R,4R)-1,8-Epoxy-p-menthane-2,4-diol	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0038978	(1beta,2beta,5beta)-p-Menth-3-ene-1,2,5-triol	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0010724	3-Oxodecanoic acid	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0033010	(1S,2S,4S,5R)-1,8-Epoxy-p-menthane-2,5-diol	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0039533	(E)--Hydroxy-8-decenoic acid	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0041376	exo,exo-1,8-Epoxy-p-menthane-2,6-diol	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0030369	3-Hydroxy-5Z-octenyl acetate	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0040204	2-Methylbutyl 3-hydroxy-2-methylidenebutanoate	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0040205	3-Methylbutyl 3-hydroxy-2-methylidenebutanoate	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0030367	Ethyl (3R,5Z)-3-hydroxy-5-octenoate	C10H18O3	M+NH4	204.1594	-2.5
	HMDB0163825	5-(1,2-dihydroxypropan-2-yl)-2-methylcyclohexan-1-one	C10H18O3	M+NH4	204.1594	-2.5
205.0112	HMDB0183285	2-{2,5-dioxo-7-oxabicyclo[4.1]hept-3-en-3-yl}acetic acid	C8H6O5	M+Na	205.0107	2.2
	HMDB0183286	2-(3,6-dioxocyclohexa-1,4-dien-1-yl)-2-hydroxyacetic acid	C8H6O5	M+Na	205.0107	2.2
	HMDB0137133	2-(2,4-dihydroxyphenyl)-2-oxoacetic acid	C8H6O5	M+Na	205.0107	2.2
	HMDB0129371	6-hydroxy-2H-1,3-benzodioxole-5-carboxylic acid	C8H6O5	M+Na	205.0107	2.2
	HMDB0183284	2-{2,5-dioxo-7-oxabicyclo[4.1]hept-3-en-1-yl}acetic acid	C8H6O5	M+Na	205.0107	2.2
205.0682	HMDB0000765	Mannitol	C6H14O6	M+Na	205.0683	-0.3
	HMDB0000247	Sorbitol	C6H14O6	M+Na	205.0683	-0.3
	HMDB0000107	Galactitol	C6H14O6	M+Na	205.0683	-0.3

	HMDB0011632	L-Iditol	C6H14O6	M+Na	205.0683	-0.3
205.0854	HMDB0179700	(3E)-3-butyldiene-7-hydroxy-1,3-dihydro-2-benzofuran-1-one	C12H12O3	M+H	205.0859	-2.5
	HMDB0177963	4,5-dihydroxy-2,3-dimethyl-1,4-dihydronaphthalen-1-one	C12H12O3	M+H	205.0859	-2.5
	HMDB0177962	4,8-dihydroxy-2,3-dimethyl-1,4-dihydronaphthalen-1-one	C12H12O3	M+H	205.0859	-2.5
	HMDB0177956	2,3-dimethylnaphthalene-1,4,5-triol	C12H12O3	M+H	205.0859	-2.5
	HMDB0177955	5-hydroxy-2,3-dimethyl-1,2,3,4-tetrahydronaphthalene-1,4-dione	C12H12O3	M+H	205.0859	-2.5
	HMDB0177474	3-methoxy-6-methylnaphthalene-1,8-diol	C12H12O3	M+H	205.0859	-2.5
	HMDB0033303	Anofinic acid	C12H12O3	M+H	205.0859	-2.5
	HMDB0035095	7-Ethoxy-4-methyl-2H-1-benzopyran-2-one	C12H12O3	M+H	205.0859	-2.5
205.0966	HMDB0000734	Indoleacrylic acid	C11H9NO2	M+NH4	205.0972	-2.7
	HMDB0030396	Tryptophan	C11H12N2O2	M+H	205.0972	-2.7
	HMDB0014892	Ethotoin	C11H12N2O2	M+H	205.0972	-2.7
	HMDB0013609	D-Tryptophan	C11H12N2O2	M+H	205.0972	-2.7
	HMDB0060967	S-nirvanol	C11H12N2O2	M+H	205.0972	-2.7
	HMDB0060878	4-Hydroxyantipyrine	C11H12N2O2	M+H	205.0972	-2.7
	HMDB0060533	Nirvanol	C11H12N2O2	M+H	205.0972	-2.7
	HMDB0013840	3-Hydroxymethylantipyrine	C11H12N2O2	M+H	205.0972	-2.7
	HMDB0000929	L-Tryptophan	C11H12N2O2	M+H	205.0972	-2.7
	HMDB0033249	6-Chloro-N-(1-methylethyl)-1,3,5-triazine-2,4-diamine	C6H10ClN5	M+NH4	205.0963	1.5
205.1217	HMDB0132944	5-(4-methoxyphenyl)-2-methylpent-1-en-3-one	C13H16O2	M+H	205.1223	-3.0
	HMDB0132949	1-(4-methoxyphenyl)-4-methylpent-1-en-3-one	C13H16O2	M+H	205.1223	-3.0
	HMDB0140968	2-[4-(2-methylpropyl)phenyl]prop-2-enoic acid	C13H16O2	M+H	205.1223	-3.0
	HMDB0140969	2-[4-(2-methylprop-2-en-1-yl)phenyl]propanoic acid	C13H16O2	M+H	205.1223	-3.0
	HMDB0183009	SCHEMBL93916	C13H16O2	M+H	205.1223	-3.0
	HMDB0175277	2-phenylprop-2-en-1-yl 2-methylpropanoate	C13H16O2	M+H	205.1223	-3.0
	HMDB0175278	SCHEMBL2968	C13H16O2	M+H	205.1223	-3.0
	HMDB0151807	SCHEMBL124142	C13H16O2	M+H	205.1223	-3.0
	HMDB0151778	(2Z)-2-[(2-hydroxyphenyl)methylidene]hexanal	C13H16O2	M+H	205.1223	-3.0
	HMDB0151777	(2Z)-6-hydroxy-2-(phenylmethylidene)hexanal	C13H16O2	M+H	205.1223	-3.0
	HMDB0151776	2-butyl-3-phenyloxirane-2-carbaldehyde	C13H16O2	M+H	205.1223	-3.0
	HMDB0151775	(2Z)-5-hydroxy-2-(phenylmethylidene)hexanal	C13H16O2	M+H	205.1223	-3.0
	HMDB0151774	(2Z)-2-[(4-hydroxyphenyl)methylidene]hexanal	C13H16O2	M+H	205.1223	-3.0
	HMDB0151773	(2Z)-2-[(3-hydroxyphenyl)methylidene]hexanal	C13H16O2	M+H	205.1223	-3.0
	HMDB0151771	SCHEMBL524131	C13H16O2	M+H	205.1223	-3.0
	HMDB0151772	3-hydroxy-2-(phenylmethylidene)hexanal	C13H16O2	M+H	205.1223	-3.0
	HMDB0031661	3-Isovalidene-3alpha,4-dihydrophthalide	C13H16O2	M+H	205.1223	-3.0
	HMDB0031553	6-(1-Hydroxyethyl)-2,2-dimethyl-2H-1-benzopyran	C13H16O2	M+H	205.1223	-3.0
	HMDB0030904	alpha,alpha-Dimethylanisalacetone	C13H16O2	M+H	205.1223	-3.0
	HMDB0036224	Benzyl 2,3-dimethyl-2-butenate	C13H16O2	M+H	205.1223	-3.0
	HMDB0037702	Butyl cinnamate	C13H16O2	M+H	205.1223	-3.0
	HMDB0037721	2-Phenylethyl 3-methyl-2-butenate	C13H16O2	M+H	205.1223	-3.0
	HMDB0041316	Cinnamyl butyrate	C13H16O2	M+H	205.1223	-3.0
	HMDB0037703	Isobutyl cinnamate	C13H16O2	M+H	205.1223	-3.0
	HMDB0033379	cis-3-Hexenyl benzoate	C13H16O2	M+H	205.1223	-3.0
	HMDB0030770	4-Hydroxy-3-(3-methyl-2-butenyl)acetophenone	C13H16O2	M+H	205.1223	-3.0
	HMDB0041317	Cinnamyl isobutyrate	C13H16O2	M+H	205.1223	-3.0
	HMDB0037628	Phenethyl tiglate	C13H16O2	M+H	205.1223	-3.0
205.1439	HMDB0039974	(1S,2S,4R,8R)-p-Menthane-1,2,8,9-tetrol	C10H20O4	M+H	205.1434	2.3
	HMDB0035133	3,7-Dimethyl-3-octene-1,2,6,7-tetrol	C10H20O4	M+H	205.1434	2.3
	HMDB0039053	(1alpha,2alpha,4betaH,6alpha,8R)-p-Menthane-2,6,8,9-tetrol	C10H20O4	M+H	205.1434	2.3
	HMDB0033217	(2xi,6xi)-7-Methyl-3-methylene-1,2,6,7-octanetetrol	C10H20O4	M+H	205.1434	2.3
	HMDB0033642	(2xi,3xi,6E)-3,7-Dimethyl-6-octene-1,2,3,8-tetrol	C10H20O4	M+H	205.1434	2.3

205.1544	HMDB0013010	N-Heptanoylglycine	C9H17NO3	M+NH4	205.1547	-1.3
	HMDB0240687	7-Keto-8-Aminopelargonic Acid	C9H17NO3	M+NH4	205.1547	-1.3
205.9249	HMDB0031258	Lenthionine	C2H4S5	M+NH4	205.9255	-2.8
206.0997	HMDB0032688	(Z)-1-(Methylthio)-5-phenyl-1-penten-3-yne	C12H12S	M+NH4	206.0998	-0.5
206.1382	HMDB0179177	5-hydroxy-4-oxononanoic acid	C9H16O4	M+NH4	206.1387	-2.3
	HMDB0179175	2-hydroxy-4-oxononanoic acid	C9H16O4	M+NH4	206.1387	-2.3
	HMDB0179176	3-hydroxy-4-oxononanoic acid	C9H16O4	M+NH4	206.1387	-2.3
	HMDB0179174	9-hydroxy-4-oxononanoic acid	C9H16O4	M+NH4	206.1387	-2.3
	HMDB0179173	8-hydroxy-4-oxononanoic acid	C9H16O4	M+NH4	206.1387	-2.3
	HMDB0059783	3-Methylsuberic acid	C9H16O4	M+NH4	206.1387	-2.3
	HMDB0059760	2,4-Dimethylpimelic acid	C9H16O4	M+NH4	206.1387	-2.3
	HMDB0059879	Diethyl glutarate	C9H16O4	M+NH4	206.1387	-2.3
	HMDB0032387	(+/-)-Methyl 5-acetoxylhexanoate	C9H16O4	M+NH4	206.1387	-2.3
	HMDB0032200	cis- and trans-Ethyl 2,4-dimethyl-1,3-dioxolane-2-acetate	C9H16O4	M+NH4	206.1387	-2.3
	HMDB0032258	(+/-)-Ethyl 3-acetoxy-2-methylbutyrate	C9H16O4	M+NH4	206.1387	-2.3
	HMDB0036233	Butyl ethyl malonate	C9H16O4	M+NH4	206.1387	-2.3
	HMDB0011717	Nonate	C9H16O4	M+NH4	206.1387	-2.3
	HMDB0059814	Diethyl methylsuccinate	C9H16O4	M+NH4	206.1387	-2.3
	HMDB0000784	Azelaic acid	C9H16O4	M+NH4	206.1387	-2.3
	HMDB0004231	Dexpanthenol	C9H19NO4	M+H	206.1387	-2.3
206.1748	HMDB0002203	3-Hydroxycapric acid	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0179929	(5E)-3,7-dimethyloct-5-ene-1,4,7-triol	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0179928	(5E)-3,7-dimethyloct-5-ene-1,3,7-triol	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0041600	Ethyl 3-hydroxyoctanoate	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0179932	(5E)-3-(hydroxymethyl)-7-methyloct-5-ene-1,7-diol	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0179931	(3E)-2,6-dimethyloct-3-ene-1,2,8-triol	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0179930	4-[3-(2-hydroxypropan-2-yl)oxiran-2-yl]-3-methylbutan-1-ol	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0094656	2s-hydroxy-decanoic acid	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0180589	SCHEMBL45681	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0180586	8-hydroxy-4-methylnonanoic acid	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0180585	AKO19123491	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0180587	4-(hydroxymethyl)nonanoic acid	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0180588	9-hydroxy-4-methylnonanoic acid	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0180106	SCHEMBL4626344	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0180104	8-Hydroxy-8-methylnonanoic acid	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0180105	9-hydroxy-8-methylnonanoic acid	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0033640	7-Methyl-3-methylene-1,6,7-octanetriol	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0038186	2,6-Dimethyl-7-octene-2,3,6-triol	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0033201	9-Hydroxydecanoic acid	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0039668	2-Hexyl-1,3-dioxan-5-ol	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0039470	(1S,2S,4R,8R)-p-Menthane-1,2,9-triol	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0039893	(1R,2R,4S)-p-Menthane-1,2,8-triol	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0033574	(1R,2R,4R,8R)-p-Menthane-2,8,9-triol	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0040329	xi-5-Hydroxydecanoic acid	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0010725	(R)-3-Hydroxydecanoic acid	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0039669	2-Hexyl-1,3-dioxolane-4-methanol	C10H20O3	M+NH4	206.1751	-1.3
	HMDB0034783	cis-p-Menthane-1,7,8-triol	C10H20O3	M+NH4	206.1751	-1.3
207.0290	HMDB0136644	5-hydroxy-2-oxo-2H-chromene-4-carboxylic acid	C10H6O5	M+H	207.0288	1.0
	HMDB0136642	7-hydroxy-2-oxo-2H-chromene-4-carboxylic acid	C10H6O5	M+H	207.0288	1.0
	HMDB0136643	8-hydroxy-2-oxo-2H-chromene-4-carboxylic acid	C10H6O5	M+H	207.0288	1.0
	HMDB0136641	2-Oxo-6-hydroxy-2H-1-benzopyran-4-carboxylic acid	C10H6O5	M+H	207.0288	1.0
	HMDB0128625	5-hydroxy-1-oxo-1H-isochromene-3-carboxylic acid	C10H6O5	M+H	207.0288	1.0
	HMDB0128624	6-hydroxy-1-oxo-1H-isochromene-3-carboxylic acid	C10H6O5	M+H	207.0288	1.0
	HMDB0128623	7-hydroxy-1-oxo-1H-isochromene-3-carboxylic acid	C10H6O5	M+H	207.0288	1.0
	HMDB0131684	4-hydroxy-2H,8H-[1,3]dioxolo[4,5-h]chromen-8-one	C10H6O5	M+H	207.0288	1.0
207.0978	HMDB0032499	Pyrrolidino-[1,2E]-4H-2,4-dimethyl-1,3,5-dithiazine	C8H15NS2	M+NH4	207.0984	-3.0
	HMDB0031574	1-Isothiocyanato-6-(methylthio)hexane	C8H15NS2	M+NH4	207.0984	-3.0
	HMDB0029070	Thr-Ser	C7H14N2O5	M+H	207.0975	1.2
	HMDB0029049	Serylthreonine	C7H14N2O5	M+H	207.0975	1.2
	HMDB0000590	Glutaryl-glycine	C7H11NO5	M+NH4	207.0975	1.2
	HMDB0001138	N-Acetyl-L-glutamic acid	C7H11NO5	M+NH4	207.0975	1.2
	HMDB0182836	4-methoxybenzyl but-3-enoate	C12H14O3	M+H	207.1016	1.6

207.1019	HMDB0177972	4,8-dihydroxy-2,3-dimethyl-1,2,3,4-tetrahydronaphthalen-1-one	C12H14O3	M+H	207.1016	1.6
	HMDB0177973	4,5-dihydroxy-2,3-dimethyl-1,2,3,4-tetrahydronaphthalen-1-one	C12H14O3	M+H	207.1016	1.6
	HMDB0172376	(3E)-3-(4-hydroxybutylidene)-1,3,4,5-tetrahydro-2-benzofuran-1-one	C12H14O3	M+H	207.1016	1.6
	HMDB0172375	(8E)-8-butylidene-3,9-dioxatricyclo[5.3,dec-1(7)-en-one	C12H14O3	M+H	207.1016	1.6
	HMDB0172374	(3E)-3-(3-hydroxybutylidene)-1,3,4,5-tetrahydro-2-benzofuran-1-one	C12H14O3	M+H	207.1016	1.6
	HMDB0172373	(3E)-3-butylidene-4-hydroxy-1,3,4,5-tetrahydro-2-benzofuran-1-one	C12H14O3	M+H	207.1016	1.6
	HMDB0172372	(3E)-3-butylidene-5-hydroxy-1,3,4,5-tetrahydro-2-benzofuran-1-one	C12H14O3	M+H	207.1016	1.6
	HMDB0132987	1-(4-methoxyphenyl)pentane-2,3-dione	C12H14O3	M+H	207.1016	1.6
	HMDB0132977	(1E)-5-hydroxy-1-(4-methoxyphenyl)pent-1-en-3-one	C12H14O3	M+H	207.1016	1.6
	HMDB0132976	1-[3-(4-methoxyphenyl)oxiran-2-yl]propan-1-one	C12H14O3	M+H	207.1016	1.6
	HMDB0132975	(1E)-4-hydroxy-1-(4-methoxyphenyl)pent-1-en-3-one	C12H14O3	M+H	207.1016	1.6
	HMDB0132974	(1E)-1-(2-hydroxy-4-methoxyphenyl)pent-1-en-3-one	C12H14O3	M+H	207.1016	1.6
	HMDB0132972	(1Z)-2-hydroxy-1-(4-methoxyphenyl)pent-1-en-3-one	C12H14O3	M+H	207.1016	1.6
	HMDB0127763	5-[(3-methoxyphenyl)methyl]oxolan-2-one	C12H14O3	M+H	207.1016	1.6
	HMDB0032348	Isoeugenyl acetate	C12H14O3	M+H	207.1016	1.6
	HMDB0030762	Ethyl trans-p-methoxycinnamate	C12H14O3	M+H	207.1016	1.6
	HMDB0034135	Isoeugenol acetate	C12H14O3	M+H	207.1016	1.6
	HMDB0031729	Phenylmethylglycidic ester	C12H14O3	M+H	207.1016	1.6
	HMDB0033594	Cuelure	C12H14O3	M+H	207.1016	1.6
	HMDB0034122	Aceteugenol	C12H14O3	M+H	207.1016	1.6
	HMDB0041410	2,3-Dihydro-6-methoxy-2,2-dimethyl-4H-1-benzopyran-4-one	C12H14O3	M+H	207.1016	1.6
	HMDB0035071	Verimol I	C12H14O3	M+H	207.1016	1.6
	HMDB0031973	(2RS,5RS)-(E)-2-(2-Phenylethenyl)-1,3-dioxan-5-ol	C12H14O3	M+H	207.1016	1.6
	HMDB0135898	4-hydroxy-3-(3-methylbut-2-en-1-yl)benzoic acid	C12H14O3	M+H	207.1016	1.6
207.1128	HMDB0163575	5-[(3Z)-3,4,5,6-tetrahydropyridin-3-ylidene[methyl]furan-2-carbaldehyde	C11H11NO2	M+NH4	207.1128	0.0
	HMDB0161234	3-(1H-indol-2-yl)propanoic acid	C11H11NO2	M+NH4	207.1128	0.0
	HMDB0014970	Phensuximide	C11H11NO2	M+NH4	207.1128	0.0
	HMDB0002302	Indole-3-propionic acid	C11H11NO2	M+NH4	207.1128	0.0
	HMDB0029738	Indole-3-methyl acetate	C11H11NO2	M+NH4	207.1128	0.0
	HMDB0163228	(5Z)-4-hydroxyundec-5-enal	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163854	6-hydroxyundec--en-2-one	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163853	7-hydroxyundec--en-2-one	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163857	SCHEMBL11481214	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163859	3-hydroxyundec--en-2-one	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163858	9-(oxiran-2-yl)nonan-2-one	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163860	1-hydroxyundec--en-2-one	C11H20O2	M+Na	207.1355	-1.7
	HMDB0175165	SCHEMBL15641446	C11H20O2	M+Na	207.1355	-1.7
	HMDB0180763	4-Hydroxy-2-undecenal	C11H20O2	M+Na	207.1355	-1.7
	HMDB0180766	(2E)-11-hydroxyundec-2-enal	C11H20O2	M+Na	207.1355	-1.7
	HMDB0180765	3-octyloxirane-2-carbaldehyde	C11H20O2	M+Na	207.1355	-1.7
	HMDB0180764	(2E)--hydroxyundec-2-enal	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163855	5-hydroxyundec--en-2-one	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163856	4-hydroxyundec--en-2-one	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163852	8-hydroxyundec--en-2-one	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163229	(5Z)--hydroxyundec-5-enal	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163227	(5Z)-7-hydroxyundec-5-enal	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163230	4-(3-pentyloxiran-2-yl)butanal	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163232	(5Z)-2-hydroxyundec-5-enal	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163234	(2E,5Z)-undeca-2,5-diene-1,1-diol	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163233	(2E,5Z)-undeca-2,5-diene-1,7-diol	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163231	(5Z)-11-hydroxyundec-5-enal	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163235	{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}methanol	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163237	(2E,5Z)-undeca-2,5-diene-1,11-diol	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163236	(2E)-4-(3-pentyloxiran-2-yl)but-2-en-1-ol	C11H20O2	M+Na	207.1355	-1.7
	HMDB0163245	5Z-undecenoic acid	C11H20O2	M+Na	207.1355	-1.7
	HMDB0038311	xi-gamma-Undecalactone	C11H20O2	M+Na	207.1355	-1.7

207.1352	HMDB0038273	2-Hexenyl valerate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0038278	cis-3-Hexenyl 3-methylbutanoate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0032308	(E)-3-Heptenyl 2-methylpropanoate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0036784	6-Hexyltetrahydro-2H-pyran-2-one	C11H20O2	M+Na	207.1355	-1.7
	HMDB0034428	Cyclohexyl 3-methylbutanoate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0034429	Cyclohexyl pentanoate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0037225	Methyl citronellate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0033724	Undecylenic acid	C11H20O2	M+Na	207.1355	-1.7
	HMDB0038277	cis-3-Hexenyl 2-methylbutanoate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0040593	2-Propenyl octanoate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0037185	Rhodinyl formate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0038274	2-Hexenyl isovalerate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0031843	2,3-Undecanedione	C11H20O2	M+Na	207.1355	-1.7
	HMDB0031062	(Z)-3-Methyl-3-decenoic acid	C11H20O2	M+Na	207.1355	-1.7
	HMDB0031272	Ethyl (E)-2-nonenoate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0031063	(Z)-3-Methyl-4-decenoic acid	C11H20O2	M+Na	207.1355	-1.7
	HMDB0031087	trans-2-Hexyl-1-cyclopropaneacetic acid	C11H20O2	M+Na	207.1355	-1.7
	HMDB0033371	Citronellyl formate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0037106	(x)-1-Nonen-3-yl acetate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0036140	5-Hexyldihydro-5-methyl-2(3H)-furanone	C11H20O2	M+Na	207.1355	-1.7
	HMDB0031691	cis-3-Hexenyl pentanoate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0031406	Ethyl 3-cyclohexylpropionate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0038906	5-Octenyl propanoate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0037309	5-Hexyldihydro-4-methyl-2(3H)-furanone	C11H20O2	M+Na	207.1355	-1.7
	HMDB0032396	Methyl 2-decenoate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0032453	cis-3-Octenyl propionate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0032320	3-Hexenyl 2-methylbutyrate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0032534	trans-2-Hexenyl 2-methylbutyrate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0032461	Pent-2-enyl hexanoate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0032404	6-Methyl-5-hepten-2-one propyleneglycol acetal	C11H20O2	M+Na	207.1355	-1.7
	HMDB0032489	Prenyl caproate	C11H20O2	M+Na	207.1355	-1.7
	HMDB0062090	butyl cyclohexanecarboxylate	C11H20O2	M+Na	207.1355	-1.7
207.1738	HMDB0133179	2-benzylheptan-1-ol	C14H22O	M+H	207.1743	-2.6
	HMDB0013816	2,4-di-tert-Butylphenol	C14H22O	M+H	207.1743	-2.6
	HMDB0061831	(Z)-alpha-Irone	C14H22O	M+H	207.1743	-2.6
	HMDB0032397	Methyl-delta-ionone	C14H22O	M+H	207.1743	-2.6
	HMDB0013825	4-(1,1,3,3-Tetramethylbutyl)-phenol	C14H22O	M+H	207.1743	-2.6
	HMDB0032528	4-(1,1,3,3-Tetramethylbutyl)-phenol	C14H22O	M+H	207.1743	-2.6
	HMDB0036023	Etaspiroene	C14H22O	M+H	207.1743	-2.6
	HMDB0035631	alpha-Irone	C14H22O	M+H	207.1743	-2.6
	HMDB0036024	-Isopropyl-2,7-dimethyl-1-oxaspiro[4.5]deca-3,6-diene	C14H22O	M+H	207.1743	-2.6
	HMDB0035245	1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1-penten-3-one	C14H22O	M+H	207.1743	-2.6
	HMDB0031737	delta-Methylionone	C14H22O	M+H	207.1743	-2.6
	HMDB0038130	1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one	C14H22O	M+H	207.1743	-2.6
207.9978	HMDB0000272	Phosphoserine	C3H8NO6P	M+Na	207.9981	-1.6
	HMDB0001721	DL-O-Phosphoserine	C3H8NO6P	M+Na	207.9981	-1.6
208.0133	HMDB0061263	Phosphoramidate Aziridinium	C4H11ClN2O2P	M+Na	208.0139	-2.8
208.1177	HMDB0166861	SCHEMBL846	C8H14O5	M+NH4	208.1179	-1.2
	HMDB0157326	2-hydroxyoctanedioic Acid	C8H14O5	M+NH4	208.1179	-1.2
	HMDB0157325	SCHEMBL596	C8H14O5	M+NH4	208.1179	-1.2
	HMDB0000325	3-Hydroxysuberic acid	C8H14O5	M+NH4	208.1179	-1.2
	HMDB0040220	Diethyl L-malate	C8H14O5	M+NH4	208.1179	-1.2
	HMDB0061681	6-(2-Hydroxyethoxy)-6-oxohexanoic acid	C8H14O5	M+NH4	208.1179	-1.2
	HMDB0014634	Miglitol	C8H17NO5	M+H	208.1179	-1.2
208.1539	HMDB0163757	3,5-dihydroxy-6-methyloctanoic acid	C9H18O4	M+NH4	208.1543	-2.1
	HMDB0169419	1-(4,6-diethyl-1,3,5-trioxan-2-yl)ethan-1-ol	C9H18O4	M+NH4	208.1543	-2.1
	HMDB0169420	2-(4,6-diethyl-1,3,5-trioxan-2-yl)ethan-1-ol	C9H18O4	M+NH4	208.1543	-2.1
	HMDB0037763	xi-3-(4-Isopropylphenyl)-2-methylpropanal	C13H18O	M+NH4	208.1696	-2.3
	HMDB0151770	2-Benzylidene-1-hexanol	C13H18O	M+NH4	208.1696	-2.3
	HMDB0151769	2-benzylhexanal	C13H18O	M+NH4	208.1696	-2.3
	HMDB0151806	2-benzylhex-5-en-1-ol	C13H18O	M+NH4	208.1696	-2.3
	HMDB0036685	2,2,6,7-Tetramethylbicyclo[4.3]nona-1(9),4-dien-8-one	C13H18O	M+NH4	208.1696	-2.3

208.1691	HMDB0013804	beta-Damascenone	C13H18O	M+NH4	208.1696	-2.3
	HMDB0036572	beta-Damascenone	C13H18O	M+NH4	208.1696	-2.3
	HMDB0036178	2-(3-Phenylpropyl)tetrahydrofuran	C13H18O	M+NH4	208.1696	-2.3
	HMDB0059904	dehydro-beta-Ionone	C13H18O	M+NH4	208.1696	-2.3
	HMDB0059906	Megastigmatrienone	C13H18O	M+NH4	208.1696	-2.3
209.0775	HMDB0060611	N-Desmethyl tapentadol	C13H21NO	M+H	208.1696	-2.4
	HMDB0166089	(3-hydroxy-4-isothiocyantobutyl)dimethylsulfanium	C7H14NOS2	M+NH4	209.0777	-0.9
209.0949	HMDB0166093	(2-hydroxy-4-isothiocyantobutyl)dimethylsulfanium	C7H14NOS2	M+NH4	209.0777	-0.9
	HMDB0011745	N-Acetyl-L-methionine	C7H13NO3S	M+NH4	209.0954	-2.6
209.1171	HMDB0133263	4-methoxy-6-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C12H16O3	M+H	209.1172	-0.6
	HMDB0164059	SCHEMBL82258	C12H16O3	M+H	209.1172	-0.6
	HMDB0183044	2-methylpropyl 2-(4-hydroxyphenyl)acetate	C12H16O3	M+H	209.1172	-0.6
	HMDB0183042	2-methylpropyl 2-(2-hydroxyphenyl)acetate	C12H16O3	M+H	209.1172	-0.6
	HMDB0183043	2-hydroxy-2-methylpropyl 2-phenylacetate	C12H16O3	M+H	209.1172	-0.6
	HMDB0183045	3-hydroxy-2-methylpropyl 2-phenylacetate	C12H16O3	M+H	209.1172	-0.6
	HMDB0183047	2-methylpropyl 2-(3-hydroxyphenyl)acetate	C12H16O3	M+H	209.1172	-0.6
	HMDB0183046	alpha-hydroxyphenylacetic acid iso-butyl ester	C12H16O3	M+H	209.1172	-0.6
	HMDB0132984	2-hydroxy-1-(4-methoxyphenyl)pentan-3-one	C12H16O3	M+H	209.1172	-0.6
	HMDB0132985	1-hydroxy-1-(4-methoxyphenyl)pentan-3-one	C12H16O3	M+H	209.1172	-0.6
	HMDB0132982	1-hydroxy-5-(4-methoxyphenyl)pentan-3-one	C12H16O3	M+H	209.1172	-0.6
	HMDB0124910	5-methoxy-2-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C12H16O3	M+H	209.1172	-0.6
	HMDB0126246	4-methoxy-2-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C12H16O3	M+H	209.1172	-0.6
	HMDB0132980	4-hydroxy-1-(4-methoxyphenyl)pentan-3-one	C12H16O3	M+H	209.1172	-0.6
	HMDB0041411	3,4-Dihydro-6-methoxy-2,2-dimethyl-2H-1-benzopyran-4-ol	C12H16O3	M+H	209.1172	-0.6
	HMDB0031469	trans-Isoasarone	C12H16O3	M+H	209.1172	-0.6
	HMDB0033778	Elemicin	C12H16O3	M+H	209.1172	-0.6
	HMDB0034991	4-Methoxybenzyl butanoate	C12H16O3	M+H	209.1172	-0.6
	HMDB0029872	gamma-Asarone	C12H16O3	M+H	209.1172	-0.6
	HMDB0030197	(Z)-3-Oxo-2-(2-pentenyl)-1-cyclopenteneacetic acid	C12H16O3	M+H	209.1172	-0.6
	HMDB0030681	5-Deoxydiplosporin	C12H16O3	M+H	209.1172	-0.6
	HMDB0038604	Amyl salicylate	C12H16O3	M+H	209.1172	-0.6
	HMDB0035224	3,4-Dihydro-6-methoxy-3,7-dimethyl-1H-2-benzopyran-8-ol	C12H16O3	M+H	209.1172	-0.6
	HMDB0040218	2-Phenoxyethyl isobutyrate	C12H16O3	M+H	209.1172	-0.6
	HMDB0029867	Isoelemicin	C12H16O3	M+H	209.1172	-0.6
	HMDB0040225	Isoamyl salicylate	C12H16O3	M+H	209.1172	-0.6
	HMDB0030150	Jasmine ketolactone	C12H16O3	M+H	209.1172	-0.6
209.1531	HMDB0178140	3-[(2Z)-but-2-en-1-yl]-6-hydroxy-2,4,4-trimethylcyclohex-2-en-1-one	C13H20O2	M+H	209.1536	-2.4
	HMDB0178138	2,4,4-trimethyl-3-[(3-methyloxiran-2-yl)methyl]cyclohex-2-en-1-one	C13H20O2	M+H	209.1536	-2.4
	HMDB0178139	6-[(2Z)-but-2-en-1-yl]-1,5,5-trimethyl-7-oxabicyclo[4.1]heptan-2-one	C13H20O2	M+H	209.1536	-2.4
	HMDB0178136	3-[(2Z)-but-2-en-1-yl]-2-(hydroxymethyl)-4,4-dimethylcyclohex-2-en-1-one	C13H20O2	M+H	209.1536	-2.4
	HMDB0178137	3-[(2Z)-4-hydroxybut-2-en-1-yl]-2,4,4-trimethylcyclohex-2-en-1-one	C13H20O2	M+H	209.1536	-2.4
	HMDB0178135	3-[(2Z)-but-2-en-1-yl]-4-(hydroxymethyl)-2,4-dimethylcyclohex-2-en-1-one	C13H20O2	M+H	209.1536	-2.4
	HMDB0163196	(2E,4E,7Z)-13-hydroxytrideca-2,4,7-trienal	C13H20O2	M+H	209.1536	-2.4
	HMDB0163195	(2E,4E)-6-(3-pentyloxiran-2-yl)hexa-2,4-dienal	C13H20O2	M+H	209.1536	-2.4
	HMDB0163194	(2E)-3-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}prop-2-enal	C13H20O2	M+H	209.1536	-2.4
	HMDB0163192	(2E,4E,7Z)-12-hydroxytrideca-2,4,7-trienal	C13H20O2	M+H	209.1536	-2.4
	HMDB0163191	(2E,4E,7Z)-9-hydroxytrideca-2,4,7-trienal	C13H20O2	M+H	209.1536	-2.4
	HMDB0163193	3-[(1E,4Z)-deca-1,4-dien-1-yl]oxirane-2-carbaldehyde	C13H20O2	M+H	209.1536	-2.4
	HMDB0163190	(2E,4E,7Z)-trideca-2,4,7-trienoic acid	C13H20O2	M+H	209.1536	-2.4
	HMDB0132947	1-(4-methoxyphenyl)-4-methylpentan-3-ol	C13H20O2	M+H	209.1536	-2.4
	HMDB0041636	(3R,8E)-3-Hydroxy-5,8-megastigmadien-7-one	C13H20O2	M+H	209.1536	-2.4
	HMDB0029668	Eremopetasinorol	C13H20O2	M+H	209.1536	-2.4
	HMDB0038047	Carvyl propionate	C13H20O2	M+H	209.1536	-2.4
	HMDB0040233	2,3,5,6,8,8a-Hexahydro-2,5,5,8a-tetramethyl-7H-1-benzopyran-7-one	C13H20O2	M+H	209.1536	-2.4
	HMDB0038529	5,9,6,9-Diepox-4-megastigmenone	C13H20O2	M+H	209.1536	-2.4
	HMDB0037776	3-Mercaptohexyl hexanoate	C13H20O2	M+H	209.1536	-2.4

	HMDB0036821	Apo-9-zeaxanthinone	C13H20O2	M+H	209.1536	-2.4
	HMDB0036686	2,2,6,7-Tetramethylbicyclo[4.3]nona-1(9),4-diene-7,8-diol	C13H20O2	M+H	209.1536	-2.4
	HMDB0031869	(S,E)-Lyratol propanoate	C13H20O2	M+H	209.1536	-2.4
	HMDB0036824	Acetal R	C13H20O2	M+H	209.1536	-2.4
	HMDB0034672	(5alpha,8beta,9beta)-5,9-Epoxy-3,6-megastigmadien-8-ol	C13H20O2	M+H	209.1536	-2.4
	HMDB0034984	(5R,6S)-5,6-Epoxy-7-megastigmen-9-one	C13H20O2	M+H	209.1536	-2.4
	HMDB0035228	Theaspirone A	C13H20O2	M+H	209.1536	-2.4
209.1895	HMDB0035862	(E)-6,-Dimethyl-9-methylene-5-undecen-2-one	C14H24O	M+H	209.1900	-2.3
	HMDB0039884	2-Cyclotetradecen-1-one	C14H24O	M+H	209.1900	-2.3
	HMDB0032215	2-Decylfuran	C14H24O	M+H	209.1900	-2.3
210.0978	HMDB0177065	Quinic acid	C7H12O6	M+NH4	210.0972	2.8
	HMDB0003072	Quinate	C7H12O6	M+NH4	210.0972	2.8
210.1258	HMDB0015171	Selegiline	C13H17N	M+Na	210.1253	2.3
	HMDB0151804	2-benzylhexan-1-ol	C13H20O	M+NH4	210.1852	-2.1
	HMDB0041615	Phenethyl isoamyl ether	C13H20O	M+NH4	210.1852	-2.1
	HMDB0032498	Pseudoionone	C13H20O	M+NH4	210.1852	-2.1
	HMDB0037139	4-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-butanone	C13H20O	M+NH4	210.1852	-2.1
	HMDB0036022	Isospirene	C13H20O	M+NH4	210.1852	-2.1
	HMDB0034959	Edulan I	C13H20O	M+NH4	210.1852	-2.1
	HMDB0035753	(R)-(E)-4,7-Megastigmadien-9-one	C13H20O	M+NH4	210.1852	-2.1
	HMDB0035682	delta-Damascone	C13H20O	M+NH4	210.1852	-2.1
	HMDB0033545	(2E,4Z,7Z)-2,4,7-Tridecatrienal	C13H20O	M+NH4	210.1852	-2.1
	HMDB0036565	beta-Ionone	C13H20O	M+NH4	210.1852	-2.1
	HMDB0036144	Cycloionone	C13H20O	M+NH4	210.1852	-2.1
	HMDB0029821	2,5-Diisopropyl-4-methylphenol	C13H20O	M+NH4	210.1852	-2.1
	HMDB0032541	4-(2,6,6-Trimethylcyclohex-1-enyl)but-2-en-4-one	C13H20O	M+NH4	210.1852	-2.1
210.1848	HMDB0029824	2,4-Diisopropyl-3-methylphenol	C13H20O	M+NH4	210.1852	-2.1
	HMDB0029822	2,5-Diisopropyl-3-methylphenol	C13H20O	M+NH4	210.1852	-2.1
	HMDB0034979	gamma-Ionone	C13H20O	M+NH4	210.1852	-2.1
	HMDB0036818	Vitispirane	C13H20O	M+NH4	210.1852	-2.1
	HMDB0031733	4-(4-Methyl-3-pentenyl)-3-cyclohexene-1-carboxaldehyde	C13H20O	M+NH4	210.1852	-2.1
	HMDB0029823	2,4-Diisopropyl-5-methylphenol	C13H20O	M+NH4	210.1852	-2.1
	HMDB0034671	(E)-5,8-Megastigmadien-4-one	C13H20O	M+NH4	210.1852	-2.1
	HMDB0036027	alpha-Damascone	C13H20O	M+NH4	210.1852	-2.1
	HMDB0029820	2,6-Diisopropyl-3-methylphenol	C13H20O	M+NH4	210.1852	-2.1
	HMDB0059883	alpha-Ionone	C13H20O	M+NH4	210.1852	-2.1
	HMDB0036684	2,4,5,7alpha-Tetrahydro-1,4,4,7a-tetramethyl-1H-inden-2-ol	C13H20O	M+NH4	210.1852	-2.1
	HMDB0029825	2,3-Diisopropyl-5-methylphenol	C13H20O	M+NH4	210.1852	-2.1
	HMDB0036031	Labienoxime	C13H23NO	M+H	210.1852	-2.1
211.0831	HMDB0036431	1,3,9-Trimethyluric acid	C8H10N4O3	M+H	211.0826	2.5
	HMDB0002123	1,3,7-Trimethyluric acid	C8H10N4O3	M+H	211.0826	2.5
	HMDB0179177	5-hydroxy-4-oxononanoic acid	C9H16O4	M+Na	211.0941	0.1
	HMDB0179175	2-hydroxy-4-oxononanoic acid	C9H16O4	M+Na	211.0941	0.1
	HMDB0179176	3-hydroxy-4-oxononanoic acid	C9H16O4	M+Na	211.0941	0.1
	HMDB0179174	9-hydroxy-4-oxononanoic acid	C9H16O4	M+Na	211.0941	0.1
	HMDB0179173	8-hydroxy-4-oxononanoic acid	C9H16O4	M+Na	211.0941	0.1
	HMDB0000784	Azelaic acid	C9H16O4	M+Na	211.0941	0.1
	HMDB0059783	3-Methylsuberic acid	C9H16O4	M+Na	211.0941	0.1
211.0941	HMDB0059760	2,4-Dimethylpimelic acid	C9H16O4	M+Na	211.0941	0.1
	HMDB0059879	Diethyl glutarate	C9H16O4	M+Na	211.0941	0.1
	HMDB0032387	(+/-)-Methyl 5-acetoxyhexanoate	C9H16O4	M+Na	211.0941	0.1
	HMDB0032200	cis- and trans-Ethyl 2,4-dimethyl-1,3-dioxolane-2-acetate	C9H16O4	M+Na	211.0941	0.1
	HMDB0032258	(+/-)-Ethyl 3-acetoxy-2-methylbutyrate	C9H16O4	M+Na	211.0941	0.1
	HMDB0036233	Butyl ethyl malonate	C9H16O4	M+Na	211.0941	0.1
	HMDB0011717	Nonate	C9H16O4	M+Na	211.0941	0.1
	HMDB0059814	Diethyl methylsuccinate	C9H16O4	M+Na	211.0941	0.1
	HMDB0037816	Dihydro-3-(1-octenyl)-2,5-furandione	C12H18O3	M+H	211.1329	-0.8
	HMDB0037135	1-Benzyloxy-1-(2-methoxyethoxy)ethane	C12H18O3	M+H	211.1329	-0.8
	HMDB0032871	Sedanonic acid	C12H18O3	M+H	211.1329	-0.8
	HMDB0032797	Jasmonic acid	C12H18O3	M+H	211.1329	-0.8

211.1327	HMDB0037735	Isoamyl 2-furonpropionate	C12H18O3	M+H	211.1329	-0.8
	HMDB0033102	Dihydro-3-(2-octenyl)-2,5-furandione	C12H18O3	M+H	211.1329	-0.8
	HMDB0037642	4-(Butoxymethyl)-2-methoxyphenol	C12H18O3	M+H	211.1329	-0.8
	HMDB0041573	3-Ethenyl-2,5-dimethyl-4-oxohex-5-en-2-yl acetate	C12H18O3	M+H	211.1329	-0.8
	HMDB0037104	(R)-8-Acetoxy-carvotanacetone	C12H18O3	M+H	211.1329	-0.8
211.1687	HMDB0182790	4-{2,2,6-trimethyl-7-oxabicyclo[4.1]heptan-1-yl}butan-2-one	C13H22O2	M+H	211.1693	-2.6
	HMDB0163206	{3-[(1E,4Z)-deca-1,4-dien-1-yl]oxiran-2-yl}methanol	C13H22O2	M+H	211.1693	-2.6
	HMDB0163203	(4E,7Z)-2-hydroxytrideca-4,7-dienal	C13H22O2	M+H	211.1693	-2.6
	HMDB0163205	(2E,4E,7Z)-trideca-2,4,7-triene-1,12-diol	C13H22O2	M+H	211.1693	-2.6
	HMDB0163202	(4E,7Z)-13-hydroxytrideca-4,7-dienal	C13H22O2	M+H	211.1693	-2.6
	HMDB0163201	(4E)-6-(3-pentyloxiran-2-yl)hex-4-enal	C13H22O2	M+H	211.1693	-2.6
	HMDB0163200	3-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}propanal	C13H22O2	M+H	211.1693	-2.6
	HMDB0163199	(4E,7Z)-12-hydroxytrideca-4,7-dienal	C13H22O2	M+H	211.1693	-2.6
	HMDB0163198	(4E,7Z)-9-hydroxytrideca-4,7-dienal	C13H22O2	M+H	211.1693	-2.6
	HMDB0163197	(4E,7Z)-3-hydroxytrideca-4,7-dienal	C13H22O2	M+H	211.1693	-2.6
	HMDB0163204	(2E,4E,7Z)-trideca-2,4,7-triene-1,9-diol	C13H22O2	M+H	211.1693	-2.6
	HMDB0163209	(2E,4E,7Z)-trideca-2,4,7-triene-1,13-diol	C13H22O2	M+H	211.1693	-2.6
	HMDB0182751	4-(2,2-dimethyl-6-methylidenecyclohexyl)-3-hydroxybutan-2-one	C13H22O2	M+H	211.1693	-2.6
	HMDB0182752	4-(2,2-dimethyl-6-methylidenecyclohexyl)-1-hydroxybutan-2-one	C13H22O2	M+H	211.1693	-2.6
	HMDB0182749	4-(1-hydroxy-2,2-dimethyl-6-methylidenecyclohexyl)butan-2-one	C13H22O2	M+H	211.1693	-2.6
	HMDB0182750	4-(5-hydroxy-2,2-dimethyl-6-methylidenecyclohexyl)butan-2-one	C13H22O2	M+H	211.1693	-2.6
	HMDB0182747	4-[2-(hydroxymethyl)-2-methyl-6-methylidenecyclohexyl]butan-2-one	C13H22O2	M+H	211.1693	-2.6
	HMDB0182748	63512--3	C13H22O2	M+H	211.1693	-2.6
	HMDB0178145	3-[(2Z)-1-hydroxybut-2-en-1-yl]-2,4,4-trimethylcyclohexan-1-one	C13H22O2	M+H	211.1693	-2.6
	HMDB0178144	3-[(2Z)-4-hydroxybut-2-en-1-yl]-2,4,4-trimethylcyclohexan-1-one	C13H22O2	M+H	211.1693	-2.6
	HMDB0178146	2,4,4-trimethyl-3-[(3-methyloxiran-2-yl)methyl]cyclohexan-1-one	C13H22O2	M+H	211.1693	-2.6
	HMDB0178147	3-[(2Z)-but-2-en-1-yl]-6-hydroxy-2,4,4-trimethylcyclohexan-1-one	C13H22O2	M+H	211.1693	-2.6
	HMDB0178143	3-[(2Z)-but-2-en-1-yl]-2-hydroxy-2,4,4-trimethylcyclohexan-1-one	C13H22O2	M+H	211.1693	-2.6
	HMDB0178142	3-[(2Z)-but-2-en-1-yl]-2-(hydroxymethyl)-4,4-dimethylcyclohexan-1-one	C13H22O2	M+H	211.1693	-2.6
	HMDB0178141	3-[(2Z)-but-2-en-1-yl]-4-(hydroxymethyl)-2,4-dimethylcyclohexan-1-one	C13H22O2	M+H	211.1693	-2.6
	HMDB0163218	(4E,7Z)-4,7-tridecadienoic acid	C13H22O2	M+H	211.1693	-2.6
	HMDB0163207	(2E)-3-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}prop-2-en-1-ol	C13H22O2	M+H	211.1693	-2.6
	HMDB0163208	(2E,4E)-6-(3-pentyloxiran-2-yl)hexa-2,4-dien-1-ol	C13H22O2	M+H	211.1693	-2.6
	HMDB0032098	Cepanone	C13H22O2	M+H	211.1693	-2.6
	HMDB0038258	Neryl propionate	C13H22O2	M+H	211.1693	-2.6
	HMDB0037307	Propyl 2,4-decadienoate	C13H22O2	M+H	211.1693	-2.6
	HMDB0037286	Citral propylene glycol acetal	C13H22O2	M+H	211.1693	-2.6
	HMDB0032052	alpha-Terpineol propanoate	C13H22O2	M+H	211.1693	-2.6
	HMDB0038249	Isobornyl propionate	C13H22O2	M+H	211.1693	-2.6
	HMDB0031014	Methyl (2E,6Z)-dodecadienoate	C13H22O2	M+H	211.1693	-2.6
	HMDB0038291	2-Propenyl cyclohexanecarboxylate	C13H22O2	M+H	211.1693	-2.6
	HMDB0030425	Linalyl propionate	C13H22O2	M+H	211.1693	-2.6
	HMDB0040232	Octahydro-2,5,5,8a-tetramethyl-7H-1-benzopyran-7-one	C13H22O2	M+H	211.1693	-2.6
	HMDB0037390	Tsibulin 1	C13H22O2	M+H	211.1693	-2.6
	HMDB0041554	Artemisyl propionate	C13H22O2	M+H	211.1693	-2.6
211.2051	HMDB0032526	(Z)-8-Tetradecenal	C14H26O	M+H	211.2056	-2.6
	HMDB0032525	Tetradec-2-enal	C14H26O	M+H	211.2056	-2.6
	HMDB0142175	2-benzylpropanedioic acid	C10H10O4	M+NH4	212.0917	-2.5
	HMDB0146403	SCHEMBL2535852	C10H10O4	M+NH4	212.0917	-2.5
	HMDB0146628	ZINC2222827	C10H10O4	M+NH4	212.0917	-2.5

212.0912

HMDB0146629	CTK4057	C10H10O4	M+NH4	212.0917	-2.5
HMDB0146630	3-(2-methoxyphenyl)oxirane-2-carboxylic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0154365	3-(3-hydroxy-2-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0166608	3-(6-hydroxy-2H-1,3-benzodioxol-5-yl)propanal	C10H10O4	M+NH4	212.0917	-2.5
HMDB0166607	3-(2H-1,3-benzodioxol-5-yl)-3-hydroxypropanal	C10H10O4	M+NH4	212.0917	-2.5
HMDB0166611	3-(2H-1,3-benzodioxol-5-yl)-2-hydroxypropanal	C10H10O4	M+NH4	212.0917	-2.5
HMDB0166609	2815-95-4	C10H10O4	M+NH4	212.0917	-2.5
HMDB0166613	6-[(1Z)-3-hydroxyprop-1-en-1-yl]-2H-1,3-benzodioxol-5-ol	C10H10O4	M+NH4	212.0917	-2.5
HMDB0166614	[3-(2H-1,3-benzodioxol-5-yl)oxiran-2-yl]methanol	C10H10O4	M+NH4	212.0917	-2.5
HMDB0178262	(2Z)-3-(3-hydroxy-5-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0141263	(2Z)-2-hydroxy-3-(3-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0141265	3-(3-methoxyphenyl)-2-oxopropanoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0140957	(2E)-3-(3-hydroxy-2-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0125096	3-(4-hydroxy-3-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0125524	(2E)-3-(3-hydroxy-5-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0125588	3-(3-hydroxy-5-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0127500	3-(4-methoxyphenyl)-2-oxopropanoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0131137	3-(3-hydroxy-4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0131173	3-(4-methoxyphenyl)oxirane-2-carboxylic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0131172	(2E)-3-(2-hydroxy-4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0131171	(2Z)-2-hydroxy-3-(4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0137510	3-(4-hydroxy-2-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0000954	Ferulic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0000955	Isoferulic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0002120	Monoethyl phthalate	C10H10O4	M+NH4	212.0917	-2.5
HMDB0030765	(-)-trans-3,4-Dihydro-4,8-dihydroxy-3-methyl-1H-2-benzopyran-1-one	C10H10O4	M+NH4	212.0917	-2.5
HMDB0039606	Repandiol	C10H10O4	M+NH4	212.0917	-2.5
HMDB0032652	Meconine	C10H10O4	M+NH4	212.0917	-2.5
HMDB0037644	3-(2-Hydroxy-3-methoxyphenyl)-2-propenoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0029663	Vanillin acetate	C10H10O4	M+NH4	212.0917	-2.5
HMDB0032614	Piperonyl acetate	C10H10O4	M+NH4	212.0917	-2.5
HMDB0165533	Ferulic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0240705	Ferulic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0059721	mono-Benzyl malonate	C10H10O4	M+NH4	212.0917	-2.5
HMDB0061686	2,5-Dihydroxycinnamic acid methyl ester	C10H10O4	M+NH4	212.0917	-2.5
HMDB0134088	3-(2-hydroxy-3-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0135741	3-(2-hydroxy-4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+NH4	212.0917	-2.5
HMDB0011754	Methyl dopa	C10H13NO4	M+H	212.0917	-2.5
HMDB0001434	3-Methoxytyrosine	C10H13NO4	M+H	212.0917	-2.5
HMDB0060747	3-O-Methyl-a-methyl dopa	C10H13NO4	M+H	212.0917	-2.5
HMDB0124918	2-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C11H14O3	M+NH4	212.1281	-2.9
HMDB0126162	3-(3-methylbut-2-en-1-yl)benzene-1,2,4-triol	C11H14O3	M+NH4	212.1281	-2.9
HMDB0126161	2-(4-hydroxy-3-methylbut-2-en-1-yl)benzene-1,3-diol	C11H14O3	M+NH4	212.1281	-2.9
HMDB0126163	2-[(3,3-dimethyloxiran-2-yl)methyl]benzene-1,3-diol	C11H14O3	M+NH4	212.1281	-2.9
HMDB0126262	2-[(2E)-4-hydroxy-3-methylbut-2-en-1-yl]benzene-1,3-diol	C11H14O3	M+NH4	212.1281	-2.9
HMDB0126462	2-[(1E)-3-hydroxy-3-methylbut-1-en-1-yl]benzene-1,3-diol	C11H14O3	M+NH4	212.1281	-2.9
HMDB0166268	76773-99-4	C11H14O3	M+NH4	212.1281	-2.9
HMDB0126464	2-[(1E)-3-methylbut-1-en-1-yl]benzene-1,3,5-triol	C11H14O3	M+NH4	212.1281	-2.9
HMDB0126465	2-[3-(propan-2-yl)oxiran-2-yl]benzene-1,3-diol	C11H14O3	M+NH4	212.1281	-2.9
HMDB0151236	[3-(4-methoxyphenyl)-2-methyloxiran-2-yl]methanol	C11H14O3	M+NH4	212.1281	-2.9
HMDB0151235	2-(3-hydroxy-2-methylprop-1-en-1-yl)-5-methoxyphenol	C11H14O3	M+NH4	212.1281	-2.9
HMDB0163606	3-hydroxy-3-methyl-2-phenylbutanoic acid	C11H14O3	M+NH4	212.1281	-2.9
HMDB0163607	4-hydroxy-3-methyl-2-phenylbutanoic acid	C11H14O3	M+NH4	212.1281	-2.9
HMDB0163609	2-hydroxy-3-methyl-2-phenylbutanoic acid	C11H14O3	M+NH4	212.1281	-2.9
HMDB0163610	SCHEMBL8733687	C11H14O3	M+NH4	212.1281	-2.9
HMDB0163612	AKO229142	C11H14O3	M+NH4	212.1281	-2.9
HMDB0163611	2-(4-hydroxyphenyl)-3-methylbutanoic acid	C11H14O3	M+NH4	212.1281	-2.9
HMDB0164134	2-Butanone, 4-hydroxy-4-(4-methoxyphenyl)-	C11H14O3	M+NH4	212.1281	-2.9
HMDB0164133	SCHEMBL13742814	C11H14O3	M+NH4	212.1281	-2.9
HMDB0164132	(4r)-hydroxy-4-(4'-methoxyphenyl)-butan-2-one	C11H14O3	M+NH4	212.1281	-2.9

212.1275	HMDB0171010	cis-4-Propenylsyringol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0182834	4-hydroxybenzyl butyrate	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0151233	2-(4-methoxybenzylidene)propane-1,3-diol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0151232	2-hydroxy-3-(4-methoxyphenyl)-2-methylpropanal	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0126466	2-[(1E)-4-hydroxy-3-methylbut-1-en-1-yl]benzene-1,3-diol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0126463	3-[(1E)-3-methylbut-1-en-1-yl]benzene-1,2,4-triol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0132270	5-(4-hydroxyphenyl)pentanoic acid	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0133192	4-(3-methylbut-2-en-1-yl)benzene-1,2,3-triol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0133191	4-(4-hydroxy-3-methylbut-2-en-1-yl)benzene-1,3-diol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0133193	5-(3-methylbut-2-en-1-yl)benzene-1,2,4-triol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0133190	4-[(2E)-4-hydroxy-3-methylbut-2-en-1-yl]benzene-1,3-diol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0133194	4-[(3,3-dimethyloxiran-2-yl)methyl]benzene-1,3-diol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0133463	4-(3-hydroxybut-1-en-1-yl)-2-methoxyphenol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0133484	3-hydroxy-4-(3-methoxyphenyl)butan-2-one	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0133515	4-(3-hydroxy-5-methoxyphenyl)butan-2-one	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0133538	1-hydroxy-4-(3-methoxyphenyl)butan-2-one	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0141323	4-hydroxy-4-(3-methoxyphenyl)butan-2-one	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0146411	3-(3-Methoxyphenyl)-2-methylpropanoic acid	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0151228	3-hydroxy-3-(4-methoxyphenyl)-2-methylpropanal	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0151230	3-hydroxy-2-[(4-methoxyphenyl)methyl]propanal	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0151229	3-(4-methoxyphenyl)-2-methylpropanoic acid	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0059944	2-(3-Methylphenyl)-1,3-dioxan-5-ol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0059943	2-(2-Methylphenyl)-1,3-dioxan-5-ol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0179740	gamma-Methoxyisoeugenol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0062055	4-hydroxy-5-phenylpentanoic acid	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0059942	[2-(4-Methylphenyl)-1,3-dioxolan-4-yl]methanol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0059945	2-(4-Methylphenyl)-1,3-dioxan-5-ol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0059940	[2-(2-Methylphenyl)-1,3-dioxolan-4-yl]methanol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0031517	(R)-3-Hydroxy-5-phenylpentanoic acid	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0032575	Butylparaben	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0034990	4-Methoxybenzyl propanoate	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0041505	5-Hydroxy-2-benzyl-1,3-dioxane	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0040730	Butyl salicylate	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0037271	2,6-Dimethoxy-4-(1-propenyl)phenol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0032590	Zingerone	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0041506	2-Benzyl-5-hydroxymethyl-1,3-dioxolane	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0036432	Isobutyl salicylate	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0034206	Ethyl 4-methylphenoxyacetate	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0041194	Methoxyeugenol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0031984	2,5-Dimethoxy-4-(2-propenyl)phenol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0041666	3-Hydroxyphenyl-valeric acid	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0059898	Ethyl 4-ethoxybenzoate	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0059941	[2-(3-Methylphenyl)-1,3-dioxolan-4-yl]methanol	C11H14O3	M+NH4	212.1281	-2.9
	HMDB0014954	Orciprenaline	C11H17NO3	M+H	212.1281	-2.9
	HMDB0015197	Isoproterenol	C11H17NO3	M+H	212.1281	-2.9
	HMDB0167331	AKO23578554	C11H17NO3	M+H	212.1281	-2.9
	HMDB0014861	Methoxamine	C11H17NO3	M+H	212.1281	-2.9
212.1640	HMDB0132986	1-(4-methoxyphenyl)pentan-3-ol	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0041610	(2,2-Diethoxyethyl)benzene	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0035801	(2S,4R)-p-Mentha-1(7),5-dien-2-ol acetate	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0037231	Perillyl acetate	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0035126	Myrtenyl acetate	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0034450	Neocnidilide	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0032567	Hexylresorcinol	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0037018	(S)-p-Mentha-1,8-dien--yl acetate	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0038046	Carvyl acetate	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0035375	Ethyl (2E,4E,7Z)-Decatrienoate	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0035376	Ethyl (2E,4Z,7Z)-Decatrienoate	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0031840	(S,Z)-Lyratol acetate	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0039685	8-Ocimenyl acetate	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0037389	(R)-2-Acetoxy-p-mentha-1,8-diene	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0038292	Menthadienyl acetate	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0041497	(S)-Neolyratyl acetate	C12H18O2	M+NH4	212.1645	-2.4

	HMDB0040439	1-(2-Furanyl)-1-octanone	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0014018	4-Hydroxypropofol	C12H18O2	M+NH4	212.1645	-2.4
	HMDB0038897	(E)-2-(2-Octenyl)cyclopentanone	C13H22O	M+NH4	212.2009	-2.8
	HMDB0182746	4-(2,2-Dimethyl-6-methylenecyclohexyl)butan-2-one	C13H22O	M+NH4	212.2009	-2.8
	HMDB0163189	(2E,4E,7Z)-trideca-2,4,7-trien-1-ol	C13H22O	M+NH4	212.2009	-2.8
	HMDB0163188	SCHEMBL15656566	C13H22O	M+NH4	212.2009	-2.8
	HMDB0178134	3-[(2Z)-but-2-en-1-yl]-2,4,4-trimethylcyclohexan-1-one	C13H22O	M+NH4	212.2009	-2.8
	HMDB0038731	4,7-Megastigmadien-9-ol	C13H22O	M+NH4	212.2009	-2.8
	HMDB0038026	Dihydro-alpha-ionone	C13H22O	M+NH4	212.2009	-2.8
	HMDB0038216	5-Isopropyl-2-(2-methylpropyl)-2-cyclohexen-1-one	C13H22O	M+NH4	212.2009	-2.8
	HMDB0032913	4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-butanone	C13H22O	M+NH4	212.2009	-2.8
	HMDB0036823	Theaspirane	C13H22O	M+NH4	212.2009	-2.8
	HMDB0036026	Octahydro-6-isopropyl-2(1H)-naphthalenone	C13H22O	M+NH4	212.2009	-2.8
	HMDB0031846	Geranylacetone	C13H22O	M+NH4	212.2009	-2.8
	HMDB0036184	7,8-Dehydro-3,4-dihydro-beta-ionol	C13H22O	M+NH4	212.2009	-2.8
	HMDB0036820	beta-Ionol	C13H22O	M+NH4	212.2009	-2.8
	HMDB0032355	(+/-)-[R-(E)]-5-Isopropyl-8-methylnona-6,8-dien-2-one	C13H22O	M+NH4	212.2009	-2.8
	HMDB0037834	Ethyl menthane carboxamide	C13H25NO	M+H	212.2009	-2.8
	HMDB0177476	6-methylnaphthalene-1,3,8-triol	C11H10O3	M+Na	213.0522	-1.9
	HMDB0166927	3-methyl-1aH,7aH-naphtho[1,2-b]oxirene-2,5-diol	C11H10O3	M+Na	213.0522	-1.9
	HMDB0166923	3-methylnaphthalene-1,4,6-triol	C11H10O3	M+Na	213.0522	-1.9
	HMDB0166925	2-(hydroxymethyl)naphthalene-1,4-diol	C11H10O3	M+Na	213.0522	-1.9
	HMDB0166924	3-methylnaphthalene-1,4,5-triol	C11H10O3	M+Na	213.0522	-1.9
	HMDB0166926	4-methyl-1aH,7aH-naphtho[1,2-b]oxirene-2,5-diol	C11H10O3	M+Na	213.0522	-1.9
	HMDB0166922	2-methylnaphthalene-1,4,6-triol	C11H10O3	M+Na	213.0522	-1.9
	HMDB0166921	691-78	C11H10O3	M+Na	213.0522	-1.9
	HMDB0129361	1-(4-methoxy-1-benzofuran-5-yl)ethan-1-one	C11H10O3	M+Na	213.0522	-1.9
	HMDB0040326	7-Hydroxy-2,5-dimethyl-4H-1-benzopyran-4-one	C11H10O3	M+Na	213.0522	-1.9
	HMDB0040938	Coixinden A	C11H10O3	M+Na	213.0522	-1.9
	HMDB0041122	(S)-2,3-Dihydro-5-hydroxy-2-methyl-1,4-naphthoquinone	C11H10O3	M+Na	213.0522	-1.9
	HMDB0032991	7-Methoxy-6-methyl-2H-1-benzopyran-2-one	C11H10O3	M+Na	213.0522	-1.9
	HMDB0040731	Avenalamic acid	C11H10O3	M+Na	213.0522	-1.9
	HMDB0039359	Methyl (Z,Z)-hydroxy-2,8-decadiene-4,6-diynoate	C11H10O3	M+Na	213.0522	-1.9
	HMDB0181530	7-methylnaphthalene-1,4,5-triol	C11H10O3	M+Na	213.0522	-1.9
	HMDB0014814	Benzyl Benzoate	C14H12O2	M+H	213.0910	-1.9
	HMDB0032039	Benzoin	C14H12O2	M+H	213.0910	-1.9
	HMDB0033601	Dihydrojasmonic acid	C12H20O3	M+H	213.1485	-2.0
	HMDB0037326	Traumatol	C12H20O3	M+H	213.1485	-2.0
	HMDB0029388	Cucurbitic acid	C12H20O3	M+H	213.1485	-2.0
	HMDB0035085	Vulgarole	C12H20O3	M+H	213.1485	-2.0
	HMDB0041572	3-Ethenyl-4-hydroxy-2,5-dimethylhex-5-en-2-yl acetate	C12H20O3	M+H	213.1485	-2.0
	HMDB0031028	Methyl (E)-2-dodecenoate	C13H24O2	M+H	213.1849	-2.4
	HMDB0032792	(E)-3-Methyl-4-decen-1-yl acetate	C13H24O2	M+H	213.1849	-2.4
	HMDB0038078	1,1-Diethoxy-2,6-nonadiene	C13H24O2	M+H	213.1849	-2.4
	HMDB0037626	1-Ethylhexyl tiglate	C13H24O2	M+H	213.1849	-2.4
	HMDB0031017	-Undecenyl acetate	C13H24O2	M+H	213.1849	-2.4
	HMDB0034286	Ethyl -undecenoate	C13H24O2	M+H	213.1849	-2.4
	HMDB0040451	Oxacyclotetradecan-2-one	C13H24O2	M+H	213.1849	-2.4
	HMDB0037907	2,6,-Tetramethyl-1-oxaspiro[4.5]decan-6-ol	C13H24O2	M+H	213.1849	-2.4
	HMDB0037226	Citronellyl propionate	C13H24O2	M+H	213.1849	-2.4
	HMDB0039805	4-(3-Hydroxybutyl)-3,3,5-trimethylcyclohexanone	C13H24O2	M+H	213.1849	-2.4
	HMDB0037187	Rhodinyl propionate	C13H24O2	M+H	213.1849	-2.4
	HMDB0031741	Coniferan	C13H24O2	M+H	213.1849	-2.4
	HMDB0012250	L-Aspartyl-4-phosphate	C4H8NO7P	M+H	214.0111	-1.5
	HMDB0062139	N-Butyl-Benzenesulfonamide	C10H15NO2S	M+H	214.0896	-2.5
	HMDB0032418	2-(4-Methyl-5-thiazolyl)ethyl butanoate	C10H15NO2S	M+H	214.0896	-2.5
	HMDB0032422	2-(4-Methyl-5-thiazolyl)ethyl isobutyrate	C10H15NO2S	M+H	214.0896	-2.5
	HMDB0030867	Dihydro-5-(2-octenyl)-2(3H)-furanone	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0038270	cis-3-Hexenyl cis-3-hexenoate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0030945	Methyl 2-undecynoate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0039522	Linalyl acetate	C12H20O2	M+NH4	214.1802	-2.1

214.1797	HMDB0040725	Fenchyl acetate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0036048	Artemisia alcohol acetate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0040397	(-)-Bornyl acetate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0040206	Allyl 3-cyclohexylpropionate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0031692	cis-3-Hexenyl trans-4-hexenoate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0031030	6-Heptyl-5,6-dihydro-2H-pyran-2-one	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0036599	Ethyl 2Z,4E-decadienoic acid	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0034903	(3R,3aR,7aS)-3-Butylhexahydro-1(3H)-isobenzofuranone	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0038280	cis-3-Hexenyl trans-2-hexenoate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0041469	Dihydrocarveol acetate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0032193	alpha-Campholene acetate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0032051	alpha-Terpineol acetate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0041494	(S)-Santolina acetate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0061816	3,7-Dimethyl-2,6-octadien-1-ylacetate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0040227	Isopulegol acetate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0037301	p-Menth-1-en-9-ol acetate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0032331	(Z)-4-Hydroxy-6-dodecenoic acid lactone	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0062144	p-Menth-1-en-4-yl acetate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0035157	geranyl acetate	C12H20O2	M+NH4	214.1802	-2.1
	HMDB0032901	Yuzu lactone	C12H20O2	M+NH4	214.1802	-2.1
214.2160	HMDB0163217	57981-61	C13H24O	M+NH4	214.2165	-2.5
	HMDB0041490	Dihydrogeranylacetone	C13H24O	M+NH4	214.2165	-2.5
	HMDB0037275	2-Tridecenal	C13H24O	M+NH4	214.2165	-2.5
	HMDB0041404	2-Methylcyclododecanone	C13H24O	M+NH4	214.2165	-2.5
	HMDB0036172	4-(2,6,6-Trimethyl-1-cyclohexenyl)-2-butanol	C13H24O	M+NH4	214.2165	-2.5
	HMDB0032247	(Z)-4-Dodecenal	C13H24O	M+NH4	214.2165	-2.5
214.9994	HMDB0174881	3-(methylsulfanyl)-3-[(1E)-prop-1-en-1-yl]disulfanyl]prop-1-ene	C7H12S3	M+Na	214.9993	0.3
215.0505	HMDB0037166	2-(Methylthiomethyl)-3-phenyl-2-propenal	C11H12OS	M+Na	215.0501	1.8
215.1272	HMDB0030986	2-Carboxy-5,7-dimethyl-4-octanolide	C11H18O4	M+H	215.1278	-2.7
	HMDB0030984	5-Hexyltetrahydro-2-oxo-3-furancarboxylic acid	C11H18O4	M+H	215.1278	-2.7
	HMDB0030985	alpha-Carboxy-delta-decalactone	C11H18O4	M+H	215.1278	-2.7
215.1637	HMDB0010727	3-Oxododecanoic acid	C12H22O3	M+H	215.1642	-2.2
	HMDB0159933	(5Z)-11-hydroxydodec-5-enoic acid	C12H22O3	M+H	215.1642	-2.2
	HMDB0159931	(5Z)-7-hydroxydodec-5-enoic acid	C12H22O3	M+H	215.1642	-2.2
	HMDB0159932	(5Z)-4-hydroxydodec-5-enoic acid	C12H22O3	M+H	215.1642	-2.2
	HMDB0159936	(5Z)-2-hydroxydodec-5-enoic acid	C12H22O3	M+H	215.1642	-2.2
	HMDB0159935	SCHEMBL14224944	C12H22O3	M+H	215.1642	-2.2
	HMDB0037398	4-Acetoxy-2-hexyltetrahydrofuran	C12H22O3	M+H	215.1642	-2.2
	HMDB0159934	4-(3-hexyloxiran-2-yl)butanoic acid	C12H22O3	M+H	215.1642	-2.2
216.0535	HMDB0172075	(2-oxo-2-propoxyethoxy)sulfonic acid	C5H10O6S	M+NH4	216.0536	-0.6
	HMDB0172073	SCHEMBL161715	C5H10O6S	M+NH4	216.0536	-0.6
	HMDB0172071	{[1-(acetyloxy)propan-2-yl]oxy}sulfonic acid	C5H10O6S	M+NH4	216.0536	-0.6
	HMDB0161211	3-methyl-2-(sulfooxy)butanoate	C5H9O6S	M+NH4	216.0536	-0.6
	HMDB0161209	3-methyl-4-(sulfooxy)butanoate	C5H9O6S	M+NH4	216.0536	-0.6
	HMDB0159994	3-(sulfooxy)pentanoic acid	C5H10O6S	M+NH4	216.0536	-0.6
	HMDB0143268	2-(sulfooxy)pentanoic acid	C5H10O6S	M+NH4	216.0536	-0.6
	HMDB0143265	5-(sulfooxy)pentanoic acid	C5H10O6S	M+NH4	216.0536	-0.6
	HMDB0143262	4-(sulfooxy)pentanoic acid	C5H10O6S	M+NH4	216.0536	-0.6
	HMDB0130850	2-methyl-4-(sulfooxy)butanoic acid	C5H10O6S	M+NH4	216.0536	-0.6
	HMDB0130847	2-[(sulfooxy)methyl]butanoic acid	C5H10O6S	M+NH4	216.0536	-0.6
	HMDB0130842	2-methyl-3-(sulfooxy)butanoic acid	C5H10O6S	M+NH4	216.0536	-0.6
	HMDB0130807	3-methyl-2-(sulfooxy)butanoic acid	C5H10O6S	M+NH4	216.0536	-0.6
	HMDB0130804	3-methyl-4-(sulfooxy)butanoic acid	C5H10O6S	M+NH4	216.0536	-0.6
	HMDB0162020	7-hydroxy-7-methyl-5H,6H,7H-cyclopenta[c]pyridine-4-carboxylic acid	C10H11NO3	M+Na	216.0631	-1.9
	HMDB0162022	5-hydroxy-7-methyl-5H,6H,7H-cyclopenta[c]pyridine-4-carboxylic acid	C10H11NO3	M+Na	216.0631	-1.9
	HMDB0162023	7-(hydroxymethyl)-5H,6H,7H-cyclopenta[c]pyridine-4-carboxylic acid	C10H11NO3	M+Na	216.0631	-1.9
	HMDB0240317	N-formyl-L-phenylalanine	C10H11NO3	M+Na	216.0631	-1.9
	HMDB0000821	Phenylacetyl glycine	C10H11NO3	M+Na	216.0631	-1.9
	HMDB0000859	Methyl hippurate	C10H11NO3	M+Na	216.0631	-1.9
	HMDB0011723	2-Methylhippuric acid	C10H11NO3	M+Na	216.0631	-1.9

216.0627	HMDB0060366	3-Carbamoyl-2-phenylpropionaldehyde	C10H11NO3	M+Na	216.0631	-1.9
	HMDB0060389	4-Hydroxy-5-phenyltetrahydro-1,3-oxazin-2-one	C10H11NO3	M+Na	216.0631	-1.9
	HMDB0034250	Betamipron	C10H11NO3	M+Na	216.0631	-1.9
	HMDB0032388	Methyl n-acetylanthranilate	C10H11NO3	M+Na	216.0631	-1.9
	HMDB0013245	m-Methylhippuric acid	C10H11NO3	M+Na	216.0631	-1.9
	HMDB0013292	p-Methylhippuric acid	C10H11NO3	M+Na	216.0631	-1.9
	HMDB0060758	4-Anilino-4-oxobutanoic acid	C10H11NO3	M+Na	216.0631	-1.9
	HMDB0000114	Glycerylphosphorylethanolamine	C5H14NO6P	M+H	216.0632	-2.1
	HMDB0059660	sn-glycero-3-Phosphoethanolamine	C5H14NO6P	M+H	216.0632	-2.1
216.1226	HMDB0135755	4-ethyl-2,6-dimethoxybenzene-1,3-diol	C10H14O4	M+NH4	216.1230	-2.0
	HMDB0131265	2,3,5-trimethoxy-6-methylphenol	C10H14O4	M+NH4	216.1230	-2.0
	HMDB0059779	2,3-Methylene suberic acid	C10H14O4	M+NH4	216.1230	-2.0
	HMDB0059768	3,4-Methylene suberic acid	C10H14O4	M+NH4	216.1230	-2.0
	HMDB0030991	5-(3E-Pentenyl)tetrahydro-2-oxo-3-furancarboxylic acid	C10H14O4	M+NH4	216.1230	-2.0
	HMDB0033093	3-(4-Hydroxy-3-methoxyphenyl)-1,2-propanediol	C10H14O4	M+NH4	216.1230	-2.0
	HMDB0034099	(2E,4E)-2,7-Dimethyl-2,4-octadienedioic acid	C10H14O4	M+NH4	216.1230	-2.0
	HMDB0004998	Guaifenesin	C10H14O4	M+NH4	216.1230	-2.0
	HMDB0177594	1-(3,4-dimethoxyphenyl)ethane-1,2-diol	C10H14O4	M+NH4	216.1230	-2.0
	HMDB0094771	2-[(1,6-dihydroxyoct-6-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094767	2-[(1,6-dihydroxyoct-2-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094765	5-hydroxyoct-7-enoylglycine	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094766	2-[(6-hydroxy-1-oxooct-1-en-2-yl)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094763	2-[(1,5-dihydroxyoct-5-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094764	2-[(1,5-dihydroxyoct-6-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094761	2-[(1,5-dihydroxyoct-3-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094762	2-[(1,5-dihydroxyoct-4-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094760	2-[(1,5-dihydroxyoct-2-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094768	2-[(1,6-dihydroxyoct-3-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094770	2-[(1,6-dihydroxyoct-5-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094769	2-[(1,6-dihydroxyoct-4-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0013124	Propenoylcarnitine	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094776	2-[(1,7-dihydroxyoct-4-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094778	2-[(1,7-dihydroxyoct-6-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094777	2-[(1,7-dihydroxyoct-5-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094779	7-hydroxyoct-7-enoylglycine	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094774	2-[(1,7-dihydroxyoct-2-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094775	2-[(1,7-dihydroxyoct-3-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094773	2-[(7-hydroxy-1-oxooct-1-en-2-yl)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094772	6-hydroxyoct-7-enoylglycine	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094757	2-[(1,4-dihydroxyoct-6-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094759	2-[(5-hydroxy-1-oxooct-1-en-2-yl)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094758	4-hydroxyoct-7-enoylglycine	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094741	2-[(1,2-dihydroxyoct-4-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094739	2-[(1,2-dihydroxyoct-2-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094740	2-[(1,2-dihydroxyoct-3-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094738	2-[(2-hydroxy-1-oxooct-1-en-3-yl)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094737	1-hydroxyoct-7-enoylglycine	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094735	2-[(carboxymethyl)amino]oct-5-enoic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094733	2-[(carboxymethyl)amino]oct-3-enoic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094734	2-[(carboxymethyl)amino]oct-4-enoic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094736	2-[(carboxymethyl)amino]oct-6-enoic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094732	2-[(carboxymethyl)amino]oct-2-enoic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094742	2-[(1,2-dihydroxyoct-5-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094744	2-hydroxyoct-7-enoylglycine	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094743	2-[(1,2-dihydroxyoct-6-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094755	2-[(1,4-dihydroxyoct-4-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094753	2-[(1,4-dihydroxyoct-2-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094754	2-[(1,4-dihydroxyoct-3-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094756	2-[(1,4-dihydroxyoct-5-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094750	2-[(1,3-dihydroxyoct-6-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094749	2-[(1,3-dihydroxyoct-5-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094752	2-[(4-hydroxy-1-oxooct-1-en-2-yl)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0

	HMDB0094751	3-hydroxyoct-7-enoylglycine	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094748	2-[(1,3-dihydroxyoct-4-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094747	2-[(1,3-dihydroxyoct-3-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094745	2-[(3-hydroxy-1-oxooct-1-en-2-yl)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
	HMDB0094746	2-[(1,3-dihydroxyoct-2-en-1-ylidene)amino]acetic acid	C10H17NO4	M+H	216.1230	-2.0
216.1589	HMDB0179399	methyl (2E,4Z)--hydroxydeca-2,4-dienoate	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0163238	(2E,5Z)--hydroxyundeca-2,5-dienoic acid	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0163242	3-[(2Z)-oct-2-en-1-yl]oxirane-2-carboxylic acid	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0163241	(2E,5Z)-7-hydroxyundeca-2,5-dienoic acid	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0163239	(2E,5Z)-11-hydroxyundeca-2,5-dienoic acid	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0163243	(2E)-4-(3-pentylloxiran-2-yl)but-2-enoic acid	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0178762	methyl (4Z,8Z)-7-hydroxydeca-4,8-dienoate	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0178765	methyl (4Z,8Z)-6-hydroxydeca-4,8-dienoate	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0178764	methyl (4Z,8Z)-3-hydroxydeca-4,8-dienoate	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0178763	methyl (4Z,8Z)--hydroxydeca-4,8-dienoate	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0178766	methyl (4Z)-7-(3-methylloxiran-2-yl)hept-4-enoate	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0178767	methyl 3-{3-[(3Z)-pent-3-en-1-yl]oxiran-2-yl}propanoate	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0178768	methyl (4Z,8Z)-2-hydroxydeca-4,8-dienoate	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0179396	methyl (2E,4Z)-9-hydroxydeca-2,4-dienoate	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0179395	methyl (4Z)-6-hydroxydeca-2,4-dienoate	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0179397	methyl 3-[(1Z)-hept-1-en-1-yl]oxirane-2-carboxylate	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0179398	methyl (2E)-3-(3-pentylloxiran-2-yl)prop-2-enoate	C11H18O3	M+NH4	216.1594	-2.4
	HMDB0013279	N-Nonanoylglycine	C11H21NO3	M+H	216.1594	-2.4
216.1953	HMDB0000529	5Z-Dodecenoic acid	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0038081	2-Octenyl butyrate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0029763	Allyl nonanoate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0040158	Hexyl 2-methyl-3-pentenoate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0033378	cis-3-Hexenyl hexanoate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0037498	1-Ethenylhexyl butanoate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0039220	Ethyl 4-decenoate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0029585	Methyl -undecenoate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0037186	Rhodinyl acetate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0040361	1,1-Dimethoxy-3,7-dimethyl-2,6-octadiene	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0036182	5,5-Dibutyl-4,5-dihydro-2(3H)furanone	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0038895	7-Hexyl-2-oxepanone	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0010729	trans-Dodec-2-enoic acid	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0037742	xi-5-Dodecanolide	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0031683	xi-Dihydro-5-octyl-2(3H)-furanone	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0037305	Methyl 9-undecenoate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0041264	Menthyl acetate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0037813	3-Heptyldihydro-5-methyl-2(3H)-furanone	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0038269	Hexyl 2E-hexenoate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0034844	Citronellyl acetate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0037329	Ethyl 2-decenoate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0041449	[(3,7-Dimethyl-6-octenyl)oxy]acetaldehyde	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0040163	Hexyl 2-methyl-4-pentenoate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0038924	2-Hexenyl hexanoate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0034160	Citronellyl acetate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0032214	cis-4-Decenyl acetate	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0032248	11-Dodecenoic acid	C12H22O2	M+NH4	216.1958	-2.3
	HMDB0032235	2,6-Dimethyl-5-heptenal propyleneglycol acetal	C12H22O2	M+NH4	216.1958	-2.3
216.2318	HMDB0062117	6,-Dimethylundecan-2-one	C13H26O	M+NH4	216.2322	-1.8
	HMDB0030928	Tridecanal	C13H26O	M+NH4	216.2322	-1.8
	HMDB0034148	2-Tridecanone	C13H26O	M+NH4	216.2322	-1.8
217.0293	HMDB0041503	Bis(2-furanylmethyl) sulfide	C10H10O2S	M+Na	217.0294	-0.3
	HMDB0166956	(5E)-5-[(5-methylthiophen-2-yl)methylidene]oxolan-2-one	C10H10O2S	M+Na	217.0294	-0.3
	HMDB0179764	3-[5-(prop-1-yn-1-yl)thiophen-2-yl]propanoic acid	C10H10O2S	M+Na	217.0294	-0.3
	HMDB0142175	2-benzylpropanedioic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0146403	SCHEMBL2535852	C10H10O4	M+Na	217.0471	-2.4
	HMDB0146628	ZINC2222827	C10H10O4	M+Na	217.0471	-2.4
	HMDB0146630	3-(2-methoxyphenyl)oxirane-2-carboxylic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0146629	CTK4057	C10H10O4	M+Na	217.0471	-2.4
	HMDB0154365	3-(3-hydroxy-2-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na	217.0471	-2.4

217.0466	HMDB0166608	3-(6-hydroxy-2H-1,3-benzodioxol-5-yl)propanal	C10H10O4	M+Na	217.0471	-2.4
	HMDB0166607	3-(2H-1,3-benzodioxol-5-yl)-3-hydroxypropanal	C10H10O4	M+Na	217.0471	-2.4
	HMDB0166611	3-(2H-1,3-benzodioxol-5-yl)-2-hydroxypropanal	C10H10O4	M+Na	217.0471	-2.4
	HMDB0166609	2815-95-4	C10H10O4	M+Na	217.0471	-2.4
	HMDB0166613	6-[(1Z)-3-hydroxyprop-1-en-1-yl]-2H-1,3-benzodioxol-5-ol	C10H10O4	M+Na	217.0471	-2.4
	HMDB0166614	[3-(2H-1,3-benzodioxol-5-yl)oxiran-2-yl]methanol	C10H10O4	M+Na	217.0471	-2.4
	HMDB0178262	(2Z)-3-(3-hydroxy-5-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0141263	(2Z)-2-hydroxy-3-(3-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0140957	(2E)-3-(3-hydroxy-2-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0125096	3-(4-hydroxy-3-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0125524	(2E)-3-(3-hydroxy-5-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0125588	3-(3-hydroxy-5-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0127500	3-(4-methoxyphenyl)-2-oxopropanoic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0131137	3-(3-hydroxy-4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0131173	3-(4-methoxyphenyl)oxirane-2-carboxylic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0131172	(2E)-3-(2-hydroxy-4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0131171	(2Z)-2-hydroxy-3-(4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0137510	3-(4-hydroxy-2-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0135741	3-(2-hydroxy-4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0061686	2,5-Dihydroxycinnamic acid methyl ester	C10H10O4	M+Na	217.0471	-2.4
	HMDB0059721	mono-Benzyl malonate	C10H10O4	M+Na	217.0471	-2.4
	HMDB0141265	3-(3-methoxyphenyl)-2-oxopropanoic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0000954	Ferulic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0000955	Isoferulic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0002120	Monoethyl phthalate	C10H10O4	M+Na	217.0471	-2.4
	HMDB0030765	(-)-trans-3,4-Dihydro-4,8-dihydroxy-3-methyl-1H-2-benzopyran-1-one	C10H10O4	M+Na	217.0471	-2.4
	HMDB0039606	Repandiol	C10H10O4	M+Na	217.0471	-2.4
	HMDB0032652	Meconine	C10H10O4	M+Na	217.0471	-2.4
	HMDB0037644	3-(2-Hydroxy-3-methoxyphenyl)-2-propenoic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0029663	Vanillin acetate	C10H10O4	M+Na	217.0471	-2.4
	HMDB0032614	Piperonyl acetate	C10H10O4	M+Na	217.0471	-2.4
	HMDB0165533	Ferulic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0240705	Ferulic acid	C10H10O4	M+Na	217.0471	-2.4
	HMDB0134088	3-(2-hydroxy-3-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na	217.0471	-2.4
217.0627	HMDB0059798	2-Hydroxyphenanthrene	C14H10O	M+Na	217.0624	1.5
	HMDB0059797	1-Hydroxyphenanthrene	C14H10O	M+Na	217.0624	1.5
	HMDB0059800	4-Hydroxyphenanthrene	C14H10O	M+Na	217.0624	1.5
	HMDB0059799	3-Hydroxyphenanthrene	C14H10O	M+Na	217.0624	1.5
	HMDB0059801	9-Hydroxyphenanthrene	C14H10O	M+Na	217.0624	1.5
217.1066	HMDB0182566	2-(1-carboxyethyl)-1-hydroxy-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0170513	3-[3-(2-carboxy-2-methylethyl)oxiran-2-yl]-2-methylpropanoic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0170511	(4E)-2-hydroxy-2,7-dimethyloct-4-enedioic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0170512	(4E)-3-hydroxy-2,7-dimethyloct-4-enedioic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0160551	(4Z)-2-hydroxydec-4-enedioic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0160550	5-[3-(2-carboxyethyl)oxiran-2-yl]pentanoic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0160548	(4Z)-6-hydroxydec-4-enedioic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0160549	(4Z)-3-hydroxydec-4-enedioic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0160547	(4Z)-8-hydroxydec-4-enedioic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0160546	(4Z)-7-hydroxydec-4-enedioic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0170514	(4E)-2-(hydroxymethyl)-7-methyloct-4-enedioic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0175347	4-hydroxy-1,2,2-trimethylcyclopentane-1,3-dicarboxylic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0182565	2-(1-carboxy-2-hydroxyethyl)-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0182564	2-(1-carboxyethyl)-3-hydroxy-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0182562	2-(1-carboxy-1-hydroxyethyl)-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0182561	5-(1-carboxyethyl)-2-hydroxy-2-methylcyclopentane-1-carboxylic acid	C10H16O5	M+H	217.1071	-2.1

	HMDB0182560	2-(1-carboxyethyl)-5-(hydroxymethyl)cyclopentane-1-carboxylic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0182563	5-(1-carboxyethyl)-3-hydroxy-2-methylcyclopentane-1-carboxylic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0175348	SCHEMBL1335666	C10H16O5	M+H	217.1071	-2.1
	HMDB0175345	2-(hydroxymethyl)-1,2-dimethylcyclopentane-1,3-dicarboxylic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0175346	5-hydroxy-1,2,2-trimethylcyclopentane-1,3-dicarboxylic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0175344	1-Hydroxymethyl-2,2-dimethyl-cyclopentane-1,3-dicarboxylic acid	C10H16O5	M+H	217.1071	-2.1
	HMDB0160552	(4Z)-9-hydroxydec-4-enedioic acid	C10H16O5	M+H	217.1071	-2.1
217.1205	HMDB0132986	1-(4-methoxyphenyl)pentan-3-ol	C12H18O2	M+Na	217.1199	2.8
	HMDB0041610	(2,2-Diethoxyethyl)benzene	C12H18O2	M+Na	217.1199	2.8
	HMDB0032567	Hexylresorcinol	C12H18O2	M+Na	217.1199	2.8
	HMDB0034450	Neocnidilide	C12H18O2	M+Na	217.1199	2.8
	HMDB0035126	Myrtenyl acetate	C12H18O2	M+Na	217.1199	2.8
	HMDB0037231	Perillyl acetate	C12H18O2	M+Na	217.1199	2.8
	HMDB0037018	(S)-p-Mentha-1,8-dien--yl acetate	C12H18O2	M+Na	217.1199	2.8
	HMDB0038046	Carvyl acetate	C12H18O2	M+Na	217.1199	2.8
	HMDB0040439	1-(2-Furanyl)-1-octanone	C12H18O2	M+Na	217.1199	2.8
	HMDB0038292	Menthadienyl acetate	C12H18O2	M+Na	217.1199	2.8
	HMDB0037389	(R)-2-Acetoxy-p-mentha-1,8-diene	C12H18O2	M+Na	217.1199	2.8
	HMDB0039685	8-Ocimenyl acetate	C12H18O2	M+Na	217.1199	2.8
	HMDB0041497	(S)-Neolylratyl acetate	C12H18O2	M+Na	217.1199	2.8
	HMDB0031840	(S,Z)-Lyratol acetate	C12H18O2	M+Na	217.1199	2.8
	HMDB0035376	Ethyl (2E,4Z,7Z)-Decatrienoate	C12H18O2	M+Na	217.1199	2.8
	HMDB0035375	Ethyl (2E,4E,7Z)-Decatrienoate	C12H18O2	M+Na	217.1199	2.8
	HMDB0014018	4-Hydroxypropofol	C12H18O2	M+Na	217.1199	2.8
	HMDB0035801	(2S,4R)-p-Mentha-1(7),5-dien-2-ol acetate	C12H18O2	M+Na	217.1199	2.8
217.1450	HMDB0033135	Pyrimethanil	C12H13N3	M+NH4	217.1448	1.1
217.1587	HMDB0036589	1,2-Dehydro-alpha-cyperone	C15H20O	M+H	217.1587	0.0
	HMDB0059863	(S)-3-Ethyl-4-methylpentanol	C15H20O	M+H	217.1587	0.0
	HMDB0035965	5beta-1,3,7(11)-Eudesmatrien-8-one	C15H20O	M+H	217.1587	0.0
	HMDB0038147	Isogermafurene	C15H20O	M+H	217.1587	0.0
	HMDB0031736	2-Hexyl-3-phenyl-2-propenal	C15H20O	M+H	217.1587	0.0
	HMDB0036769	Furanodiene	C15H20O	M+H	217.1587	0.0
	HMDB0035612	(R)-ar-Turmerone	C15H20O	M+H	217.1587	0.0
	HMDB0036108	1,3,5,11-Bisabolatetraen--one	C15H20O	M+H	217.1587	0.0
217.1793	HMDB0002059	12-Hydroxydodecanoic acid	C12H24O3	M+H	217.1798	-2.4
	HMDB0000387	(S)-3-hydroxylauric acid	C12H24O3	M+H	217.1798	-2.4
	HMDB0010728	(R)-3-Hydroxydodecanoic acid	C12H24O3	M+H	217.1798	-2.4
	HMDB0040169	xi-5-Hydroxydodecanoic acid	C12H24O3	M+H	217.1798	-2.4
	HMDB0062032	3-hydroxy-2,4,4-trimethylpentyl 2-methylpropanoate	C12H24O3	M+H	217.1798	-2.4
218.1381	HMDB0170504	SCHEMBL4585236	C10H16O4	M+NH4	218.1387	-2.7
	HMDB0061295	526-51-6	C10H16O4	M+NH4	218.1387	-2.7
	HMDB0013227	cis-5-Decenedioic acid	C10H16O4	M+NH4	218.1387	-2.7
	HMDB0034491	Camphoric acid	C10H16O4	M+NH4	218.1387	-2.7
	HMDB0034971	(1R,2R,3S,1'R)-Nepetalinic acid	C10H16O4	M+NH4	218.1387	-2.7
	HMDB0036715	Matsutakic acid A	C10H16O4	M+NH4	218.1387	-2.7
	HMDB0030990	alpha-Carboxy-delta-nonalactone	C10H16O4	M+NH4	218.1387	-2.7
	HMDB0030989	5-Pentyltetrahydro-2-oxo-3-furancarboxylic acid	C10H16O4	M+NH4	218.1387	-2.7
	HMDB0000603	cis-4-Decenedioic acid	C10H16O4	M+NH4	218.1387	-2.7
	HMDB0062514	Propionylcarnitine	C10H19NO4	M+H	218.1387	-2.7
	HMDB0000824	Levocarnitine propionate hydrochloride	C10H20NO4	M+H	218.1387	-2.7
218.1746	HMDB0037179	3-Nonanon-1-yl acetate	C11H20O3	M+NH4	218.1751	-2.1
	HMDB0165684	8-hydroxyundec--enoic acid	C11H20O3	M+NH4	218.1751	-2.1
	HMDB0165686	6-hydroxyundec--enoic acid	C11H20O3	M+NH4	218.1751	-2.1
	HMDB0165685	7-hydroxyundec--enoic acid	C11H20O3	M+NH4	218.1751	-2.1
	HMDB0165689	3-hydroxy--undecenoic acid	C11H20O3	M+NH4	218.1751	-2.1
	HMDB0165687	5-hydroxyundec--enoic acid	C11H20O3	M+NH4	218.1751	-2.1
	HMDB0165688	4-hydroxyundec--enoic acid	C11H20O3	M+NH4	218.1751	-2.1
	HMDB0165690	9-(oxiran-2-yl)nonanoic Acid	C11H20O3	M+NH4	218.1751	-2.1
	HMDB0032662	(S)-9-Hydroxy--undecenoic acid	C11H20O3	M+NH4	218.1751	-2.1
	HMDB0036029	Clarycet	C11H20O3	M+NH4	218.1751	-2.1

	HMDB0165691	2-hydroxy--undecenoic acid	C11H20O3	M+NH4	218.1751	-2.1
218.2109	HMDB0168119	11-hydroxydodecanal	C12H24O2	M+NH4	218.2115	-2.5
	HMDB0168120	12-hydroxydodecanal	C12H24O2	M+NH4	218.2115	-2.5
	HMDB0168121	2-hydroxydodecanal	C12H24O2	M+NH4	218.2115	-2.5
	HMDB0034128	Isopropyl nonanoate	C12H24O2	M+NH4	218.2115	-2.5
	HMDB0034136	Octyl butanoate	C12H24O2	M+NH4	218.2115	-2.5
	HMDB0036225	Pentyl heptanoate	C12H24O2	M+NH4	218.2115	-2.5
	HMDB0034137	Octyl 2-methylpropanoate	C12H24O2	M+NH4	218.2115	-2.5
	HMDB0030998	Ethyl decanoate	C12H24O2	M+NH4	218.2115	-2.5
	HMDB0040166	Decyl acetate	C12H24O2	M+NH4	218.2115	-2.5
	HMDB0033619	Hexyl hexanoate	C12H24O2	M+NH4	218.2115	-2.5
	HMDB0035410	(R)-Dihydrocitronellol acetate	C12H24O2	M+NH4	218.2115	-2.5
	HMDB0032310	2-Heptyl butyrate	C12H24O2	M+NH4	218.2115	-2.5
	HMDB0032440	Nonanal propyleneglycol acetal	C12H24O2	M+NH4	218.2115	-2.5
	HMDB0061988	2-ethylhexyl butanoate	C12H24O2	M+NH4	218.2115	-2.5
	HMDB0059868	Isobutyl octanoate	C12H24O2	M+NH4	218.2115	-2.5
	HMDB0000638	Dodecanoic acid	C12H24O2	M+NH4	218.2115	-2.5
219.0260	HMDB0126031	(2E)-3-(2,3,4-trihydroxyphenyl)prop-2-enoic acid	C9H8O5	M+Na	219.0264	-1.8
	HMDB0125584	3-(3,4,5-trihydroxyphenyl)prop-2-enoic acid	C9H8O5	M+Na	219.0264	-1.8
	HMDB0125523	1-Sinapoylglucose	C9H8O5	M+Na	219.0264	-1.8
	HMDB0125373	3-(3,4-dihydroxyphenyl)-2-oxopropanoic acid	C9H8O5	M+Na	219.0264	-1.8
	HMDB0126041	(2E)-3-(2,4,5-trihydroxyphenyl)prop-2-enoic acid	C9H8O5	M+Na	219.0264	-1.8
	HMDB0131758	3-(2,4-dihydroxyphenyl)-2-oxopropanoic acid	C9H8O5	M+Na	219.0264	-1.8
	HMDB0132449	3-(3,5-dihydroxyphenyl)-2-oxopropanoic acid	C9H8O5	M+Na	219.0264	-1.8
	HMDB0137120	2-(2-hydroxy-4-methoxyphenyl)-2-oxoacetic acid	C9H8O5	M+Na	219.0264	-1.8
	HMDB0137166	3-(2,3,4-trihydroxyphenyl)prop-2-enoic acid	C9H8O5	M+Na	219.0264	-1.8
	HMDB0146801	hydroxycaffeic acid	C9H8O5	M+Na	219.0264	-1.8
	HMDB0030800	3-Methoxy-4,5-methylenedioxybenzoic acid	C9H8O5	M+Na	219.0264	-1.8
	HMDB0059809	4-Hydroxy-benzenepropanedioate	C9H8O5	M+Na	219.0264	-1.8
	HMDB0132521	3-(2,4,5-trihydroxyphenyl)prop-2-enoic acid	C9H8O5	M+Na	219.0264	-1.8
	HMDB0178261	CHEMBL1765653	C9H8O5	M+Na	219.0264	-1.8
219.1410	HMDB0038945	(S)-3-Mercaptohexyl pentanoate	C11H22O2S	M+H	219.1413	-1.5
	HMDB0038946	(S)-3-Methylthiohexyl butyrate	C11H22O2S	M+H	219.1413	-1.5
219.1738	HMDB0134122	(2Z)-2-(phenylmethylidene)octan-1-ol	C15H22O	M+H	219.1743	-2.5
	HMDB0134121	2-benzylactanal	C15H22O	M+H	219.1743	-2.5
	HMDB0094674	1-Phenylnonan-1-one	C15H22O	M+H	219.1743	-2.5
	HMDB0035643	beta-Sinensal	C15H22O	M+H	219.1743	-2.5
	HMDB0038215	alpha-Sinensal	C15H22O	M+H	219.1743	-2.5
	HMDB0036201	(E)-,11-Dihydro-alpha-atlantone	C15H22O	M+H	219.1743	-2.5
	HMDB0038187	beta-Atlantone	C15H22O	M+H	219.1743	-2.5
	HMDB0036797	Mustakone	C15H22O	M+H	219.1743	-2.5
	HMDB0036733	Vulgarone A	C15H22O	M+H	219.1743	-2.5
	HMDB0036667	Zerumbone	C15H22O	M+H	219.1743	-2.5
	HMDB0036813	alpha-Santalal	C15H22O	M+H	219.1743	-2.5
	HMDB0035081	(5alpha,11)-Eudesmadien-2-one	C15H22O	M+H	219.1743	-2.5
	HMDB0036718	beta-Santalal	C15H22O	M+H	219.1743	-2.5
	HMDB0036109	1,3,5-Bisabolatrien--one	C15H22O	M+H	219.1743	-2.5
	HMDB0035747	Patchoulone	C15H22O	M+H	219.1743	-2.5
	HMDB0040686	Isohumbertiol	C15H22O	M+H	219.1743	-2.5
	HMDB0038164	Vulgarone B	C15H22O	M+H	219.1743	-2.5
	HMDB0037000	alpha-Turmerone	C15H22O	M+H	219.1743	-2.5
	HMDB0038195	Xanthorrhizol	C15H22O	M+H	219.1743	-2.5
	HMDB0038200	Calamusenone	C15H22O	M+H	219.1743	-2.5
	HMDB0038511	Bisacumol	C15H22O	M+H	219.1743	-2.5
	HMDB0013687	Nookatone	C15H22O	M+H	219.1743	-2.5
	HMDB0035657	Solavetivone	C15H22O	M+H	219.1743	-2.5
	HMDB0035786	Valerenal	C15H22O	M+H	219.1743	-2.5
	HMDB0037061	(+)-4,11-Eudesmadien-3-one	C15H22O	M+H	219.1743	-2.5
	HMDB0035835	Furanoeremophilane	C15H22O	M+H	219.1743	-2.5
	HMDB0037068	Curlone	C15H22O	M+H	219.1743	-2.5
	HMDB0039637	beta-Elementone	C15H22O	M+H	219.1743	-2.5
	HMDB0036071	Dendrolasin	C15H22O	M+H	219.1743	-2.5
	HMDB0036443	Rotundone	C15H22O	M+H	219.1743	-2.5
	HMDB0038201	4,7(11)-Guaiadien-8-one	C15H22O	M+H	219.1743	-2.5
	HMDB0035082	(5beta,7beta,beta)-3,11-Eudesmadien-2-one	C15H22O	M+H	219.1743	-2.5

	HMDB0013693	AC1L1WLS	C15H22O	M+H	219.1743	-2.5
219.9913	HMDB0006492	4-Nitrophenyl sulfate	C6H5NO6S	M+H	219.9910	1.2
220.0365	HMDB0182899	5-Chloroorsellinic acid	C8H7ClO4	M+NH4	220.0371	-2.8
	HMDB0060440	Benzoyl phosphate	C7H7O5P	M+NH4	220.0369	-2.0
220.1175	HMDB0062766	4-ethylamino-6-isopropylamino-1,3,5-triazin-2-ol	C8H15N5O	M+Na	220.1169	2.8
	HMDB0033092	3-(1-Hydroxymethyl-1-propenyl)pentanedioic acid	C9H14O5	M+NH4	220.1179	-2.0
	HMDB0032306	Diethyl oxalpropionate	C9H14O5	M+NH4	220.1179	-2.0
	HMDB0000210	Pantothenic acid	C9H17NO5	M+H	220.1179	-2.0
	HMDB0062717	Pantothenic acid	C9H17NO5	M+H	220.1179	-2.0
220.1539	HMDB0062180	(2S,5S)-2-[(2R)-butan-2-yl]-5-hydroxy-4-oxohexanoic acid	C10H18O4	M+NH4	220.1543	-2.0
	HMDB0059719	Heptylmalonic acid	C10H18O4	M+NH4	220.1543	-2.0
	HMDB0059754	3-Methylazelaic acid	C10H18O4	M+NH4	220.1543	-2.0
	HMDB0040196	Oxalic acid dibutyl ester	C10H18O4	M+NH4	220.1543	-2.0
	HMDB0031510	R-2-Hydroxy-3-methylbutanoic acid 3-Methylbutanoyl	C10H18O4	M+NH4	220.1543	-2.0
	HMDB0000792	Sebacic acid	C10H18O4	M+NH4	220.1543	-2.0
	HMDB0059708	2-Ethylsuberic acid	C10H18O4	M+NH4	220.1543	-2.0
	HMDB0014563	Miglustat	C10H21NO4	M+H	220.1543	-2.0
220.1902	HMDB0032443	3-Hydroxynonyl acetate	C11H22O3	M+NH4	220.1907	-2.4
	HMDB0166976	Methyl 9-hydroxydecanoate	C11H22O3	M+NH4	220.1907	-2.4
	HMDB0166977	Methyl -hydroxydecanoate	C11H22O3	M+NH4	220.1907	-2.4
	HMDB0175162	SCHEMBL9794217	C11H22O3	M+NH4	220.1907	-2.4
	HMDB0175163	SCHEMBL8984439	C11H22O3	M+NH4	220.1907	-2.4
	HMDB0175164	2-hydroxy-9-methyldecanoic acid	C11H22O3	M+NH4	220.1907	-2.4
	HMDB0183924	4-hydroxy-4,8-dimethylnonanoic acid	C11H22O3	M+NH4	220.1907	-2.4
	HMDB0183927	9-hydroxy-4,8-dimethylnonanoic acid	C11H22O3	M+NH4	220.1907	-2.4
	HMDB0183926	4-(hydroxymethyl)-8-methylnonanoic acid	C11H22O3	M+NH4	220.1907	-2.4
	HMDB0183925	8-hydroxy-4,8-dimethylnonanoic acid	C11H22O3	M+NH4	220.1907	-2.4
	HMDB0061654	3-hydroxyundecanoic acid	C11H22O3	M+NH4	220.1907	-2.4
	HMDB0059736	2-Hydroxyundecanoate	C11H22O3	M+NH4	220.1907	-2.4
	HMDB0183928	2-hydroxy-4,8-dimethylnonanoic acid	C11H22O3	M+NH4	220.1907	-2.4
220.2273	HMDB0037310	1,1-Dimethoxydecane	C12H26O2	M+NH4	220.2271	0.9
	HMDB0032153	Acetaldehyde diisoamyl acetal	C12H26O2	M+NH4	220.2271	0.9
	HMDB0168123	1,12-Dodecanediol	C12H26O2	M+NH4	220.2271	0.9
	HMDB0168122	158-99-2	C12H26O2	M+NH4	220.2271	0.9
221.0418	HMDB0131426	2-(3,4-dihydroxy-5-methoxyphenyl)acetic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0130476	2-(2,5-dihydroxy-4-methoxyphenyl)acetic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0126489	3-(2,4,5-trihydroxyphenyl)propanoic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0126478	3-(2,4-dihydroxyphenyl)-3-hydroxypropanoic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0125529	3-(3,4,5-trihydroxyphenyl)propanoic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0125024	2-(2,4,5-trihydroxyphenyl)propanoic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0142084	2-hydroxy-3,4-dimethoxybenzoic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0137136	2-hydroxy-2-(2-hydroxy-4-methoxyphenyl)acetic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0137823	2-(2,3,4-trihydroxyphenyl)propanoic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0142087	4-hydroxy-2,3-dimethoxybenzoic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0180893	1-(2,3,4-trihydroxy-6-methoxyphenyl)ethan-1-one	C9H10O5	M+Na	221.0420	-1.1
	HMDB0180892	Ethanone, 1-(3,4,6-trihydroxy-2-methoxyphenyl)-	C9H10O5	M+Na	221.0420	-1.1
	HMDB0157241	ZINC34716	C9H10O5	M+Na	221.0420	-1.1
	HMDB0157242	3695-24-7	C9H10O5	M+Na	221.0420	-1.1
	HMDB0150485	4,6-dihydroxy-3-methoxy-2-methylbenzoic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0149149	2-HYDROXY-4,5-DIMETHOXYBENZOIC ACID	C9H10O5	M+Na	221.0420	-1.1
	HMDB0146916	SCHEMBL11141488	C9H10O5	M+Na	221.0420	-1.1
	HMDB0140947	3-hydroxy-2,4-dimethoxybenzoic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0029170	3-Hydroxy-4-methoxymandelate	C9H10O5	M+Na	221.0420	-1.1
	HMDB0133489	2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0041662	3,4-O-Dimethylgallic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0033836	Ethyl gallate	C9H10O5	M+Na	221.0420	-1.1
	HMDB0003503	3-(3,4-Dihydroxyphenyl)lactic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0002085	Syringic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0146890	AC1NT14U	C9H10O5	M+Na	221.0420	-1.1
	HMDB0000291	Vanillylmandelic acid	C9H10O5	M+Na	221.0420	-1.1
	HMDB0151802	(2Z)-2-[(2-hydroxyphenyl)methylidene]hexanoic acid	C13H16O3	M+H	221.1172	-2.8
	HMDB0151801	(2Z)-6-hydroxy-2-(phenylmethylidene)hexanoic acid	C13H16O3	M+H	221.1172	-2.8
	HMDB0151799	(2Z)-5-hydroxy-2-(phenylmethylidene)hexanoic acid	C13H16O3	M+H	221.1172	-2.8
	HMDB0151798	(2Z)-2-[(4-hydroxyphenyl)methylidene]hexanoic acid	C13H16O3	M+H	221.1172	-2.8

221.1166	HMDB0151800	2-butyl-3-phenyloxirane-2-carboxylic acid	C13H16O3	M+H	221.1172	-2.8
	HMDB0151797	(2Z)-2-[(3-hydroxyphenyl)methylidene]hexanoic acid	C13H16O3	M+H	221.1172	-2.8
	HMDB0151796	(2Z)-3-hydroxy-2-(phenylmethylidene)hexanoic acid	C13H16O3	M+H	221.1172	-2.8
	HMDB0132948	1-(4-methoxyphenyl)-4-methylpentane-2,3-dione	C13H16O3	M+H	221.1172	-2.8
	HMDB0132939	4-hydroxy-1-(4-methoxyphenyl)-4-methylpent-1-en-3-one	C13H16O3	M+H	221.1172	-2.8
	HMDB0132936	1-[3-(4-methoxyphenyl)oxiran-2-yl]-2-methylpropan-1-one	C13H16O3	M+H	221.1172	-2.8
	HMDB0132935	1-(2-hydroxy-4-methoxyphenyl)-4-methylpent-1-en-3-one	C13H16O3	M+H	221.1172	-2.8
	HMDB0132937	5-hydroxy-1-(4-methoxyphenyl)-4-methylpent-1-en-3-one	C13H16O3	M+H	221.1172	-2.8
	HMDB0132933	(1Z)-2-hydroxy-1-(4-methoxyphenyl)-4-methylpent-1-en-3-one	C13H16O3	M+H	221.1172	-2.8
	HMDB0061942	cis-3-Hexenyl salicylate	C13H16O3	M+H	221.1172	-2.8
	HMDB0061823	3-Hexenyl salicylic acid	C13H16O3	M+H	221.1172	-2.8
	HMDB0040424	Ethyl 2-benzylacetoacetate	C13H16O3	M+H	221.1172	-2.8
221.1514	HMDB0037492	Ethyl methyl-p-tolylglycidate	C13H16O3	M+H	221.1172	-2.8
	HMDB0032589	1-(5-Acetyl-2-hydroxyphenyl)-3-methyl-1-butanone	C13H16O3	M+H	221.1172	-2.8
	HMDB0240348	SCHEMBL934365	C10H13N5	M+NH4	221.1509	2.2
	HMDB0000529	5Z-Dodecenoic acid	C12H22O2	M+Na	221.1512	0.9
	HMDB0038081	2-Octenyl butyrate	C12H22O2	M+Na	221.1512	0.9
	HMDB0029763	Allyl nonanoate	C12H22O2	M+Na	221.1512	0.9
	HMDB0040158	Hexyl 2-methyl-3-pentenoate	C12H22O2	M+Na	221.1512	0.9
	HMDB0033378	cis-3-Hexenyl hexanoate	C12H22O2	M+Na	221.1512	0.9
	HMDB0037498	1-Ethenylhexyl butanoate	C12H22O2	M+Na	221.1512	0.9
	HMDB0039220	Ethyl 4-decenoate	C12H22O2	M+Na	221.1512	0.9
	HMDB0029585	Methyl -undecenoate	C12H22O2	M+Na	221.1512	0.9
	HMDB0037186	Rhodinyl acetate	C12H22O2	M+Na	221.1512	0.9
	HMDB0040361	1,1-Dimethoxy-3,7-dimethyl-2,6-octadiene	C12H22O2	M+Na	221.1512	0.9
	HMDB0036182	5,5-Dibutyl-4,5-dihydro-2(3H)furanone	C12H22O2	M+Na	221.1512	0.9
	HMDB0038895	7-Hexyl-2-oxepanone	C12H22O2	M+Na	221.1512	0.9
	HMDB0010729	trans-Dodec-2-enoic acid	C12H22O2	M+Na	221.1512	0.9
	HMDB0037742	xi-5-Dodecanolide	C12H22O2	M+Na	221.1512	0.9
	HMDB0031683	xi-Dihydro-5-octyl-2(3H)-furanone	C12H22O2	M+Na	221.1512	0.9
	HMDB0037305	Methyl 9-undecenoate	C12H22O2	M+Na	221.1512	0.9
	HMDB0041264	Menthyl acetate	C12H22O2	M+Na	221.1512	0.9
	HMDB0037813	3-Heptyldihydro-5-methyl-2(3H)-furanone	C12H22O2	M+Na	221.1512	0.9
	HMDB0038269	Hexyl 2E-hexenoate	C12H22O2	M+Na	221.1512	0.9
	HMDB0034844	Citronellyl acetate	C12H22O2	M+Na	221.1512	0.9
	HMDB0037329	Ethyl 2-decenoate	C12H22O2	M+Na	221.1512	0.9
	HMDB0041449	[(3,7-Dimethyl-6-octenyl)oxy]acetaldehyde	C12H22O2	M+Na	221.1512	0.9
	HMDB0032235	2,6-Dimethyl-5-heptenal propyleneglycol acetal	C12H22O2	M+Na	221.1512	0.9
	HMDB0032248	11-Dodecenoic acid	C12H22O2	M+Na	221.1512	0.9
	HMDB0032214	cis-4-Decenyl acetate	C12H22O2	M+Na	221.1512	0.9
	HMDB0034160	Citronellyl acetate	C12H22O2	M+Na	221.1512	0.9
	HMDB0040163	Hexyl 2-methyl-4-pentenoate	C12H22O2	M+Na	221.1512	0.9
	HMDB0038924	2-Hexenyl hexanoate	C12H22O2	M+Na	221.1512	0.9
	HMDB0182057	5-{2,3-dimethyltricyclo[2.2.1,]heptan-3-yl}-2-methylpent-2-en-1-ol	C15H24O	M+H	221.1900	-2.7
	HMDB0134152	2-benzyl octan-1-ol	C15H24O	M+H	221.1900	-2.7
	HMDB0182055	[2-methyl-3-(4-methylpent-3-en-1-yl)tricyclo[2.2.1,heptan-3-yl]methanol	C15H24O	M+H	221.1900	-2.7
	HMDB0182054	[7-methyl-7-(4-methylpent-3-en-1-yl)tricyclo[2.2.1,heptan-1-yl]methanol	C15H24O	M+H	221.1900	-2.7
	HMDB0182874	4a-methyl-8-methylidene-2-(prop-1-en-2-yl)-decahydronaphthalen-2-ol	C15H24O	M+H	221.1900	-2.7
	HMDB0182875	2-(4a-methyl-8-methylidene-decahydronaphthalen-2-yl)-2-methyloxirane	C15H24O	M+H	221.1900	-2.7
	HMDB0036420	spathulenol	C15H24O	M+H	221.1900	-2.7
	HMDB0182154	1-(6-methylhept-5-en-2-yl)-4-methylidenebicyclo[3.1]hexan-6-ol	C15H24O	M+H	221.1900	-2.7
	HMDB0182153	5-(6-methylhept-5-en-2-yl)-2-methylidenebicyclo[3.1]hexan-1-ol	C15H24O	M+H	221.1900	-2.7

HMDB0182155	6-methyl-2-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-5-en-1-ol	C15H24O	M+H	221.1900	-2.7
HMDB0182060	1,7-dimethyl-7-(4-methylpent-3-en-1-yl)tricyclo[2.2.1,heptan-3-ol	C15H24O	M+H	221.1900	-2.7
HMDB0182059	1-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-4-methylpent-3-en-2-ol	C15H24O	M+H	221.1900	-2.7
HMDB0182058	.alpha.-Santalol	C15H24O	M+H	221.1900	-2.7
HMDB0182056	1-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-4-methylpent-3-en-1-ol	C15H24O	M+H	221.1900	-2.7
HMDB0182062	santal--en-2-ol	C15H24O	M+H	221.1900	-2.7
HMDB0182147	6-methyl-2-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-5-en-2-ol	C15H24O	M+H	221.1900	-2.7
HMDB0182150	2-methyl-6-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-2-en-4-ol	C15H24O	M+H	221.1900	-2.7
HMDB0182148	1-(6-methylhept-5-en-2-yl)-4-methylidenebicyclo[3.1]hexan-3-ol	C15H24O	M+H	221.1900	-2.7
HMDB0182151	1-(6-methylhept-5-en-2-yl)-4-methylidenebicyclo[3.1]hexan-2-ol	C15H24O	M+H	221.1900	-2.7
HMDB0182149	2-methyl-6-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-2-en-1-ol	C15H24O	M+H	221.1900	-2.7
HMDB0182152	2,2-dimethyl-3-(3-{4-methylidenebicyclo[3.1]hexan-1-yl}butyl)oxirane	C15H24O	M+H	221.1900	-2.7
HMDB0060295	3,7,7,-tetramethyl-2-oxatetracyclo[7.3,?蜜dodecane	C15H24O	M+H	221.1900	-2.7
HMDB0035645	Epoxyguaiene	C15H24O	M+H	221.1900	-2.7
HMDB0040763	Neoaclarimarine E	C15H24O	M+H	221.1900	-2.7
HMDB0033826	2,6-Di-tert-butyl-4-methylphenol	C15H24O	M+H	221.1900	-2.7
HMDB0038123	1,5-Epoxy-4(14)-salvialene	C15H24O	M+H	221.1900	-2.7
HMDB0038134	Bisabolene oxide	C15H24O	M+H	221.1900	-2.7
HMDB0039532	(6Z,9Z,12Z)-6,9,12-Pentadecatrien-2-one	C15H24O	M+H	221.1900	-2.7
HMDB0035718	Isocyperol	C15H24O	M+H	221.1900	-2.7
HMDB0038193	Isoshyobunone	C15H24O	M+H	221.1900	-2.7
HMDB0036717	trans-beta-Santalol	C15H24O	M+H	221.1900	-2.7
HMDB0038208	Humuladienone	C15H24O	M+H	221.1900	-2.7
HMDB0036788	beta-Betulenol	C15H24O	M+H	221.1900	-2.7
HMDB0035020	Acolamone	C15H24O	M+H	221.1900	-2.7
HMDB0037395	11-Copaen-4-ol	C15H24O	M+H	221.1900	-2.7
HMDB0035720	Isoacolamone	C15H24O	M+H	221.1900	-2.7
HMDB0039711	Aromadendrene epoxide	C15H24O	M+H	221.1900	-2.7
HMDB0036118	(3S,6E)-6-Caryophyllen-15-al	C15H24O	M+H	221.1900	-2.7
HMDB0035306	Epishyobunone	C15H24O	M+H	221.1900	-2.7
HMDB0034940	Mammea E/BB	C15H24O	M+H	221.1900	-2.7
HMDB0030232	(2R,6S,7S,Z)-beta-Santala-3(15),-dien-12-ol	C15H24O	M+H	221.1900	-2.7
HMDB0036793	3,15-Epoxy-6-caryophyllene	C15H24O	M+H	221.1900	-2.7
HMDB0035097	beta-Costol	C15H24O	M+H	221.1900	-2.7
HMDB0036789	Caryophyllene alpha-oxide	C15H24O	M+H	221.1900	-2.7
HMDB0038160	7(14)-Isodaucen--one	C15H24O	M+H	221.1900	-2.7
HMDB0035704	Acorenone	C15H24O	M+H	221.1900	-2.7
HMDB0037069	Acoragermacrone	C15H24O	M+H	221.1900	-2.7
HMDB0034661	alpha-Valerenol	C15H24O	M+H	221.1900	-2.7
HMDB0038211	Humulenol I	C15H24O	M+H	221.1900	-2.7
HMDB0036716	beta-Santalol	C15H24O	M+H	221.1900	-2.7
HMDB0038512	Bisacurool	C15H24O	M+H	221.1900	-2.7
HMDB0035391	Preisocalamendiol	C15H24O	M+H	221.1900	-2.7
HMDB0038210	Humulene epoxide II	C15H24O	M+H	221.1900	-2.7
HMDB0032220	Dihydronootkatone	C15H24O	M+H	221.1900	-2.7
HMDB0037811	Vetiverol	C15H24O	M+H	221.1900	-2.7
HMDB0013688	Nootkatol	C15H24O	M+H	221.1900	-2.7
HMDB0034718	Isospathulenol	C15H24O	M+H	221.1900	-2.7
HMDB0060356	2-trans,6-trans-Farnesal	C15H24O	M+H	221.1900	-2.7
HMDB0037392	4(15)-Copaen-11-ol	C15H24O	M+H	221.1900	-2.7
HMDB0035026	alpha-Cyperol	C15H24O	M+H	221.1900	-2.7
HMDB0035793	Fukinone	C15H24O	M+H	221.1900	-2.7
HMDB0038212	Humulenol II	C15H24O	M+H	221.1900	-2.7
HMDB0035739	(R)-2,7(14),9-Bisabolatrien-11-ol	C15H24O	M+H	221.1900	-2.7
HMDB0038146	Calacone	C15H24O	M+H	221.1900	-2.7

	HMDB0036798	8alpha-3-Copaen-8-ol	C15H24O	M+H	221.1900	-2.7
	HMDB0036402	alpha-Bergamotenol	C15H24O	M+H	221.1900	-2.7
	HMDB0036192	Apritone	C15H24O	M+H	221.1900	-2.7
	HMDB0038119	Eremofukinone	C15H24O	M+H	221.1900	-2.7
	HMDB0038982	4-Nonylphenol	C15H24O	M+H	221.1900	-2.7
	HMDB0059836	Cabreuva oxide D	C15H24O	M+H	221.1900	-2.7
	HMDB0182061	3-(2-{2,3-dimethyltricyclo[2.2.1,]heptan-3-yl}ethyl)-2,2-dimethyloxirane	C15H24O	M+H	221.1900	-2.7
	HMDB0182873	[1-methylidene-7-(prop-1-en-2-yl)-decahydronaphthalen-4a-yl]methanol	C15H24O	M+H	221.1900	-2.7
222.1694	HMDB0039974	(1S,2S,4R,8R)-p-Menthane-1,2,8,9-tetrol	C10H20O4	M+NH4	222.1700	-2.6
	HMDB0035133	3,7-Dimethyl-3-octene-1,2,6,7-tetrol	C10H20O4	M+NH4	222.1700	-2.6
	HMDB0039053	(1alpha,2alpha,4betaH,6alpha,8R)-p-Menthane-2,6,8,9-tetrol	C10H20O4	M+NH4	222.1700	-2.6
	HMDB0033217	(2xi,6xi)-7-Methyl-3-methylene-1,2,6,7-octanetetrol	C10H20O4	M+NH4	222.1700	-2.6
	HMDB0033642	(2xi,3xi,6E)-3,7-Dimethyl-6-octene-1,2,3,8-tetrol	C10H20O4	M+NH4	222.1700	-2.6
222.1847	HMDB0133154	2-benzylheptanal	C14H20O	M+NH4	222.1852	-2.4
	HMDB0036170	2-Benzylidene-1-heptanol	C14H20O	M+NH4	222.1852	-2.4
	HMDB0031776	(6R,7S)-6,7-Epoxy-1,3-tetradecadiyne	C14H20O	M+NH4	222.1852	-2.4
	HMDB0041482	3-Benzyl-4-heptanone	C14H20O	M+NH4	222.1852	-2.4
	HMDB0030188	N-Isobutyl-2,4,8-decatrienamide	C14H23NO	M+H	222.1852	-2.4
	HMDB0038840	Sarmentine	C14H23NO	M+H	222.1852	-2.4
	HMDB0032240	N-3,7-Dimethyl-2,6-octadienylcyclopropylcarboxamide	C14H23NO	M+H	222.1852	-2.4
222.9877	HMDB0184683	(4,5-dihydroxyoxolan-3-yl)oxidanesulfonic acid	C4H8O7S	M+Na	222.9883	-2.7
	HMDB0159606	2-hydroxy-3-(sulfooxy)butanoic acid	C4H8O7S	M+Na	222.9883	-2.7
	HMDB0159605	3-hydroxy-2-(sulfooxy)butanoic acid	C4H8O7S	M+Na	222.9883	-2.7
	HMDB0157675	4-hydroxy-2-(sulfooxy)butanoic acid	C4H8O7S	M+Na	222.9883	-2.7
	HMDB0157674	2-hydroxy-4-(sulfooxy)butanoic acid	C4H8O7S	M+Na	222.9883	-2.7
	HMDB0157265	4-hydroxy-3-(sulfooxy)butanoic acid	C4H8O7S	M+Na	222.9883	-2.7
	HMDB0157264	3-hydroxy-4-(sulfooxy)butanoic acid	C4H8O7S	M+Na	222.9883	-2.7
	HMDB0154804	3-hydroxy-2-[(sulfooxy)methyl]propanoic acid	C4H8O7S	M+Na	222.9883	-2.7
	HMDB0154801	2-Hydroxy-2-methyl-3-(sulfooxy)propionic acid	C4H8O7S	M+Na	222.9883	-2.7
	HMDB0184682	(2,4-dihydroxyoxolan-3-yl)oxidanesulfonic acid	C4H8O7S	M+Na	222.9883	-2.7
223.0631	HMDB0163327	{[(5E)-7-oxooct-5-en-2-yl]oxy}sulfonic acid	C8H14O5S	M+H	223.0635	-1.7
	HMDB0163325	{[(5E)-7-oxooct-5-en-4-yl]oxy}sulfonic acid	C8H14O5S	M+H	223.0635	-1.7
	HMDB0163331	{[(5E)-7-oxooct-5-en-1-yl]oxy}sulfonic acid	C8H14O5S	M+H	223.0635	-1.7
	HMDB0163333	{[(3E)-2-oxooct-3-en-1-yl]oxy}sulfonic acid	C8H14O5S	M+H	223.0635	-1.7
223.0742	HMDB0029058	Threoninyl-Cysteine	C7H14N2O4S	M+H	223.0747	-2.3
	HMDB0000099	L-Cystathionine	C7H14N2O4S	M+H	223.0747	-2.3
	HMDB0000455	Allocystathionine	C7H14N2O4S	M+H	223.0747	-2.3
	HMDB0028785	Cysteinyl-Threonine	C7H14N2O4S	M+H	223.0747	-2.3
	HMDB0135689	4-(4-hydroxy-3,5-dimethoxyphenyl)but-3-en-2-one	C12H14O4	M+H	223.0965	-2.6
	HMDB0135906	3,4-dihydroxy-5-(3-methylbut-2-en-1-yl)benzoic acid	C12H14O4	M+H	223.0965	-2.6
	HMDB0164056	4-(2-hydroxy-3-oxobutyl)phenyl acetate	C12H14O4	M+H	223.0965	-2.6
	HMDB0170845	2-methoxy-4-[(oxiran-2-yl)methyl]phenyl acetate	C12H14O4	M+H	223.0965	-2.6
	HMDB0170846	2-methoxy-4-(prop-2-en-1-yl)phenyl 2-hydroxyacetate	C12H14O4	M+H	223.0965	-2.6
	HMDB0170974	4-[(1Z)-3-hydroxyprop-1-en-1-yl]-2-methoxyphenyl acetate	C12H14O4	M+H	223.0965	-2.6
	HMDB0170976	3-hydroxy-2-methoxy-4-[(1Z)-prop-1-en-1-yl]phenyl acetate	C12H14O4	M+H	223.0965	-2.6
	HMDB0170977	5-hydroxy-2-methoxy-4-[(1Z)-prop-1-en-1-yl]phenyl acetate	C12H14O4	M+H	223.0965	-2.6
	HMDB0170978	1-acetoxy-2-methoxy-4-(3-methyl-oxiranyl)-benzene	C12H14O4	M+H	223.0965	-2.6
	HMDB0170979	2-methoxy-4-[(1Z)-prop-1-en-1-yl]phenyl 2-hydroxyacetate	C12H14O4	M+H	223.0965	-2.6
	HMDB0164058	4-(1-hydroxy-3-oxobutyl)phenyl acetate	C12H14O4	M+H	223.0965	-2.6
	HMDB0164057	4-(4-hydroxy-3-oxobutyl)phenyl acetate	C12H14O4	M+H	223.0965	-2.6
	HMDB0164055	4-(3-oxobutyl)phenyl 2-hydroxyacetate	C12H14O4	M+H	223.0965	-2.6
	HMDB0127824	5-[(3-hydroxy-4-methoxyphenyl)methyl]oxolan-2-one	C12H14O4	M+H	223.0965	-2.6
	HMDB0131281	2-Hydroxy-3-(4-methoxyphenyl)propenoic acid ethyl ester	C12H14O4	M+H	223.0965	-2.6

223.0959	HMDB0131284	ethyl 3-(4-methoxyphenyl)oxirane-2-carboxylate	C12H14O4	M+H	223.0965	-2.6
	HMDB0131283	ethyl (2E)-3-(2-hydroxy-4-methoxyphenyl)prop-2-enoate	C12H14O4	M+H	223.0965	-2.6
	HMDB0131285	2-hydroxyethyl (2E)-3-(4-methoxyphenyl)prop-2-enoate	C12H14O4	M+H	223.0965	-2.6
	HMDB0135900	4-hydroxy-3-(4-hydroxy-3-methylbut-2-en-1-yl)benzoic acid	C12H14O4	M+H	223.0965	-2.6
	HMDB0135904	3-[(3,3-dimethyloxiran-2-yl)methyl]-4-hydroxybenzoic acid	C12H14O4	M+H	223.0965	-2.6
	HMDB0135902	4-hydroxy-3-(4-hydroxy-3-methylbut-2-en-1-yl)benzoic acid	C12H14O4	M+H	223.0965	-2.6
	HMDB0002056	Monoisobutyl phthalic acid	C12H14O4	M+H	223.0965	-2.6
	HMDB0094660	Diethyl phthalic acid	C12H14O4	M+H	223.0965	-2.6
	HMDB0038563	(Z)-3-(2,4,5-Trimethoxyphenyl)-2-propenal	C12H14O4	M+H	223.0965	-2.6
	HMDB0041379	2,3-Dihydro-3-hydroxy-6-methoxy-2,2-dimethyl-4H-1-benzopyran-4-one	C12H14O4	M+H	223.0965	-2.6
	HMDB0033776	Apiole	C12H14O4	M+H	223.0965	-2.6
	HMDB0031668	Dihydrodeoxy-8-epiaustdiol	C12H14O4	M+H	223.0965	-2.6
	HMDB0034056	5-(3,4-Methylenedioxyphenyl)pentanoic acid	C12H14O4	M+H	223.0965	-2.6
	HMDB0037681	Vanillin isobutyrate	C12H14O4	M+H	223.0965	-2.6
	HMDB0029470	Isodillapiole	C12H14O4	M+H	223.0965	-2.6
	HMDB0037130	Piperonyl isobutyrate	C12H14O4	M+H	223.0965	-2.6
	HMDB0030725	Dillapiol	C12H14O4	M+H	223.0965	-2.6
	HMDB0013247	Monobutylphthalate	C12H14O4	M+H	223.0965	-2.6
	HMDB0029226	5'-(3'-Methoxy-4'-hydroxyphenyl)-gamma-valerolactone	C12H14O4	M+H	223.0965	-2.6
	HMDB0060606	Hydralazine acetone hydrazone	C11H12N4	M+Na	223.0954	2.2
223.1117	HMDB0094704	N-propanoyl-L-methionine	C8H15NO3S	M+NH4	223.1111	2.7
223.1686	HMDB0035593	Rishitin	C14H22O2	M+H	223.1693	-2.9
	HMDB0036790	Kobusone	C14H22O2	M+H	223.1693	-2.9
	HMDB0036791	Isokobusone	C14H22O2	M+H	223.1693	-2.9
	HMDB0037820	Acetaldehyde butyl phenethyl acetal	C14H22O2	M+H	223.1693	-2.9
	HMDB0040178	2,6-Di-tert-butyl-1,4-benzenediol	C14H22O2	M+H	223.1693	-2.9
	HMDB0037605	(betaH,11xi)-11-Hydroxy-13-nor-6-eremophilen-8-one	C14H22O2	M+H	223.1693	-2.9
223.2053	HMDB0036197	(-)-alpha-Bisabolol	C15H26O	M+H	223.2056	-1.5
	HMDB0041575	Isokessane	C15H26O	M+H	223.2056	-1.5
	HMDB0036452	alpha-cadinol	C15H26O	M+H	223.2056	-1.5
	HMDB0041629	(3S,6E)-nerolidol	C15H26O	M+H	223.2056	-1.5
	HMDB0036646	Cedrelanol	C15H26O	M+H	223.2056	-1.5
	HMDB0036445	Bulnesol	C15H26O	M+H	223.2056	-1.5
	HMDB0035662	Nerolidol	C15H26O	M+H	223.2056	-1.5
	HMDB0036579	Carotol	C15H26O	M+H	223.2056	-1.5
	HMDB0035711	Panasinsanol A	C15H26O	M+H	223.2056	-1.5
	HMDB0039744	Ginsenol	C15H26O	M+H	223.2056	-1.5
	HMDB0037066	beta-Caryophyllene alcohol	C15H26O	M+H	223.2056	-1.5
	HMDB0036679	Faurinone	C15H26O	M+H	223.2056	-1.5
	HMDB0036908	Sesquiceneol	C15H26O	M+H	223.2056	-1.5
	HMDB0059841	Cubenol	C15H26O	M+H	223.2056	-1.5
	HMDB0038167	Maaliolalcohol	C15H26O	M+H	223.2056	-1.5
	HMDB0038213	Humulol	C15H26O	M+H	223.2056	-1.5
	HMDB0035663	(S)-Nerolidol	C15H26O	M+H	223.2056	-1.5
	HMDB0030938	beta-Triticene	C15H26O	M+H	223.2056	-1.5
	HMDB0036645	Globulol	C15H26O	M+H	223.2056	-1.5
	HMDB0035199	Sesquisabinene hydrate	C15H26O	M+H	223.2056	-1.5
	HMDB0036732	Licoagroaurone	C15H26O	M+H	223.2056	-1.5
	HMDB0037031	Epicubenol	C15H26O	M+H	223.2056	-1.5
	HMDB0033239	Pogostol	C15H26O	M+H	223.2056	-1.5
	HMDB0035351	4beta-8-Daucen-4-ol	C15H26O	M+H	223.2056	-1.5
	HMDB0037394	p-Hydroxynonanophenone	C15H26O	M+H	223.2056	-1.5
	HMDB0036642	Isointermedeol	C15H26O	M+H	223.2056	-1.5
	HMDB0036198	(+)-alpha-Bisabolol	C15H26O	M+H	223.2056	-1.5
	HMDB0035021	(-)-Pacifigorgiol	C15H26O	M+H	223.2056	-1.5
	HMDB0035364	6-Epi-beta-bisabolol	C15H26O	M+H	223.2056	-1.5
	HMDB0004305	Farnesol	C15H26O	M+H	223.2056	-1.5
	HMDB0036447	Guaiooxide	C15H26O	M+H	223.2056	-1.5

	HMDB0039538	(6Z,9Z)-6,9-Pentadecadien-2-one	C15H26O	M+H	223.2056	-1.5
	HMDB0059849	(Z)-Farnesol	C15H26O	M+H	223.2056	-1.5
	HMDB0036421	(-)-Valeranone	C15H26O	M+H	223.2056	-1.5
	HMDB0037234	Koraiol	C15H26O	M+H	223.2056	-1.5
	HMDB0034982	-Epijunenol	C15H26O	M+H	223.2056	-1.5
	HMDB0040422	Chamomillool	C15H26O	M+H	223.2056	-1.5
	HMDB0037067	Zingiberenol	C15H26O	M+H	223.2056	-1.5
	HMDB0030939	alpha-Triticene	C15H26O	M+H	223.2056	-1.5
	HMDB0035383	Panasinsanol B	C15H26O	M+H	223.2056	-1.5
	HMDB0035811	Shyobunol	C15H26O	M+H	223.2056	-1.5
	HMDB0034951	Valerianol	C15H26O	M+H	223.2056	-1.5
	HMDB0036580	5,8-Epoxydaucane	C15H26O	M+H	223.2056	-1.5
	HMDB0035868	Rosifoliol	C15H26O	M+H	223.2056	-1.5
	HMDB0036111	beta-Bisabolol	C15H26O	M+H	223.2056	-1.5
224.0630	HMDB0061289	1-(2,4-difluorophenyl)-2-(1H-1,2,4-triazol-1-yl)ethan-1-one	C10H7F2N3O	M+H	224.0630	0.0
224.1122	HMDB0033584	Diethyl tartrate	C8H14O6	M+NH4	224.1129	-2.9
	HMDB0240354	N-acetyl-D-galactosaminitol	C8H17NO6	M+H	224.1129	-3.0
225.0586	HMDB0151306	(2E)-2-(methanesulfinylmethyl)-3-phenylprop-2-enoic acid	C11H12O3S	M+H	225.0580	2.7
	HMDB0151305	(2E)-3-(4-hydroxyphenyl)-2-[(methylsulfonyl)methyl]prop-2-enoic acid	C11H12O3S	M+H	225.0580	2.7
	HMDB0151304	(2E)-3-(3-hydroxyphenyl)-2-[(methylsulfonyl)methyl]prop-2-enoic acid	C11H12O3S	M+H	225.0580	2.7
	HMDB0151308	(2E)-3-(2-hydroxyphenyl)-2-[(methylsulfonyl)methyl]prop-2-enoic acid	C11H12O3S	M+H	225.0580	2.7
	HMDB0151307	2-[(methylsulfonyl)methyl]-3-phenyloxirane-2-carboxylic acid	C11H12O3S	M+H	225.0580	2.7
225.0909	HMDB0030411	(2R,2'S)-Isobuteine	C7H13NO4S	M+NH4	225.0904	2.4
	HMDB0031200	2-Methyl-2-[(1-oxo-2-propenyl)amino]-1-propanesulfonic acid	C7H13NO4S	M+NH4	225.0904	2.4
	HMDB0240343	AC-MET(O)-OH	C7H13NO4S	M+NH4	225.0904	2.4
	HMDB0135602	3-(4-hydroxyphenyl)-1-phenylprop-2-en-1-one	C15H12O2	M+H	225.0910	-0.5
	HMDB0135404	(2E)-1-(3-hydroxyphenyl)-3-phenylprop-2-en-1-one	C15H12O2	M+H	225.0910	-0.5
	HMDB0135600	3-(3-hydroxyphenyl)-1-phenylprop-2-en-1-one	C15H12O2	M+H	225.0910	-0.5
	HMDB0135604	1-(3-hydroxyphenyl)-3-phenylprop-2-en-1-one	C15H12O2	M+H	225.0910	-0.5
	HMDB0135607	(2E)-1-(4-hydroxyphenyl)-3-phenylprop-2-en-1-one	C15H12O2	M+H	225.0910	-0.5
	HMDB0141385	(2E)-3-(3-hydroxyphenyl)-1-phenylprop-2-en-1-one	C15H12O2	M+H	225.0910	-0.5
	HMDB0141386	(2E)-3-(4-hydroxyphenyl)-1-phenylprop-2-en-1-one	C15H12O2	M+H	225.0910	-0.5
	HMDB0141387	2-benzoyl-3-phenyloxirane	C15H12O2	M+H	225.0910	-0.5
	HMDB0032584	4-Hydroxychalcone	C15H12O2	M+H	225.0910	-0.5
	HMDB0135599	1-(2-hydroxyphenyl)-3-phenylprop-2-en-1-one	C15H12O2	M+H	225.0910	-0.5
	HMDB0135603	1-(4-hydroxyphenyl)-3-phenylprop-2-en-1-one	C15H12O2	M+H	225.0910	-0.5
225.1269	HMDB0135562	2-phenyl-2-(2-phenylethyl)oxirane	C16H16O	M+H	225.1274	-2.2
	HMDB0135561	4-(3-phenylbut-3-en-1-yl)phenol	C16H16O	M+H	225.1274	-2.2
	HMDB0135560	3-(3-phenylbut-3-en-1-yl)phenol	C16H16O	M+H	225.1274	-2.2
	HMDB0135559	3-(4-phenylbut-1-en-2-yl)phenol	C16H16O	M+H	225.1274	-2.2
	HMDB0135555	2-(4-phenylbut-1-en-2-yl)phenol	C16H16O	M+H	225.1274	-2.2
	HMDB0135557	1,3-diphenylbut-3-en-1-ol	C16H16O	M+H	225.1274	-2.2
	HMDB0135556	2-(3-phenylbut-3-en-1-yl)phenol	C16H16O	M+H	225.1274	-2.2
	HMDB0135558	4-(4-phenylbut-1-en-2-yl)phenol	C16H16O	M+H	225.1274	-2.2
	HMDB0135554	1,3-diphenylbut-3-en-2-ol	C16H16O	M+H	225.1274	-2.2
	HMDB0134567	4-(2-phenylcyclobutyl)phenol	C16H16O	M+H	225.1274	-2.2
	HMDB0134565	2-(2-phenylcyclobutyl)phenol	C16H16O	M+H	225.1274	-2.2
	HMDB0134566	3-(2-phenylcyclobutyl)phenol	C16H16O	M+H	225.1274	-2.2
	HMDB0134568	1,2-diphenylcyclobutan-1-ol	C16H16O	M+H	225.1274	-2.2
	HMDB0163216	(2E,4E)-6-(3-pentyloxiran-2-yl)hexa-2,4-dienoic acid	C13H20O3	M+H	225.1485	-1.0
	HMDB0163215	(2E)-3-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}prop-2-enoic acid	C13H20O3	M+H	225.1485	-1.0
	HMDB0163211	(2E,4E,7Z)-13-hydroxytrideca-2,4,7-trienoic acid	C13H20O3	M+H	225.1485	-1.0
	HMDB0163213	(2E,4E,7Z)-9-hydroxytrideca-2,4,7-trienoic acid	C13H20O3	M+H	225.1485	-1.0
	HMDB0163214	3-[(1E,4Z)-deca-1,4-dien-1-yl]oxirane-2-carboxylic acid	C13H20O3	M+H	225.1485	-1.0
	HMDB0163210	(2E,4E,7Z)-12-hydroxytrideca-2,4,7-trienoic acid	C13H20O3	M+H	225.1485	-1.0
	HMDB0112084	3-(3-methyl-5-pentylfuran-2-yl)propanoic acid	C13H20O3	M+H	225.1485	-1.0

225.1483	HMDB0037730	Furfuryl octanoate	C13H20O3	M+H	225.1485	-1.0
	HMDB0037726	Octyl 2-furoate	C13H20O3	M+H	225.1485	-1.0
	HMDB0036583	Methyl jasmonate	C13H20O3	M+H	225.1485	-1.0
	HMDB0032679	Annuionone A	C13H20O3	M+H	225.1485	-1.0
	HMDB0037736	3-Methylbutyl 2-furanbutanoate	C13H20O3	M+H	225.1485	-1.0
	HMDB0034564	13-Oxo-9,11-tridecadienoic acid	C13H20O3	M+H	225.1485	-1.0
	HMDB0032689	Annuionone C	C13H20O3	M+H	225.1485	-1.0
	HMDB0029670	Epoxyeremopetasinorol	C13H20O3	M+H	225.1485	-1.0
	HMDB0037244	(8alpha,beta,11beta)-3-Hydroxy-4,15-dinor-1(5)-xanthen-12,8-olide	C13H20O3	M+H	225.1485	-1.0
225.1844	HMDB0030427	Linalyl butyrate	C14H24O2	M+H	225.1849	-2.2
	HMDB0038260	Geranyl 2-methylpropanoate	C14H24O2	M+H	225.1849	-2.2
	HMDB0038246	Bornyl butyrate	C14H24O2	M+H	225.1849	-2.2
	HMDB0037814	2-Propenyl cyclohexanepentanoate	C14H24O2	M+H	225.1849	-2.2
	HMDB0030426	Linalyl isobutyrate	C14H24O2	M+H	225.1849	-2.2
	HMDB0031015	Ethyl (2E,6Z)-dodecadienoate	C14H24O2	M+H	225.1849	-2.2
	HMDB0038259	Neryl butyrate	C14H24O2	M+H	225.1849	-2.2
	HMDB0032524	Terpinyl isobutyrate	C14H24O2	M+H	225.1849	-2.2
	HMDB0036424	Allyl undecylenate	C14H24O2	M+H	225.1849	-2.2
	HMDB0032053	alpha-Terpineol butanoate	C14H24O2	M+H	225.1849	-2.2
	HMDB0032342	Isobornyl isobutyrate	C14H24O2	M+H	225.1849	-2.2
	HMDB0000560	Goshuyic acid	C14H24O2	M+H	225.1849	-2.2
	HMDB0039129	Goshuyic acid	C14H24O2	M+H	225.1849	-2.2
225.2207	HMDB0031111	5,-Pentadecadien-1-ol	C15H28O	M+H	225.2213	-2.6
	HMDB0032218	(+/-)-Dihydrofarnesol	C15H28O	M+H	225.2213	-2.6
	HMDB0040377	3-Pentadecenal	C15H28O	M+H	225.2213	-2.6
226.0842	HMDB0002096	3-Indolebutyric acid	C12H13NO2	M+Na	226.0838	1.6
	HMDB0015611	Methsuximide	C12H13NO2	M+Na	226.0838	1.6
	HMDB0039656	5-(2-Furanyl)-1,2,3,4,5,6-hexahydro-7H-cyclopenta[b]pyridin-7-one	C12H13NO2	M+Na	226.0838	1.6
	HMDB0041526	Isosalsolidine	C12H13NO2	M+Na	226.0838	1.6
	HMDB0240623	methyl 3-(1H-indol-3-yl)propanoate	C12H13NO2	M+Na	226.0838	1.6
226.0932	HMDB0012210	Dihydrolipoate	C8H16O2S2	M+NH4	226.0930	0.9
	HMDB0060589	Aminofurantoin	C8H8N4O3	M+NH4	226.0935	-1.2
	HMDB0014925	Aciclovir	C8H11N5O3	M+H	226.0935	-1.2
226.1109	HMDB0170972	(oct-7-en-1-yloxy)sulfonic acid	C8H16O4S	M+NH4	226.1108	0.7
	HMDB0172324	(oct-7-en-2-yloxy)sulfonic acid	C8H16O4S	M+NH4	226.1108	0.7
226.1221	HMDB0003066	Chalcone	C15H12O	M+NH4	226.1226	-2.4
	HMDB0135598	1,3-diphenylprop-2-en-1-one	C15H12O	M+NH4	226.1226	-2.4
	HMDB0060323	1-Methoxyphenanthrene	C15H12O	M+NH4	226.1226	-2.4
226.1796	HMDB0178135	3-[(2Z)-but-2-en-1-yl]-4-(hydroxymethyl)-2,4-dimethylcyclohex-2-en-1-one	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0178139	6-[(2Z)-but-2-en-1-yl]-1,5,5-trimethyl-7-oxabicyclo[4.1]heptan-2-one	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0178137	3-[(2Z)-4-hydroxybut-2-en-1-yl]-2,4,4-trimethylcyclohex-2-en-1-one	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0178136	3-[(2Z)-but-2-en-1-yl]-2-(hydroxymethyl)-4,4-dimethylcyclohex-2-en-1-one	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0178138	2,4,4-trimethyl-3-[(3-methyloxiran-2-yl)methyl]cyclohex-2-en-1-one	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0178140	3-[(2Z)-but-2-en-1-yl]-6-hydroxy-2,4,4-trimethylcyclohex-2-en-1-one	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0163196	(2E,4E,7Z)-13-hydroxytrideca-2,4,7-trienal	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0163195	(2E,4E)-6-(3-pentyloxiran-2-yl)hexa-2,4-dienal	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0132947	1-(4-methoxyphenyl)-4-methylpentan-3-ol	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0163190	(2E,4E,7Z)-trideca-2,4,7-trienoic acid	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0163194	(2E)-3-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}prop-2-enal	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0163192	(2E,4E,7Z)-12-hydroxytrideca-2,4,7-trienal	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0163193	3-[(1E,4Z)-deca-1,4-dien-1-yl]oxirane-2-carbaldehyde	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0163191	(2E,4E,7Z)-9-hydroxytrideca-2,4,7-trienal	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0038047	Carvyl propionate	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0029668	Eremopetasinorol	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0041636	(3R,8E)-3-Hydroxy-5,8-megastigmadien-7-one	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0040233	2,3,5,6,8,8a-Hexahydro-2,5,5,8a-tetramethyl-7H-1-benzopyran-7-one	C13H20O2	M+NH4	226.1802	-2.4

	HMDB0038529	5,9:6,9-Diepoxy-4-megastigmenene	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0035228	Theaspirone A	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0034984	(5R,6S)-5,6-Epoxy-7-megastigmen-9-one	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0034672	(5alpha,8beta,9beta)-5,9-Epoxy-3,6-megastigmadien-8-ol	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0036824	Acetal R	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0036686	2,2,6,7-Tetramethylbicyclo[4.3]nona-1(9),4-diene-7,8-diol	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0036821	Apo-9-zeaxanthinone	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0037776	3-Mercaptohexyl hexanoate	C13H20O2	M+NH4	226.1802	-2.4
226.2161	HMDB0031869	(S,E)-Lyratol propanoate	C13H20O2	M+NH4	226.1802	-2.4
	HMDB0035862	(E)-6,-Dimethyl-9-methylene-5-undecen-2-one	C14H24O	M+NH4	226.2165	-1.9
	HMDB0032215	2-Decylfuran	C14H24O	M+NH4	226.2165	-1.9
227.1273	HMDB0039884	2-Cyclotetradecen-1-one	C14H24O	M+NH4	226.2165	-1.9
	HMDB0040705	Allixin	C12H18O4	M+H	227.1278	-2.1
227.1637	HMDB0059729	3,4-Methylenesecbacic acid	C12H18O4	M+H	227.1278	-2.1
	HMDB0176431	(9E,11E)-13-hydroxytrideca-9,11-dienoic acid	C13H22O3	M+H	227.1642	-2.1
	HMDB0176430	(9E)-13-oxotridec-9-enoic acid	C13H22O3	M+H	227.1642	-2.1
	HMDB0037562	Riesling acetal	C13H22O3	M+H	227.1642	-2.1
	HMDB0040615	4,5-Dihydrovomifoliol	C13H22O3	M+H	227.1642	-2.1
227.2000	HMDB0031740	Methyl dihydrojasmonate	C13H22O3	M+H	227.1642	-2.1
	HMDB0062248	(9E)-tetradecenoic acid	C14H26O2	M+H	227.2006	-2.4
	HMDB0094671	cyclohexyl octanoate	C14H26O2	M+H	227.2006	-2.4
	HMDB0062243	cis-tetradec-7-enoic acid	C14H26O2	M+H	227.2006	-2.4
	HMDB0037189	Rhodinyl isobutyrate	C14H26O2	M+H	227.2006	-2.4
	HMDB0037188	Rhodinyl butyrate	C14H26O2	M+H	227.2006	-2.4
	HMDB0031073	12-Methyl-13-tridecanolide	C14H26O2	M+H	227.2006	-2.4
	HMDB0034561	Houttuynin	C14H26O2	M+H	227.2006	-2.4
	HMDB0038056	delta-Tetradecalactone	C14H26O2	M+H	227.2006	-2.4
	HMDB0030921	(R)-14-Methyloxacyclotetradecan-2-one	C14H26O2	M+H	227.2006	-2.4
	HMDB0031029	Ethyl (E)-2-dodecenoate	C14H26O2	M+H	227.2006	-2.4
	HMDB0037633	xi-Tetrahydro-3-nonyl-2H-pyran-2-one	C14H26O2	M+H	227.2006	-2.4
	HMDB0010732	trans-Tetra-dec-2-enoic acid	C14H26O2	M+H	227.2006	-2.4
	HMDB0005051	Tsuzuic acid	C14H26O2	M+H	227.2006	-2.4
	HMDB0002000	Myristoleic acid	C14H26O2	M+H	227.2006	-2.4
	HMDB0000521	5Z-Tetradecenoic acid	C14H26O2	M+H	227.2006	-2.4
	HMDB0037227	Citronellyl butyrate	C14H26O2	M+H	227.2006	-2.4
	HMDB0037228	Citronellyl isobutyrate	C14H26O2	M+H	227.2006	-2.4
	HMDB0061991	Menthyl butyrate	C14H26O2	M+H	227.2006	-2.4
	HMDB0032152	Acetaldehyde di-cis-3-hexenyl acetal	C14H26O2	M+H	227.2006	-2.4
	HMDB0032321	2-Hexenyl octanoate	C14H26O2	M+H	227.2006	-2.4
	HMDB0040228	1,1-Diethoxy-3,7-dimethyl-2,6-octadiene	C14H26O2	M+H	227.2006	-2.4
	HMDB0037369	Butyl 2-decenoate	C14H26O2	M+H	227.2006	-2.4
	HMDB0000499	5-Tetradecenoic acid	C14H26O2	M+H	227.2006	-2.4
228.1014	HMDB0161858	7-methoxy-6-methyl-9H-carbazol-2-ol	C14H13NO2	M+H	228.1019	-2.2
	HMDB0161860	2-methoxy-3-methyl-9H-carbazol-1-ol	C14H13NO2	M+H	228.1019	-2.2
	HMDB0161862	2-methoxy-3-methyl-9H-carbazol-4-ol	C14H13NO2	M+H	228.1019	-2.2
	HMDB0161861	7-methoxy-6-methyl-9H-carbazol-1-ol	C14H13NO2	M+H	228.1019	-2.2
	HMDB0161859	O-Methylmukonal	C14H13NO2	M+H	228.1019	-2.2
	HMDB0161863	7-methoxy-6-methyl-9H-carbazol-4-ol	C14H13NO2	M+H	228.1019	-2.2
	HMDB0041444	Mukoline	C14H13NO2	M+H	228.1019	-2.2
	HMDB0033452	Koenoline	C14H13NO2	M+H	228.1019	-2.2
228.1588	HMDB0161857	7-methoxy-6-methyl-9H-carbazol-3-ol	C14H13NO2	M+H	228.1019	-2.2
	HMDB0037816	Dihydro-3-(1-octenyl)-2,5-furandione	C12H18O3	M+NH4	228.1594	-2.7
	HMDB0037135	1-Benzyloxy-1-(2-methoxyethoxy)ethane	C12H18O3	M+NH4	228.1594	-2.7
	HMDB0032871	Sedanonic acid	C12H18O3	M+NH4	228.1594	-2.7
	HMDB0032797	Jasmonic acid	C12H18O3	M+NH4	228.1594	-2.7
	HMDB0037735	Isoamyl 2-furonpropionate	C12H18O3	M+NH4	228.1594	-2.7
	HMDB0033102	Dihydro-3-(2-octenyl)-2,5-furandione	C12H18O3	M+NH4	228.1594	-2.7
	HMDB0037642	4-(Butoxymethyl)-2-methoxyphenol	C12H18O3	M+NH4	228.1594	-2.7
	HMDB0041573	3-Ethenyl-2,5-dimethyl-4-oxohex-5-en-2-yl acetate	C12H18O3	M+NH4	228.1594	-2.7
	HMDB0037104	(R)-8-Acetoxycarvotanacetone	C12H18O3	M+NH4	228.1594	-2.7
	HMDB0182790	4-{2,2,6-trimethyl-7-oxabicyclo[4.1]heptan-1-yl}butan-2-one	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0163203	(4E,7Z)-2-hydroxytrideca-4,7-dienal	C13H22O2	M+NH4	228.1958	-2.6

228.1952	HMDB0163204	(2E,4E,7Z)-trideca-2,4,7-triene-1,9-diol	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0163200	3-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}propanal	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0163202	(4E,7Z)-13-hydroxytrideca-4,7-dienal	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0163199	(4E,7Z)-12-hydroxytrideca-4,7-dienal	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0163201	(4E)-6-(3-pentyloxiran-2-yl)hex-4-enal	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0163198	(4E,7Z)-9-hydroxytrideca-4,7-dienal	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0163197	(4E,7Z)-3-hydroxytrideca-4,7-dienal	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0163206	{3-[(1E,4Z)-deca-1,4-dien-1-yl]oxiran-2-yl}methanol	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0163205	(2E,4E,7Z)-trideca-2,4,7-triene-1,12-diol	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0182750	4-(5-hydroxy-2,2-dimethyl-6-methylidenecyclohexyl)butan-2-one	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0182752	4-(2,2-dimethyl-6-methylidenecyclohexyl)-1-hydroxybutan-2-one	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0182751	4-(2,2-dimethyl-6-methylidenecyclohexyl)-3-hydroxybutan-2-one	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0182749	4-(1-hydroxy-2,2-dimethyl-6-methylidenecyclohexyl)butan-2-one	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0182748	63512--3	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0182747	4-[2-(hydroxymethyl)-2-methyl-6-methylidenecyclohexyl]butan-2-one	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0178145	3-[(2Z)-1-hydroxybut-2-en-1-yl]-2,4,4-trimethylcyclohexan-1-one	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0178147	3-[(2Z)-but-2-en-1-yl]-6-hydroxy-2,4,4-trimethylcyclohexan-1-one	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0178146	2,4,4-trimethyl-3-[(3-methyloxiran-2-yl)methyl]cyclohexan-1-one	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0178144	3-[(2Z)-4-hydroxybut-2-en-1-yl]-2,4,4-trimethylcyclohexan-1-one	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0178141	3-[(2Z)-but-2-en-1-yl]-4-(hydroxymethyl)-2,4-dimethylcyclohexan-1-one	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0178142	3-[(2Z)-but-2-en-1-yl]-2-(hydroxymethyl)-4,4-dimethylcyclohexan-1-one	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0178143	3-[(2Z)-but-2-en-1-yl]-2-hydroxy-2,4,4-trimethylcyclohexan-1-one	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0163218	(4E,7Z)-4,7-tridecadienoic acid	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0163207	(2E)-3-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}prop-2-en-1-ol	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0163209	(2E,4E,7Z)-trideca-2,4,7-triene-1,13-diol	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0163208	(2E,4E)-6-(3-pentyloxiran-2-yl)hexa-2,4-dien-1-ol	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0041554	Artemisyl propionate	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0032098	Cepanone	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0038258	Neryl propionate	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0037307	Propyl 2,4-decadienoate	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0037286	Citral propylene glycol acetal	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0032052	alpha-Terpineol propanoate	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0038249	Isobornyl propionate	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0031014	Methyl (2E,6Z)-dodecadienoate	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0038291	2-Propenyl cyclohexanebutanoate	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0030425	Linalyl propionate	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0040232	Octahydro-2,5,5,8a-tetramethyl-7H-1-benzopyran-7-one	C13H22O2	M+NH4	228.1958	-2.6
	HMDB0037390	Tsibulin 1	C13H22O2	M+NH4	228.1958	-2.6
229.1429	HMDB0164279	2-[2-(4-hydroxypentyl)-3-oxocyclopentyl]acetic acid	C12H20O4	M+H	229.1434	-2.3
	HMDB0164283	2-hydroxy-2-(3-oxo-2-pentylcyclopentyl)acetic acid	C12H20O4	M+H	229.1434	-2.3
	HMDB0164284	2-(2-hydroxy-3-oxo-2-pentylcyclopentyl)acetic acid	C12H20O4	M+H	229.1434	-2.3
	HMDB0164282	2-(4-hydroxy-3-oxo-2-pentylcyclopentyl)acetic acid	C12H20O4	M+H	229.1434	-2.3
	HMDB0164280	2-(5-hydroxy-3-oxo-2-pentylcyclopentyl)acetic acid	C12H20O4	M+H	229.1434	-2.3
	HMDB0030994	5-Heptyltetrahydro-2-oxo-3-furancarboxylic acid	C12H20O4	M+H	229.1434	-2.3
	HMDB0164281	2-[2-(5-hydroxypentyl)-3-oxocyclopentyl]acetic acid	C12H20O4	M+H	229.1434	-2.3
	HMDB0000933	Traumatic acid	C12H20O4	M+H	229.1434	-2.3
229.1795	HMDB0040004	Menthone 1,3-glyceryl ketal	C13H24O3	M+H	229.1798	-1.4
	HMDB0037212	Menthyl lactate	C13H24O3	M+H	229.1798	-1.4
	HMDB0036139	Menthone 1,2-glyceryl ketal	C13H24O3	M+H	229.1798	-1.4
	HMDB0035881	11-Hydroxy-9-tridecenoic acid	C13H24O3	M+H	229.1798	-1.4
	HMDB0172394	SCHEMBL1959824	C14H28O2	M+H	229.2162	-1.3

229.2159	HMDB0176318	1-hydroxytetradecan-3-one	C14H28O2	M+H	229.2162	-1.3
	HMDB0172395	2-hydroxy-tetradecaldehyde	C14H28O2	M+H	229.2162	-1.3
	HMDB0172393	SCHEMBL4937612	C14H28O2	M+H	229.2162	-1.3
	HMDB0033788	Ethyl dodecanoate	C14H28O2	M+H	229.2162	-1.3
	HMDB0034461	Heptyl heptanoate	C14H28O2	M+H	229.2162	-1.3
	HMDB0037495	3-Methylbutyl nonanoate	C14H28O2	M+H	229.2162	-1.3
	HMDB0038034	Nonyl isovalerate	C14H28O2	M+H	229.2162	-1.3
	HMDB0031072	12-Methyltridecanoic acid	C14H28O2	M+H	229.2162	-1.3
	HMDB0037312	Decyl butanoate	C14H28O2	M+H	229.2162	-1.3
	HMDB0036216	Hexyl octanoate	C14H28O2	M+H	229.2162	-1.3
	HMDB0002221	2,6,-Trimethylundecanoic acid	C14H28O2	M+H	229.2162	-1.3
	HMDB0038969	Dodecyl acetate	C14H28O2	M+H	229.2162	-1.3
	HMDB0032318	Hexanal octane-1,3-diol acetal	C14H28O2	M+H	229.2162	-1.3
	HMDB0032548	Undecanal propyleneglycol acetal	C14H28O2	M+H	229.2162	-1.3
	HMDB0061781	-Methyltridecanoic acid	C14H28O2	M+H	229.2162	-1.3
	HMDB0059865	Isobutyl decanoate	C14H28O2	M+H	229.2162	-1.3
	HMDB0000806	Myristic acid	C14H28O2	M+H	229.2162	-1.3
230.1026	HMDB0180901	Ethanone, 1-(4,6-dihydroxy-2,3-dimethoxyphenyl)-	C10H12O5	M+NH4	230.1023	1.3
	HMDB0133486	3-hydroxy-3-(4-hydroxy-3-methoxyphenyl)propanoic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0125013	2-(2,5-dihydroxy-4-methoxyphenyl)propanoic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0125520	3-(2,4-dihydroxy-5-methoxyphenyl)propanoic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0159047	13443-54-4	C10H12O5	M+NH4	230.1023	1.3
	HMDB0157250	2-(3-hydroxy-2,4-dimethoxyphenyl)acetic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0154359	3-(2,5-dihydroxy-3-methoxyphenyl)propanoic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0154357	3-(2,6-dihydroxy-3-methoxyphenyl)propanoic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0151902	3-(3,4-dihydroxy-2-methoxyphenyl)propanoic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0141332	3-(3,5-dihydroxy-4-methoxyphenyl)propanoic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0140911	3-(2,3-dihydroxy-4-methoxyphenyl)propanoic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0140910	3-(2,5-dihydroxy-4-methoxyphenyl)propanoic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0137878	2-(2,4-dihydroxy-5-methoxyphenyl)propanoic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0131466	SCHEMBL316	C10H12O5	M+NH4	230.1023	1.3
	HMDB0129354	2-(2,3-dihydroxy-4-methoxyphenyl)propanoic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0125540	3-(2,4-dihydroxy-3-methoxyphenyl)propanoic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0125526	3-(3,4-dihydroxy-5-methoxyphenyl)propanoic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0060557	beta-(2-Methoxyphenoxy)-lactic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0041661	3,4-Dihydroxyphenyllactic acid methyl ester	C10H12O5	M+NH4	230.1023	1.3
	HMDB0041665	3-Hydroxy-4-methoxyphenyllactic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0041663	3-(3,4-Dihydroxyphenyl)-2-methoxypropionic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0033835	Propyl gallate	C10H12O5	M+NH4	230.1023	1.3
	HMDB0031704	Danielone	C10H12O5	M+NH4	230.1023	1.3
	HMDB0034493	Valtrate	C10H12O5	M+NH4	230.1023	1.3
	HMDB0033839	Eudesmic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0041286	2,3-Dihydroxy-1-(4-hydroxy-3-methoxyphenyl)-1-propanone	C10H12O5	M+NH4	230.1023	1.3
	HMDB0000913	Vanillactic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0131424	2-(4-hydroxy-3,5-dimethoxyphenyl)acetic acid	C10H12O5	M+NH4	230.1023	1.3
	HMDB0182125	SCHEMBL3676418	C10H12O5	M+NH4	230.1023	1.3
	HMDB0142083	2,3,4-trimethoxybenzoic acid	C10H12O5	M+NH4	230.1023	1.3
230.1170	HMDB0032039	Benzoin	C14H12O2	M+NH4	230.1176	-2.4
	HMDB0014814	Benzyl Benzoate	C14H12O2	M+NH4	230.1176	-2.4
230.1381	HMDB0153808	2-(3-hydroxy-3-methylbutyl)benzene-1,3,5-triol	C11H16O4	M+NH4	230.1387	-2.5
	HMDB0169511	2-(1-hydroxyethyl)-3,5-dimethoxy-6-methylphenol	C11H16O4	M+NH4	230.1387	-2.5
	HMDB0059744	3,4-Methyleneazelaic acid	C11H16O4	M+NH4	230.1387	-2.5
	HMDB0013126	Butenylcarnitine	C11H19NO4	M+H	230.1387	-2.5
230.1746	HMDB0035085	Vulgarole	C12H20O3	M+NH4	230.1751	-2.0
	HMDB0029388	Cucurbitic acid	C12H20O3	M+NH4	230.1751	-2.0
	HMDB0037326	Traumatin	C12H20O3	M+NH4	230.1751	-2.0
	HMDB0033601	Dihydrojasmonic acid	C12H20O3	M+NH4	230.1751	-2.0
	HMDB0041572	3-Ethenyl-4-hydroxy-2,5-dimethylhex-5-en-2-yl acetate	C12H20O3	M+NH4	230.1751	-2.0
	HMDB0013267	N-Decanoylglycine	C12H23NO3	M+H	230.1751	-2.0
	HMDB0037226	Citronellyl propionate	C13H24O2	M+NH4	230.2115	-2.4
	HMDB0037907	2,6,,,-Tetramethyl-1-oxaspiro[4.5]decan-6-ol	C13H24O2	M+NH4	230.2115	-2.4
	HMDB0040451	Oxacyclotetradecan-2-one	C13H24O2	M+NH4	230.2115	-2.4
	HMDB0034286	Ethyl -undecenoate	C13H24O2	M+NH4	230.2115	-2.4

230.2109	HMDB0031017	-Undecenyl acetate	C13H24O2	M+NH4	230.2115	-2.4
	HMDB0037626	1-Ethylhexyl tiglate	C13H24O2	M+NH4	230.2115	-2.4
	HMDB0038078	1,1-Diethoxy-2,6-nonadiene	C13H24O2	M+NH4	230.2115	-2.4
	HMDB0032792	(E)-3-Methyl-4-decen-1-yl acetate	C13H24O2	M+NH4	230.2115	-2.4
	HMDB0031028	Methyl (E)-2-dodecenoate	C13H24O2	M+NH4	230.2115	-2.4
	HMDB0039805	4-(3-Hydroxybutyl)-3,3,5-trimethylcyclohexanone	C13H24O2	M+NH4	230.2115	-2.4
	HMDB0037187	Rhodinyl propionate	C13H24O2	M+NH4	230.2115	-2.4
	HMDB0031741	Coniferan	C13H24O2	M+NH4	230.2115	-2.4
230.2475	HMDB0061955	(E)-9-Tetradecen-1-ol	C14H28O	M+NH4	230.2478	-1.5
	HMDB0032432	12-Methyltridecanal	C14H28O	M+NH4	230.2478	-1.5
	HMDB0034283	Tetradecanal	C14H28O	M+NH4	230.2478	-1.5
	HMDB0030924	2-Tetradecanone	C14H28O	M+NH4	230.2478	-1.5
231.1340	HMDB0029128	Valylhydroxyproline	C10H18N2O4	M+H	231.1339	0.3
	HMDB0240320	AC-LYS(AC)-OH	C10H18N2O4	M+H	231.1339	0.3
	HMDB0028876	Hydroxypropyl-L-Valine	C10H18N2O4	M+H	231.1339	0.3
	HMDB0185203	2-amino-1-(4-hydroxy-3-methoxyphenyl)propane-1,3-diol	C10H15NO4	M+NH4	231.1339	0.3
	HMDB0185197	2-(2-amino-1-hydroxypropyl)-5-methoxybenzene-1,4-diol	C10H15NO4	M+NH4	231.1339	0.3
	HMDB0155125	2-[1-hydroxy-2-(methylamino)ethyl]-5-methoxybenzene-1,4-diol	C10H15NO4	M+NH4	231.1339	0.3
	HMDB0125517	2-(2,6-dihydroxy-3,4-dimethoxycyclohexylidene)acetonitrile	C10H15NO4	M+NH4	231.1339	0.3
231.1585	HMDB0000623	Dodecanedioic acid	C12H22O4	M+H	231.1591	-2.5
	HMDB0041614	Dipropyl hexanedioate	C12H22O4	M+H	231.1591	-2.5
	HMDB0041613	Bis(1-methylethyl) hexanedioate	C12H22O4	M+H	231.1591	-2.5
	HMDB0030143	Talaromycin A	C12H22O4	M+H	231.1591	-2.5
231.2314	HMDB0038678	1,1-Dihexyloxyethane	C14H30O2	M+H	231.2319	-2.0
	HMDB0032246	Dodecanal dimethyl acetal	C14H30O2	M+H	231.2319	-2.0
	HMDB0172396	1,13-tetradecandiol	C14H30O2	M+H	231.2319	-2.0
	HMDB0172397	1,14-Tetradecandiol	C14H30O2	M+H	231.2319	-2.0
232.1538	HMDB0030985	alpha-Carboxy-delta-decalactone	C11H18O4	M+NH4	232.1543	-2.3
	HMDB0030986	2-Carboxy-5,7-dimethyl-4-octanolide	C11H18O4	M+NH4	232.1543	-2.3
	HMDB0030984	5-Hexyltetrahydro-2-oxo-3-furancarboxylic acid	C11H18O4	M+NH4	232.1543	-2.3
	HMDB0062606	Isobutyryl-L-carnitine	C11H21NO4	M+H	232.1543	-2.3
	HMDB0002013	Butyrylcarnitine	C11H21NO4	M+H	232.1543	-2.3
	HMDB0062510	Butyrylcarnitine	C11H21NO4	M+H	232.1543	-2.3
	HMDB0000736	[(2R)-3-carboxy-2-[(2-methylpropanoyl)oxy]propyl]trimethylazanium	C11H22NO4	M+H	232.1543	-2.3
	HMDB0062556	[(2R)-3-carboxy-2-[(2-methylpropanoyl)oxy]propyl]trimethylazanium	C11H22NO4	M+H	232.1543	-2.3
232.1902	HMDB0010727	3-Oxododecanoic acid	C12H22O3	M+NH4	232.1907	-2.2
	HMDB0159933	(5Z)-11-hydroxydodec-5-enoic acid	C12H22O3	M+NH4	232.1907	-2.2
	HMDB0159932	(5Z)-4-hydroxydodec-5-enoic acid	C12H22O3	M+NH4	232.1907	-2.2
	HMDB0159931	(5Z)-7-hydroxydodec-5-enoic acid	C12H22O3	M+NH4	232.1907	-2.2
	HMDB0159936	(5Z)-2-hydroxydodec-5-enoic acid	C12H22O3	M+NH4	232.1907	-2.2
	HMDB0159935	SCHEMBL14224944	C12H22O3	M+NH4	232.1907	-2.2
	HMDB0037398	4-Acetoxy-2-hexyltetrahydrofuran	C12H22O3	M+NH4	232.1907	-2.2
	HMDB0159934	4-(3-hexyloxiran-2-yl)butanoic acid	C12H22O3	M+NH4	232.1907	-2.2
233.1044	HMDB0015656	Naphazoline	C14H14N2	M+Na	233.1049	-2.2
	HMDB0094777	2-[(1,7-dihydroxyoct-5-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
	HMDB0094761	2-[(1,5-dihydroxyoct-3-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
	HMDB0094759	2-[(5-hydroxy-1-oxooct-1-en-2-yl)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
	HMDB0094760	2-[(1,5-dihydroxyoct-2-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
	HMDB0094757	2-[(1,4-dihydroxyoct-6-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
	HMDB0094758	4-hydroxyoct-7-enoylglycine	C10H17NO4	M+NH4	233.1496	-1.2
	HMDB0094756	2-[(1,4-dihydroxyoct-5-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
	HMDB0094755	2-[(1,4-dihydroxyoct-4-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
	HMDB0094754	2-[(1,4-dihydroxyoct-3-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
	HMDB0094753	2-[(1,4-dihydroxyoct-2-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
	HMDB0094752	2-[(4-hydroxy-1-oxooct-1-en-2-yl)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
	HMDB0094750	2-[(1,3-dihydroxyoct-6-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2

233.1493

HMDB0094751	3-hydroxyoct-7-enoylglycine	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094749	2-[(1,3-dihydroxyoct-5-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094746	2-[(1,3-dihydroxyoct-2-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094762	2-[(1,5-dihydroxyoct-4-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094764	2-[(1,5-dihydroxyoct-6-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094776	2-[(1,7-dihydroxyoct-4-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094778	2-[(1,7-dihydroxyoct-6-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094779	7-hydroxyoct-7-enoylglycine	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094775	2-[(1,7-dihydroxyoct-3-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094774	2-[(1,7-dihydroxyoct-2-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094772	6-hydroxyoct-7-enoylglycine	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094768	2-[(1,6-dihydroxyoct-3-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094769	2-[(1,6-dihydroxyoct-4-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094770	2-[(1,6-dihydroxyoct-5-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094771	2-[(1,6-dihydroxyoct-6-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094767	2-[(1,6-dihydroxyoct-2-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094766	2-[(6-hydroxy-1-oxooct-1-en-2-yl)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094765	5-hydroxyoct-7-enoylglycine	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094763	2-[(1,5-dihydroxyoct-5-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094748	2-[(1,3-dihydroxyoct-4-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094747	2-[(1,3-dihydroxyoct-3-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094745	2-[(3-hydroxy-1-oxooct-1-en-2-yl)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094733	2-[(carboxymethyl)amino]oct-3-enoic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094734	2-[(carboxymethyl)amino]oct-4-enoic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094732	2-[(carboxymethyl)amino]oct-2-enoic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094773	2-[(7-hydroxy-1-oxooct-1-en-2-yl)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0013124	Propenoylcarnitine	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094736	2-[(carboxymethyl)amino]oct-6-enoic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094735	2-[(carboxymethyl)amino]oct-5-enoic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094744	2-hydroxyoct-7-enoylglycine	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094741	2-[(1,2-dihydroxyoct-4-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094743	2-[(1,2-dihydroxyoct-6-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094739	2-[(1,2-dihydroxyoct-2-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094742	2-[(1,2-dihydroxyoct-5-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094738	2-[(2-hydroxy-1-oxooct-1-en-3-yl)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094737	1-hydroxyoct-7-enoylglycine	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0094740	2-[(1,2-dihydroxyoct-3-en-1-ylidene)amino]acetic acid	C10H17NO4	M+NH4	233.1496	-1.2
HMDB0029065	Thr-Leu	C10H20N2O4	M+H	233.1496	-1.2
HMDB0013075	Spermic acid 2	C10H20N2O4	M+H	233.1496	-1.2
HMDB0028917	Isoleucyl-Threonine	C10H20N2O4	M+H	233.1496	-1.2
HMDB0028939	Leucyl-Threonine	C10H20N2O4	M+H	233.1496	-1.2
HMDB0029064	TI dipeptide	C10H20N2O4	M+H	233.1496	-1.2
HMDB0170512	(4E)-3-hydroxy-2,7-dimethyloct-4-enedioic acid	C10H16O5	M+NH4	234.1336	-2.5
HMDB0170511	(4E)-2-hydroxy-2,7-dimethyloct-4-enedioic acid	C10H16O5	M+NH4	234.1336	-2.5
HMDB0160552	(4Z)-9-hydroxydec-4-enedioic acid	C10H16O5	M+NH4	234.1336	-2.5
HMDB0160551	(4Z)-2-hydroxydec-4-enedioic acid	C10H16O5	M+NH4	234.1336	-2.5
HMDB0160549	(4Z)-3-hydroxydec-4-enedioic acid	C10H16O5	M+NH4	234.1336	-2.5
HMDB0175347	4-hydroxy-1,2,2-trimethylcyclopentane-1,3-dicarboxylic acid	C10H16O5	M+NH4	234.1336	-2.5
HMDB0160550	5-[3-(2-carboxyethyl)oxiran-2-yl]pentanoic acid	C10H16O5	M+NH4	234.1336	-2.5
HMDB0160548	(4Z)-6-hydroxydec-4-enedioic acid	C10H16O5	M+NH4	234.1336	-2.5
HMDB0160546	(4Z)-7-hydroxydec-4-enedioic acid	C10H16O5	M+NH4	234.1336	-2.5
HMDB0170514	(4E)-2-(hydroxymethyl)-7-methyloct-4-enedioic acid	C10H16O5	M+NH4	234.1336	-2.5
HMDB0170513	3-[3-(2-carboxy-2-methylethyl)oxiran-2-yl]-2-methylpropanoic acid	C10H16O5	M+NH4	234.1336	-2.5
HMDB0182564	2-(1-carboxyethyl)-3-hydroxy-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M+NH4	234.1336	-2.5
HMDB0182566	2-(1-carboxyethyl)-1-hydroxy-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M+NH4	234.1336	-2.5

234.1330	HMDB0182565	2-(1-carboxy-2-hydroxyethyl)-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M+NH4	234.1336	-2.5
	HMDB0182561	5-(1-carboxyethyl)-2-hydroxy-2-methylcyclopentane-1-carboxylic acid	C10H16O5	M+NH4	234.1336	-2.5
	HMDB0182563	5-(1-carboxyethyl)-3-hydroxy-2-methylcyclopentane-1-carboxylic acid	C10H16O5	M+NH4	234.1336	-2.5
	HMDB0182562	2-(1-carboxy-1-hydroxyethyl)-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M+NH4	234.1336	-2.5
	HMDB0182560	2-(1-carboxyethyl)-5-(hydroxymethyl)cyclopentane-1-carboxylic acid	C10H16O5	M+NH4	234.1336	-2.5
	HMDB0175348	SCHEMBL1335666	C10H16O5	M+NH4	234.1336	-2.5
	HMDB0175345	2-(hydroxymethyl)-1,2-dimethylcyclopentane-1,3-dicarboxylic acid	C10H16O5	M+NH4	234.1336	-2.5
	HMDB0175346	5-hydroxy-1,2,2-trimethylcyclopentane-1,3-dicarboxylic acid	C10H16O5	M+NH4	234.1336	-2.5
	HMDB0175344	1-Hydroxymethyl-2,2-dimethyl-cyclopentane-1,3-dicarboxylic acid	C10H16O5	M+NH4	234.1336	-2.5
	HMDB0160547	(4Z)-8-hydroxydec-4-enedioic acid	C10H16O5	M+NH4	234.1336	-2.5
	HMDB0013125	Hydroxypropionylcarnitine	C10H19NO5	M+H	234.1336	-2.6
234.1483	HMDB0133178	(2Z)-2-(phenylmethylidene)hept-6-enoic acid	C14H16O2	M+NH4	234.1489	-2.4
	HMDB0040833	3-[4-Hydroxy-3-(3-methyl-2-butenyl)phenyl]-2-propenal	C14H16O2	M+NH4	234.1489	-2.4
	HMDB0034684	Thalictroidine	C14H19NO2	M+H	234.1489	-2.4
	HMDB0015647	Dexmethylphenidate	C14H19NO2	M+H	234.1489	-2.4
	HMDB0041958	Normeperidine	C14H19NO2	M+H	234.1489	-2.4
	HMDB0014566	Methylphenidate	C14H19NO2	M+H	234.1489	-2.4
234.2058	HMDB0002059	12-Hydroxydodecanoic acid	C12H24O3	M+NH4	234.2064	-2.4
	HMDB0000387	(S)-3-hydroxylauric acid	C12H24O3	M+NH4	234.2064	-2.4
	HMDB0010728	(R)-3-Hydroxydodecanoic acid	C12H24O3	M+NH4	234.2064	-2.4
	HMDB0040169	xi-5-Hydroxydodecanoic acid	C12H24O3	M+NH4	234.2064	-2.4
	HMDB0062032	3-hydroxy-2,4,4-trimethylpentyl 2-methylpropanoate	C12H24O3	M+NH4	234.2064	-2.4
235.1686	HMDB0134131	2-[hydroxy(phenyl)methyl]octanal	C15H22O2	M+H	235.1693	-2.8
	HMDB0134135	2-benzyl-8-hydroxyoctanal	C15H22O2	M+H	235.1693	-2.8
	HMDB0134132	2-[(3-hydroxyphenyl)methyl]octanal	C15H22O2	M+H	235.1693	-2.8
	HMDB0134134	2-benzyl-7-hydroxyoctanal	C15H22O2	M+H	235.1693	-2.8
	HMDB0177700	(1E)-1-ethylidene-5-hydroxy-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O2	M+H	235.1693	-2.8
	HMDB0183493	(8aR)-4-hydroxy-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O2	M+H	235.1693	-2.8
	HMDB0177624	(1Z)-1-ethylidene-5-hydroxy-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O2	M+H	235.1693	-2.8
	HMDB0150675	2,5,5,8a-tetramethyl-6-oxo-1,4,4a,5,6,7,8,8a-octahydronaphthalene-1-carbaldehyde	C15H22O2	M+H	235.1693	-2.8
	HMDB0134153	2-benzyl-octanoic acid	C15H22O2	M+H	235.1693	-2.8
	HMDB0134133	2-[(4-hydroxyphenyl)methyl]octanal	C15H22O2	M+H	235.1693	-2.8
	HMDB0134136	2-benzyl-2-hydroxyoctanal	C15H22O2	M+H	235.1693	-2.8
	HMDB0134138	2-(phenylmethylidene)octane-1,3-diol	C15H22O2	M+H	235.1693	-2.8
	HMDB0134139	3-[(1Z)-2-hexyl-3-hydroxyprop-1-en-1-yl]phenol	C15H22O2	M+H	235.1693	-2.8
	HMDB0134137	2-[(2-hydroxyphenyl)methyl]octanal	C15H22O2	M+H	235.1693	-2.8
	HMDB0134142	(2-hexyl-3-phenyloxiran-2-yl)methanol	C15H22O2	M+H	235.1693	-2.8
	HMDB0134140	4-[(1Z)-2-hexyl-3-hydroxyprop-1-en-1-yl]phenol	C15H22O2	M+H	235.1693	-2.8
	HMDB0134141	(2Z)-2-(phenylmethylidene)octane-1,7-diol	C15H22O2	M+H	235.1693	-2.8
	HMDB0134143	(2Z)-2-(phenylmethylidene)octane-1,8-diol	C15H22O2	M+H	235.1693	-2.8
	HMDB0240643	3,5-di-tert-butyl-4-hydroxybenzaldehyde	C15H22O2	M+H	235.1693	-2.8
	HMDB0035408	1,-Epoxygermacrone	C15H22O2	M+H	235.1693	-2.8
	HMDB0036466	Zerumbone oxide	C15H22O2	M+H	235.1693	-2.8
	HMDB0036647	Isocurcumenol	C15H22O2	M+H	235.1693	-2.8
	HMDB0038698	xi-2-Hydroxy-1,3,5-bisabolatrien-9-one	C15H22O2	M+H	235.1693	-2.8
	HMDB0037710	4-Methylphenyl octanoate	C15H22O2	M+H	235.1693	-2.8
	HMDB0035639	Petasalbin	C15H22O2	M+H	235.1693	-2.8
	HMDB0037391	p-Hydroxynonanophenone	C15H22O2	M+H	235.1693	-2.8
	HMDB0033252	Curcumanolide A	C15H22O2	M+H	235.1693	-2.8
	HMDB0038914	4,6-Decadiyn-1-ol isovalerate	C15H22O2	M+H	235.1693	-2.8
	HMDB0035869	alpha-Rotunol	C15H22O2	M+H	235.1693	-2.8
	HMDB0039621	beta-Santalal acid	C15H22O2	M+H	235.1693	-2.8

	HMDB0034562	9-Pentadecene-12,14-diyne-1,11-diol	C15H22O2	M+H	235.1693	-2.8
	HMDB0036449	(1alpha,4beta,5beta)-4-Hydroxy-7(11),(14)-guaiaadien-8-one	C15H22O2	M+H	235.1693	-2.8
	HMDB0033960	Curcumenol	C15H22O2	M+H	235.1693	-2.8
	HMDB0035935	Dihydroisoolantolactone	C15H22O2	M+H	235.1693	-2.8
	HMDB0031349	Epiacoronene	C15H22O2	M+H	235.1693	-2.8
	HMDB0035413	(4alpha,5alpha)-11-Eremophilene-2,9-dione	C15H22O2	M+H	235.1693	-2.8
	HMDB0036392	(Z)-alpha-Bergamotenoic acid	C15H22O2	M+H	235.1693	-2.8
	HMDB0034956	Oxysolavetivone	C15H22O2	M+H	235.1693	-2.8
	HMDB0038190	Rishitinol	C15H22O2	M+H	235.1693	-2.8
	HMDB0038795	7,9-Illudadiene-3,14-diol	C15H22O2	M+H	235.1693	-2.8
	HMDB0036390	3-Phenylpropyl hexanoate	C15H22O2	M+H	235.1693	-2.8
	HMDB0032081	4,-Longipinanedione	C15H22O2	M+H	235.1693	-2.8
	HMDB0036035	Acutissimin A	C15H22O2	M+H	235.1693	-2.8
	HMDB0035889	Germacrone 4,5-epoxide	C15H22O2	M+H	235.1693	-2.8
	HMDB0037739	7-(1,3-Cyclohexadienyl)-5-hydroxy-2,6-dimethyl-2-hepten-4-one	C15H22O2	M+H	235.1693	-2.8
	HMDB0036427	Procurcumenol	C15H22O2	M+H	235.1693	-2.8
	HMDB0035794	beta-Costic acid	C15H22O2	M+H	235.1693	-2.8
	HMDB0035407	Dehydrocurdione	C15H22O2	M+H	235.1693	-2.8
	HMDB0037038	Cyclodehydroisolibimin	C15H22O2	M+H	235.1693	-2.8
	HMDB0041036	Sugeonol	C15H22O2	M+H	235.1693	-2.8
	HMDB0038796	2,7(14)-Illudadiene-,15-diol	C15H22O2	M+H	235.1693	-2.8
	HMDB0034742	Saussurea lactone	C15H22O2	M+H	235.1693	-2.8
	HMDB0033253	Curcumenone	C15H22O2	M+H	235.1693	-2.8
	HMDB0030016	Valerenic acid	C15H22O2	M+H	235.1693	-2.8
	HMDB0037640	2-Methyl-4-phenyl-2-butyl 2-methylpropanoate	C15H22O2	M+H	235.1693	-2.8
	HMDB0035202	7-Hydroxycostal	C15H22O2	M+H	235.1693	-2.8
	HMDB0038198	3,7-Bisaboladiene-2,8-dione	C15H22O2	M+H	235.1693	-2.8
235.2053	HMDB0175555	(2E,6E)-6-methyl-2-(4-methylpent-3-en-1-yl)nona-2,6,8-trien-1-ol	C16H26O	M+H	235.2056	-1.4
	HMDB0175552	(3E,7Z)-4,8,12-trimethyltrideca-1,3,7,11-tetraen-5-ol	C16H26O	M+H	235.2056	-1.4
	HMDB0175553	(2Z,5Z)-6,-dimethyl-2-(prop-2-en-1-ylidene)undeca-5,9-dien-1-ol	C16H26O	M+H	235.2056	-1.4
	HMDB0175554	(6Z,E)-2,6,-trimethyltrideca-2,6,,12-tetraen-5-ol	C16H26O	M+H	235.2056	-1.4
	HMDB0175559	(6Z,E)-2,6,-trimethyltrideca-2,6,,12-tetraen-4-ol	C16H26O	M+H	235.2056	-1.4
	HMDB0175558	(3E,7Z)-4,8,12-trimethyltrideca-1,3,7,11-tetraen-6-ol	C16H26O	M+H	235.2056	-1.4
	HMDB0175556	(6Z,E)-2,6,-trimethyltrideca-2,6,,12-tetraen-1-ol	C16H26O	M+H	235.2056	-1.4
	HMDB0175557	(2E,6Z,E)-2,6,-trimethyltrideca-2,6,,12-tetraen-1-ol	C16H26O	M+H	235.2056	-1.4
	HMDB0175563	3-[(3Z,7E)-3,7-dimethyldeca-3,7,9-trien-1-yl]-2,2-dimethyloxirane	C16H26O	M+H	235.2056	-1.4
	HMDB0175560	2-[(3Z)-4,8-dimethylnona-3,7-dien-1-yl]-3-ethenyl-2-methyloxirane	C16H26O	M+H	235.2056	-1.4
	HMDB0175561	2-[(1E,5Z)-2,6,-trimethylundeca-1,5,9-trien-1-yl]oxirane	C16H26O	M+H	235.2056	-1.4
	HMDB0040179	2,6-Di-tert-butyl-4-ethylphenol	C16H26O	M+H	235.2056	-1.4
	HMDB0175562	2-methyl-3-[(3E)-3-methylhexa-3,5-dien-1-yl]-2-(4-methylpent-3-en-1-yl)oxirane	C16H26O	M+H	235.2056	-1.4
236.1123	HMDB0029592	Triacetin	C9H14O6	M+NH4	236.1129	-2.4
	HMDB0134121	2-benzyloctanal	C15H22O	M+NH4	236.2009	-2.5
	HMDB0134122	(2Z)-2-(phenylmethylidene)octan-1-ol	C15H22O	M+NH4	236.2009	-2.5
	HMDB0094674	1-Phenylnonan-1-one	C15H22O	M+NH4	236.2009	-2.5
	HMDB0035643	beta-Sinensal	C15H22O	M+NH4	236.2009	-2.5
	HMDB0038215	alpha-Sinensal	C15H22O	M+NH4	236.2009	-2.5
	HMDB0038164	Vulgarone B	C15H22O	M+NH4	236.2009	-2.5
	HMDB0036201	(E)-,11-Dihydro-alpha-atlantone	C15H22O	M+NH4	236.2009	-2.5
	HMDB0038187	beta-Atlantone	C15H22O	M+NH4	236.2009	-2.5
	HMDB0036797	Mustakone	C15H22O	M+NH4	236.2009	-2.5
	HMDB0036733	Vulgarone A	C15H22O	M+NH4	236.2009	-2.5
	HMDB0036667	Zerumbone	C15H22O	M+NH4	236.2009	-2.5
	HMDB0036813	alpha-Santalal	C15H22O	M+NH4	236.2009	-2.5
	HMDB0035081	(5alpha,alpha)-3,7(11)-Eudesmadien-2-one	C15H22O	M+NH4	236.2009	-2.5
	HMDB0036718	beta-Santalal	C15H22O	M+NH4	236.2009	-2.5
	HMDB0036109	1,3,5-Bisabolatrien--one	C15H22O	M+NH4	236.2009	-2.5
	HMDB0035747	Patchoulenone	C15H22O	M+NH4	236.2009	-2.5

236.2003	HMDB0040686	Isohumbertiol	C15H22O	M+NH4	236.2009	-2.5
	HMDB0037000	alpha-Turmerone	C15H22O	M+NH4	236.2009	-2.5
	HMDB0038195	Xanthorrhizol	C15H22O	M+NH4	236.2009	-2.5
	HMDB0038200	Calamusenone	C15H22O	M+NH4	236.2009	-2.5
	HMDB0038511	Bisacumol	C15H22O	M+NH4	236.2009	-2.5
	HMDB0013687	Nookatone	C15H22O	M+NH4	236.2009	-2.5
	HMDB0035657	Solavetivone	C15H22O	M+NH4	236.2009	-2.5
	HMDB0035786	Valerenal	C15H22O	M+NH4	236.2009	-2.5
	HMDB0037061	(+)-4,11-Eudesmadien-3-one	C15H22O	M+NH4	236.2009	-2.5
	HMDB0035835	Furanoeremophilane	C15H22O	M+NH4	236.2009	-2.5
	HMDB0037068	Curlone	C15H22O	M+NH4	236.2009	-2.5
	HMDB0039637	beta-Elementone	C15H22O	M+NH4	236.2009	-2.5
	HMDB0036071	Dendrolasin	C15H22O	M+NH4	236.2009	-2.5
	HMDB0036443	Rotundone	C15H22O	M+NH4	236.2009	-2.5
	HMDB0038201	4,7(11)-Guaiadien-8-one	C15H22O	M+NH4	236.2009	-2.5
	HMDB0035082	(5beta,7beta,beta)-3,11-Eudesmadien-2-one	C15H22O	M+NH4	236.2009	-2.5
	HMDB0013693	AC1L1WLS	C15H22O	M+NH4	236.2009	-2.5
237.0114	HMDB0014841	Methazolamide	C5H8N4O3S2	M+H	237.0111	1.4
237.0221	HMDB0181067	[(2-methyl-3-sulfanyl)pentyl]oxy]sulfonic acid	C6H14O4S2	M+Na	237.0226	-2.0
237.0755	HMDB0137293	3-(4,7-dimethoxy-2H-1,3-benzodioxol-5-yl)prop-2-enal	C12H12O5	M+H	237.0757	-1.1
	HMDB0169150	7-hydroxy-2,2-dimethyl-4-oxo-chroman-6-carboxylic acid	C12H12O5	M+H	237.0757	-1.1
	HMDB0166280	(4Z)-5-(2H-1,3-benzodioxol-5-yl)-3-hydroxypent-4-enoic acid	C12H12O5	M+H	237.0757	-1.1
	HMDB0166281	3-[3-(2H-1,3-benzodioxol-5-yl)oxiran-2-yl]propanoic acid	C12H12O5	M+H	237.0757	-1.1
	HMDB0166282	(4Z)-5-(2H-1,3-benzodioxol-5-yl)-2-hydroxypent-4-enoic acid	C12H12O5	M+H	237.0757	-1.1
	HMDB0166279	(4Z)-5-(6-hydroxy-2H-1,3-benzodioxol-5-yl)pent-4-enoic acid	C12H12O5	M+H	237.0757	-1.1
	HMDB0128676	3-(6,7-dimethoxy-2H-1,3-benzodioxol-5-yl)prop-2-enal	C12H12O5	M+H	237.0757	-1.1
	HMDB0030582	Dillapional	C12H12O5	M+H	237.0757	-1.1
	HMDB0033096	Apional	C12H12O5	M+H	237.0757	-1.1
	HMDB0030858	Austdiol	C12H12O5	M+H	237.0757	-1.1
	HMDB0040407	(S)-2,3-Dihydro-7-hydroxy-2-methyl-4-oxo-4H-1-benzopyran-5-acetic acid	C12H12O5	M+H	237.0757	-1.1
237.1116	HMDB0140425	4-hydroxy-3-methoxy-5-(3-methylbut-2-en-1-yl)benzoic acid	C13H16O4	M+H	237.1121	-2.3
	HMDB0162477	2-[(3,5-dihydroxyphenyl)methyl]-6-methyloxan-4-one	C13H16O4	M+H	237.1121	-2.3
	HMDB0150433	3,5-dihydroxy-2-(hydroxymethyl)-4-(3-methylbut-2-en-1-yl)benzaldehyde	C13H16O4	M+H	237.1121	-2.3
	HMDB0150432	2,4-dihydroxy-6-(hydroxymethyl)-3-(3-methylbut-2-en-1-yl)benzaldehyde	C13H16O4	M+H	237.1121	-2.3
	HMDB0135908	2-hydroxy-2-[4-hydroxy-3-(3-methylbut-2-en-1-yl)phenyl]acetic acid	C13H16O4	M+H	237.1121	-2.3
	HMDB0124833	4-hydroxy-2-methoxy-3-(3-methylbut-2-en-1-yl)benzoic acid	C13H16O4	M+H	237.1121	-2.3
	HMDB0060564	Carboxy-ibuprofen	C13H16O4	M+H	237.1121	-2.3
	HMDB0037683	Ethyl vanillin isobutyrate	C13H16O4	M+H	237.1121	-2.3
237.1451	HMDB0000210	Pantothenic acid	C9H17NO5	M+NH4	237.1445	2.5
	HMDB0062717	Pantothenic acid	C9H17NO5	M+NH4	237.1445	2.5
	HMDB0182083	2-(3-{2,3-dimethyltricyclo[2.2.1]heptan-3-yl}propylidene)propane-1,3-diol	C15H24O2	M+H	237.1849	-2.6
	HMDB0166723	396--2	C15H24O2	M+H	237.1849	-2.6
	HMDB0137903	6-hydroxy-5,5,8a-trimethyl-2-methylidene-decahydronaphthalene-1-carbaldehyde	C15H24O2	M+H	237.1849	-2.6
	HMDB0150688	5-(hydroxymethyl)-1,1,4a,6-tetramethyl-1,2,3,4,4a,5,8,8a-octahydronaphthalen-2-one	C15H24O2	M+H	237.1849	-2.6
	HMDB0163044	(2Z)-5-(5-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl)-3-methylpent-2-enal	C15H24O2	M+H	237.1849	-2.6
	HMDB0166721	2,4-di-tert-butyl-6-methylbenzene-1,3-diol	C15H24O2	M+H	237.1849	-2.6
	HMDB0166722	UNII-7B7Y8CEM7E	C15H24O2	M+H	237.1849	-2.6
	HMDB0177916	4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-7-ol	C15H24O2	M+H	237.1849	-2.6

HMDB0177917	2-[(3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl)methylidene]propane-1,3-diol	C15H24O2	M+H	237.1849	-2.6
HMDB0177914	(2E)-3-[3-(hydroxymethyl)-7-methyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl]-2-methylprop-2-en-1-ol	C15H24O2	M+H	237.1849	-2.6
HMDB0177915	(2E)-3-[7-(hydroxymethyl)-3-methyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl]-2-methylprop-2-en-1-ol	C15H24O2	M+H	237.1849	-2.6
HMDB0182081	(2Z)-5-[3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-en-1-ol	C15H24O2	M+H	237.1849	-2.6
HMDB0182080	(2Z)-5-[2-(hydroxymethyl)-3-methyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-en-1-ol	C15H24O2	M+H	237.1849	-2.6
HMDB0182086	[3-(2-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl}ethyl)-2-methyloxiran-2-yl]methanol	C15H24O2	M+H	237.1849	-2.6
HMDB0182084	(2Z)-5-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-ene-1,4-diol	C15H24O2	M+H	237.1849	-2.6
HMDB0182082	(2Z)-5-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-ene-1,5-diol	C15H24O2	M+H	237.1849	-2.6
HMDB0182085	7-[(3Z)-5-hydroxy-4-methylpent-3-en-1-yl]-1,7-dimethyltricyclo[2.2.1,heptan-3-ol	C15H24O2	M+H	237.1849	-2.6
HMDB0182087	3-[(3Z)-5-hydroxy-4-methylpent-3-en-1-yl]-2,3-dimethyltricyclo[2.2.1,heptan-1-ol	C15H24O2	M+H	237.1849	-2.6
HMDB0179231	1,1,4,7-tetramethyl-1H,1aH,2H,3H,5H,6H,7H,7aH,7bH-cyclopropa[e]azulene-7,7b-diol	C15H24O2	M+H	237.1849	-2.6
HMDB0179230	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,7a-diol	C15H24O2	M+H	237.1849	-2.6
HMDB0177918	4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-2-ol	C15H24O2	M+H	237.1849	-2.6
HMDB0177919	4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-1-ol	C15H24O2	M+H	237.1849	-2.6
HMDB0177920	[3-(3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl)-2-methyloxiran-2-yl]methanol	C15H24O2	M+H	237.1849	-2.6
HMDB0179225	2-(hydroxymethyl)-1,1,5-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-ol	C15H24O2	M+H	237.1849	-2.6
HMDB0179224	1-(hydroxymethyl)-1,2,5-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-ol	C15H24O2	M+H	237.1849	-2.6
HMDB0179226	5-(hydroxymethyl)-1,1,2-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-ol	C15H24O2	M+H	237.1849	-2.6
HMDB0179228	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,6-diol	C15H24O2	M+H	237.1849	-2.6
HMDB0179229	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,3-diol	C15H24O2	M+H	237.1849	-2.6
HMDB0179227	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,4-diol	C15H24O2	M+H	237.1849	-2.6
HMDB0002352	Capsidiol	C15H24O2	M+H	237.1849	-2.6
HMDB0035827	Aubergenone	C15H24O2	M+H	237.1849	-2.6
HMDB0035040	7-Hydroxycostol	C15H24O2	M+H	237.1849	-2.6
HMDB0037393	(3xi,7(11)Z)-7(11)-Copaene-4,12-diol	C15H24O2	M+H	237.1849	-2.6
HMDB0035301	4alpha,5alpha-Epoxy-11-eudesmen-3a-ol	C15H24O2	M+H	237.1849	-2.6
HMDB0030916	2-Hydroxyacorenone	C15H24O2	M+H	237.1849	-2.6
HMDB0032048	2,6-Di-tert-butyl-4-hydroxymethylphenol	C15H24O2	M+H	237.1849	-2.6
HMDB0036680	Cyperolone	C15H24O2	M+H	237.1849	-2.6
HMDB0035032	Epilubimin	C15H24O2	M+H	237.1849	-2.6
HMDB0035127	(-)-Myrtenyl isovalerate	C15H24O2	M+H	237.1849	-2.6
HMDB0035648	Isolubimin	C15H24O2	M+H	237.1849	-2.6
HMDB0036446	(4alpha,alpha)-1(5),6-Guaiadiene	C15H24O2	M+H	237.1849	-2.6
HMDB0032681	alpha-4,5-Seco-11-eudesmene-4,5-dione	C15H24O2	M+H	237.1849	-2.6

	HMDB0031348	Epiacorone	C15H24O2	M+H	237.1849	-2.6
	HMDB0030891	(2E,6E)-1-Hydroxy-2,6,-farnesatrien-9-one	C15H24O2	M+H	237.1849	-2.6
	HMDB0039688	Tuberone	C15H24O2	M+H	237.1849	-2.6
	HMDB0035147	Rishitinone	C15H24O2	M+H	237.1849	-2.6
	HMDB0030920	Acorusnol	C15H24O2	M+H	237.1849	-2.6
	HMDB0039525	Isomelitic acid A	C15H24O2	M+H	237.1849	-2.6
	HMDB0036668	Humulene-8-hydroperoxide	C15H24O2	M+H	237.1849	-2.6
	HMDB0036687	Tanavulgarol	C15H24O2	M+H	237.1849	-2.6
	HMDB0038144	Petasitolone	C15H24O2	M+H	237.1849	-2.6
	HMDB0032292	Geranyl tiglate	C15H24O2	M+H	237.1849	-2.6
	HMDB0038122	5-Methyl-5-hexen-2-one	C15H24O2	M+H	237.1849	-2.6
	HMDB0038027	beta-Ionyl acetate	C15H24O2	M+H	237.1849	-2.6
	HMDB0034722	3-Hydroxy-1,-bisaboladien-9-one	C15H24O2	M+H	237.1849	-2.6
	HMDB0038178	Davanone	C15H24O2	M+H	237.1849	-2.6
	HMDB0036549	Apotrichothecene	C15H24O2	M+H	237.1849	-2.6
	HMDB0037906	Hernandulcin	C15H24O2	M+H	237.1849	-2.6
	HMDB0034714	Curdione	C15H24O2	M+H	237.1849	-2.6
	HMDB0033104	Calamensesquiterpinenol	C15H24O2	M+H	237.1849	-2.6
	HMDB0033083	(4S)-Dihydrocurcumenone	C15H24O2	M+H	237.1849	-2.6
	HMDB0040712	Humulene diepoxide A	C15H24O2	M+H	237.1849	-2.6
237.2207	HMDB0031851	3-(5,6,6-Trimethylbicyclo[2.2.1]hept-1-yl)cyclohexanol	C16H28O	M+H	237.2213	-2.5
	HMDB0036831	Ambrionide	C16H28O	M+H	237.2213	-2.5
238.1434	HMDB0151802	(2Z)-2-[(2-hydroxyphenyl)methylidene]hexanoic acid	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0151801	(2Z)-6-hydroxy-2-(phenylmethylidene)hexanoic acid	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0151797	(2Z)-2-[(3-hydroxyphenyl)methylidene]hexanoic acid	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0151800	2-butyl-3-phenyloxirane-2-carboxylic acid	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0151799	(2Z)-5-hydroxy-2-(phenylmethylidene)hexanoic acid	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0151798	(2Z)-2-[(4-hydroxyphenyl)methylidene]hexanoic acid	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0151796	(2Z)-3-hydroxy-2-(phenylmethylidene)hexanoic acid	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0132948	1-(4-methoxyphenyl)-4-methylpentane-2,3-dione	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0132939	4-hydroxy-1-(4-methoxyphenyl)-4-methylpent-1-en-3-one	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0132937	5-hydroxy-1-(4-methoxyphenyl)-4-methylpent-1-en-3-one	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0132936	1-[3-(4-methoxyphenyl)oxiran-2-yl]-2-methylpropan-1-one	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0132933	(1Z)-2-hydroxy-1-(4-methoxyphenyl)-4-methylpent-1-en-3-one	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0032589	1-(5-Acetyl-2-hydroxyphenyl)-3-methyl-1-butanone	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0132935	1-(2-hydroxy-4-methoxyphenyl)-4-methylpent-1-en-3-one	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0061942	cis-3-Hexenyl salicylate	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0061823	3-Hexenyl salicylic acid	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0040424	Ethyl 2-benzylacetoacetate	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0037492	Ethyl methyl-p-tolylglycidate	C13H16O3	M+NH4	238.1438	-1.5
	HMDB0164379	1-{4-[(2E)-4-methyl-5-oxoxolan-2-ylidene]butyl}pyrrolidin-2-one	C13H19NO3	M+H	238.1438	-1.5
238.1796	HMDB0133180	2-benzylheptanoic acid	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0126515	2-(phenylmethylidene)heptane-1,3-diol	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0126516	3-[(1Z)-3-hydroxy-2-pentylprop-1-en-1-yl]phenol	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0133170	2-[(2-hydroxyphenyl)methyl]heptanal	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0133169	2-benzyl-2-hydroxyheptanal	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0133168	2-benzyl-7-hydroxyheptanal	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0133166	2-[(4-hydroxyphenyl)methyl]heptanal	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0133167	2-benzyl-6-hydroxyheptanal	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0133164	2-[hydroxy(phenyl)methyl]heptanal	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0133165	2-[(3-hydroxyphenyl)methyl]heptanal	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0126518	(2Z)-2-(phenylmethylidene)heptane-1,6-diol	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0126519	(2-pentyl-3-phenyloxiran-2-yl)methanol	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0126520	(2Z)-2-(phenylmethylidene)heptane-1,7-diol	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0126517	4-[(1Z)-3-hydroxy-2-pentylprop-1-en-1-yl]phenol	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0037714	Hexyl phenylacetate	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0037718	2-Phenylethyl hexanoate	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0013817	2,6-Di-tert-butylbenzoquinone	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0040226	2-Methyl-1-phenyl-2-propanyl butyrate	C14H20O2	M+NH4	238.1802	-2.3

	HMDB0040217	3,4-Dihydro-2,2,5,7,8-pentamethyl-2H-1-benzopyran-6-ol	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0036389	3-Phenylpropyl isovalerate	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0037606	13-Nor-6-eremophilene-8,11-dione	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0038996	(Z)-6-Tetradecene-1,3-diyne-5,8-diol	C14H20O2	M+NH4	238.1802	-2.3
238.2161	HMDB0039539	13-Tetradecene-1,3-diyne-6,7-diol	C14H20O2	M+NH4	238.1802	-2.3
	HMDB0182057	5-{2,3-dimethyltricyclo[2.2.1,]heptan-3-yl}-2-methylpent-2-en-1-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0134152	2-benzyl-octan-1-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182054	[7-methyl-7-(4-methylpent-3-en-1-yl)tricyclo[2.2.1,heptan-1-yl]methanol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182055	[2-methyl-3-(4-methylpent-3-en-1-yl)tricyclo[2.2.1,heptan-3-yl]methanol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182874	4a-methyl-8-methylidene-2-(prop-1-en-2-yl)-decahydronaphthalen-2-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182875	2-(4a-methyl-8-methylidene-decahydronaphthalen-2-yl)-2-methyloxirane	C15H24O	M+NH4	238.2165	-1.8
	HMDB0036420	spathulenol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182154	1-(6-methylhept-5-en-2-yl)-4-methylidenebicyclo[3.1]hexan-6-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182155	6-methyl-2-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-5-en-1-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182153	5-(6-methylhept-5-en-2-yl)-2-methylidenebicyclo[3.1]hexan-1-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182056	1-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-4-methylpent-3-en-1-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182058	.alpha.-Santalol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182060	1,7-dimethyl-7-(4-methylpent-3-en-1-yl)tricyclo[2.2.1,heptan-3-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182059	1-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-4-methylpent-3-en-2-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182062	santal--en-2-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182147	6-methyl-2-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-5-en-2-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182150	2-methyl-6-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-2-en-4-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182148	1-(6-methylhept-5-en-2-yl)-4-methylidenebicyclo[3.1]hexan-3-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182149	2-methyl-6-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-2-en-1-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182151	1-(6-methylhept-5-en-2-yl)-4-methylidenebicyclo[3.1]hexan-2-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182152	2,2-dimethyl-3-(3-{4-methylidenebicyclo[3.1]hexan-1-yl}butyl)oxirane	C15H24O	M+NH4	238.2165	-1.8
	HMDB0035645	Epoxyguaiane	C15H24O	M+NH4	238.2165	-1.8
	HMDB0040763	Neocrimarine E	C15H24O	M+NH4	238.2165	-1.8
	HMDB0033826	2,6-Di-tert-butyl-4-methylphenol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0038123	1,5-Epoxy-4(14)-salvialene	C15H24O	M+NH4	238.2165	-1.8
	HMDB0038134	Bisabolene oxide	C15H24O	M+NH4	238.2165	-1.8
	HMDB0039532	(6Z,9Z,12Z)-6,9,12-Pentadecatrien-2-one	C15H24O	M+NH4	238.2165	-1.8
	HMDB0035718	Isocyperol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0038193	Isoshyobunone	C15H24O	M+NH4	238.2165	-1.8
	HMDB0036717	trans-beta-Santalol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0038208	Humuladienone	C15H24O	M+NH4	238.2165	-1.8
	HMDB0036788	beta-Betulenol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0038160	7(14)-Isodaucen--one	C15H24O	M+NH4	238.2165	-1.8
	HMDB0035020	Acolamone	C15H24O	M+NH4	238.2165	-1.8
	HMDB0037395	11-Copaen-4-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0035720	Isoacolamone	C15H24O	M+NH4	238.2165	-1.8
	HMDB0039711	Aromadendrene epoxide	C15H24O	M+NH4	238.2165	-1.8
	HMDB0036118	(3S,6E)-6-Caryophyllen-15-al	C15H24O	M+NH4	238.2165	-1.8
	HMDB0035306	Epishyobunone	C15H24O	M+NH4	238.2165	-1.8
	HMDB0034940	Mammea E/BB	C15H24O	M+NH4	238.2165	-1.8
	HMDB0030232	(2R,6S,7S,Z)-beta-Santala-3(15),-dien-12-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0036793	3,15-Epoxy-6-caryophyllene	C15H24O	M+NH4	238.2165	-1.8

	HMDB0035097	beta-Costol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0036789	Caryophyllene alpha-oxide	C15H24O	M+NH4	238.2165	-1.8
	HMDB0035704	Acorenone	C15H24O	M+NH4	238.2165	-1.8
	HMDB0037069	Acoragermacrone	C15H24O	M+NH4	238.2165	-1.8
	HMDB0034661	alpha-Valerenol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0038211	Humulenol I	C15H24O	M+NH4	238.2165	-1.8
	HMDB0036716	beta-Santalol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0038512	Bisacurool	C15H24O	M+NH4	238.2165	-1.8
	HMDB0035391	Preisocalamendiol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0038210	Humulene epoxide II	C15H24O	M+NH4	238.2165	-1.8
	HMDB0032220	Dihydronootkatone	C15H24O	M+NH4	238.2165	-1.8
	HMDB0037811	Vetiverol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0013688	Nootkatol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0059836	Cabreuva oxide D	C15H24O	M+NH4	238.2165	-1.8
	HMDB0034718	Isospathulenol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0060356	2-trans,6-trans-Farnesal	C15H24O	M+NH4	238.2165	-1.8
	HMDB0035026	alpha-Cyperol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0035793	Fukinone	C15H24O	M+NH4	238.2165	-1.8
	HMDB0038212	Humulenol II	C15H24O	M+NH4	238.2165	-1.8
	HMDB0035739	(R)-2,7(14),9-Bisabolatrien-11-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0038146	Calacone	C15H24O	M+NH4	238.2165	-1.8
	HMDB0036798	8alpha-3-Copaen-8-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0036402	alpha-Bergamotenol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0036192	Apritone	C15H24O	M+NH4	238.2165	-1.8
	HMDB0038119	Eremofukinone	C15H24O	M+NH4	238.2165	-1.8
	HMDB0038982	4-Nonylphenol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0037392	4(15)-Copaen-11-ol	C15H24O	M+NH4	238.2165	-1.8
	HMDB0060295	3,7,7,-tetramethyl-2-oxatetracyclo[7.3.2.0.0]dodecane	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182061	3-(2-{2,3-dimethyltricyclo[2.2.1]heptan-3-yl}ethyl)-2,2-dimethyloxirane	C15H24O	M+NH4	238.2165	-1.8
	HMDB0182873	[1-methylidene-7-(prop-1-en-2-yl)-decahydronaphthalen-4a-yl]methanol	C15H24O	M+NH4	238.2165	-1.8
239.0675	HMDB0148941	AKO226343	C13H12O3	M+Na	239.0679	-1.5
	HMDB0148933	4-hydroxy-6-styryl-5,6-dihydro-pyran-2-one	C13H12O3	M+Na	239.0679	-1.5
	HMDB0130033	3-[(1E)-4-hydroxybut-1-en-1-yl]-1H-isochromen-1-one	C13H12O3	M+Na	239.0679	-1.5
	HMDB0130030	3-[(1E)-but-1-en-1-yl]-6-hydroxy-1H-isochromen-1-one	C13H12O3	M+Na	239.0679	-1.5
	HMDB0130032	3-[(1E)-but-1-en-1-yl]-5-hydroxy-1H-isochromen-1-one	C13H12O3	M+Na	239.0679	-1.5
	HMDB0130029	3-[(1E)-but-1-en-1-yl]-7-hydroxy-1H-isochromen-1-one	C13H12O3	M+Na	239.0679	-1.5
	HMDB0130028	3-[(1E)-3-hydroxybut-1-en-1-yl]-1H-isochromen-1-one	C13H12O3	M+Na	239.0679	-1.5
	HMDB0130031	3-(3-ethyloxiran-2-yl)-1H-isochromen-1-one	C13H12O3	M+Na	239.0679	-1.5
	HMDB0013989	O-Desmethylnaproxen	C13H12O3	M+Na	239.0679	-1.5
	HMDB0038017	Ethyl 2-phenyl-3-furancarboxylate	C13H12O3	M+Na	239.0679	-1.5
	HMDB0037723	2-Phenylethyl 2-furancarboxylate	C13H12O3	M+Na	239.0679	-1.5
	HMDB0032656	(Z)-6-(2-Methoxyvinyl)-7-methyl-2H-1-benzopyran-2-one	C13H12O3	M+Na	239.0679	-1.5
	HMDB0030647	Artemidinol	C13H12O3	M+Na	239.0679	-1.5
	HMDB0032035	6-(3,4-Methylenedioxyphenyl)-3,5-hexadien-2-one	C13H12O3	M+Na	239.0679	-1.5
239.0944	HMDB0171051	{[1-(oxiran-2-yl)heptyl]oxy}sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0171055	[(9-hydroxynon-1-en-3-yl)oxy]sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0171054	[(7-hydroxynon-8-en-1-yl)oxy]sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0179179	[(4-oxononyl)oxy]sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0179823	[(8-oxononan-2-yl)oxy]sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0179827	[(2-oxononyl)oxy]sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0179825	[(8-oxononyl)oxy]sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0179829	[(2-oxononan-3-yl)oxy]sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0163492	[(2E)-2-hexylidene-3-hydroxypropoxy]sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0171048	[(8-hydroxynon-1-en-3-yl)oxy]sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0163508	{[(2Z)-8-hydroxy-2-methyloct-2-en-1-yl]oxy}sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0163507	{[(6Z)-8-hydroxy-7-methyloct-6-en-1-yl]oxy}sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0163504	[(2-methyl-3-pentyloxiran-2-yl)methoxy]sulfonic acid	C9H18O5S	M+H	239.0948	-1.6

	HMDB0163501	{[(6Z)-8-hydroxy-7-methyloct-6-en-2-yl]oxy}sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0163500	{[(2Z)-7-hydroxy-2-methyloct-2-en-1-yl]oxy}sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0163497	{[(2Z)-1-hydroxy-2-methyloct-2-en-4-yl]oxy}sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0163493	[(2Z)-2-hexylidene-3-hydroxypropoxy]sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0163496	{[(2Z)-4-hydroxy-2-methyloct-2-en-1-yl]oxy}sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
	HMDB0171047	[(7-hydroxynon-8-en-2-yl)oxy]sulfonic acid	C9H18O5S	M+H	239.0948	-1.6
239.1395	HMDB0014562	Secobarbital	C12H18N2O3	M+H	239.1390	2.0
	HMDB0139940	N-(3-aminopropyl)-3-(3,4-dihydroxyphenyl)propanimidic acid	C12H18N2O3	M+H	239.1390	2.0
	HMDB0014798	Metaxalone	C12H15NO3	M+NH4	239.1390	2.0
	HMDB0031770	Carbofuran	C12H15NO3	M+NH4	239.1390	2.0
	HMDB0033701	Hydrocotarnine	C12H15NO3	M+NH4	239.1390	2.0
	HMDB0139892	3-(4-hydroxyphenyl)-N-(3-oxopropyl)propanimidic	C12H15NO3	M+NH4	239.1390	2.0
239.1640	HMDB0112083	3-(3,4-dimethyl-5-pentylfuran-2-yl)-propanoic acid	C14H22O3	M+H	239.1642	-0.7
	HMDB0038256	Geranyl acetoacetate	C14H22O3	M+H	239.1642	-0.7
239.2002	HMDB0182767	2-(1-hydroxypropan-2-yl)-4a-methyl-8-methylidene-decahydronaphthalen-1-ol	C15H26O2	M+H	239.2006	-1.5
	HMDB0182764	4a-(hydroxymethyl)-8-methylidene-2-(propan-2-yl)-decahydronaphthalen-1-ol	C15H26O2	M+H	239.2006	-1.5
	HMDB0182219	7-(2-hydroxypropan-2-yl)-1,8a-dimethyl-1,2,3,5,6,7,8,8a-octahydronaphthalen-1-ol	C15H26O2	M+H	239.2006	-1.5
	HMDB0182220	3-(2-hydroxypropan-2-yl)-4a,5-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalen-1-ol	C15H26O2	M+H	239.2006	-1.5
	HMDB0182221	6-(2-hydroxypropan-2-yl)-4,4a-dimethyl-2,3,4,4a,5,6,7,8-octahydronaphthalen-2-ol	C15H26O2	M+H	239.2006	-1.5
	HMDB0182218	2-[8-(hydroxymethyl)-8a-methyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl]propan-2-ol	C15H26O2	M+H	239.2006	-1.5
	HMDB0182217	2-[8a-(hydroxymethyl)-8-methyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl]propan-2-ol	C15H26O2	M+H	239.2006	-1.5
	HMDB0179265	2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O2	M+H	239.2006	-1.5
	HMDB0041589	alpha-Kessyl alcohol	C15H26O2	M+H	239.2006	-1.5
	HMDB0062130	methyl tetradec-13-ynoate	C15H26O2	M+H	239.2006	-1.5
	HMDB0036730	Tricyclohumuladiol	C15H26O2	M+H	239.2006	-1.5
	HMDB0038196	alpha-Bisabolol oxide A	C15H26O2	M+H	239.2006	-1.5
	HMDB0037284	5(1->)-Abeo-1,12-patchoulanediol	C15H26O2	M+H	239.2006	-1.5
	HMDB0036880	1,6,9-Farnesatriene-3,11-diol	C15H26O2	M+H	239.2006	-1.5
	HMDB0037279	2,-Bisaboladiene-1,4-diol	C15H26O2	M+H	239.2006	-1.5
	HMDB0034673	Calamendiol	C15H26O2	M+H	239.2006	-1.5
	HMDB0031383	(3S,4S,6R,7S)-1,-Bisaboladiene-3,4-diol	C15H26O2	M+H	239.2006	-1.5
	HMDB0038250	Isobornyl isovalerate	C15H26O2	M+H	239.2006	-1.5
	HMDB0033228	Guaidiol	C15H26O2	M+H	239.2006	-1.5
	HMDB0036032	3beta-7-Drimene-3,11-diol	C15H26O2	M+H	239.2006	-1.5
	HMDB0031384	beta-Kessyl alcohol	C15H26O2	M+H	239.2006	-1.5
	HMDB0035887	Germacrenone	C15H26O2	M+H	239.2006	-1.5
	HMDB0039130	Methyl (Z,Z)-5,8-tetradecadienoate	C15H26O2	M+H	239.2006	-1.5
	HMDB0038247	Bornyl valerate	C15H26O2	M+H	239.2006	-1.5
	HMDB0040273	Terpenyl isovalerate	C15H26O2	M+H	239.2006	-1.5
	HMDB0032343	Isobornyl 2-methylbutyrate	C15H26O2	M+H	239.2006	-1.5
	HMDB0032209	Citronellyl trans-2-methyl-2-butenate	C15H26O2	M+H	239.2006	-1.5
	HMDB0032291	Geranyl 2-methylbutyrate	C15H26O2	M+H	239.2006	-1.5
	HMDB0035287	Daucol	C15H26O2	M+H	239.2006	-1.5
	HMDB0038136	Curcumadiol	C15H26O2	M+H	239.2006	-1.5
	HMDB0038138	alpha-Bisabolol oxide C	C15H26O2	M+H	239.2006	-1.5
	HMDB0038197	alpha-Bisabolol oxide B	C15H26O2	M+H	239.2006	-1.5
	HMDB0030428	Linalyl isovalerate	C15H26O2	M+H	239.2006	-1.5
	HMDB0037195	2-Propenyl cyclohexanhexanoate	C15H26O2	M+H	239.2006	-1.5
	HMDB0040281	Geranyl valerate	C15H26O2	M+H	239.2006	-1.5
	HMDB0029350	Geranyl 3-methylbutanoate	C15H26O2	M+H	239.2006	-1.5
	HMDB0032054	alpha-Terpinyol pentanoate	C15H26O2	M+H	239.2006	-1.5

	HMDB0038248	Bornyl isovalerate	C15H26O2	M+H	239.2006	-1.5
	HMDB0039745	(2E,6E,9xi)-Farnesol	C15H26O2	M+H	239.2006	-1.5
	HMDB0182766	4a-methyl-8-methylidene-2-(propan-2-yl)-decahydronaphthalene-1,7-diol	C15H26O2	M+H	239.2006	-1.5
	HMDB0182222	2-(8,8a-dimethyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl)propane-1,2-diol	C15H26O2	M+H	239.2006	-1.5
	HMDB0182765	2-(2-hydroxypropan-2-yl)-4a-methyl-8-methylidene-decahydronaphthalen-1-ol	C15H26O2	M+H	239.2006	-1.5
239.2365	HMDB0060482	Hexadecenal	C16H30O	M+H	239.2369	-1.8
	HMDB0034181	3-Methylcyclopentadecanone	C16H30O	M+H	239.2369	-1.8
	HMDB0037544	2-Dodecylcyclobutanone	C16H30O	M+H	239.2369	-1.8
240.0909	HMDB0174725	[(1E)-3-(butan-2-ylsulfanyl)prop-1-en-1-yl]dimethylsulfanium	C9H19S3	M+NH4	240.0909	0.0
	HMDB0033072	(E)-1-Propenyl 1-(propylthio)propyl disulfide	C9H18S3	M+NH4	240.0909	0.1
	HMDB0033041	1-(1-Propenylthio)propyl propyl disulfide	C9H18S3	M+NH4	240.0909	0.1
	HMDB0040262	2,4,6-Triethyl-1,3,5-trithiane	C9H18S3	M+NH4	240.0909	0.1
	HMDB0040243	2,2,4,4,6,6-Hexamethyl-1,3,5-trithiane	C9H18S3	M+NH4	240.0909	0.1
240.1232	HMDB0135689	4-(4-hydroxy-3,5-dimethoxyphenyl)but-3-en-2-one	C12H14O4	M+NH4	240.1230	0.7
	HMDB0135906	3,4-dihydroxy-5-(3-methylbut-2-en-1-yl)benzoic acid	C12H14O4	M+NH4	240.1230	0.7
	HMDB0164056	4-(2-hydroxy-3-oxobutyl)phenyl acetate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0164058	4-(1-hydroxy-3-oxobutyl)phenyl acetate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0170845	2-methoxy-4-[(oxiran-2-yl)methyl]phenyl acetate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0170846	2-methoxy-4-(prop-2-en-1-yl)phenyl 2-hydroxyacetate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0170974	4-[(1Z)-3-hydroxyprop-1-en-1-yl]-2-methoxyphenyl acetate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0170976	3-hydroxy-2-methoxy-4-[(1Z)-prop-1-en-1-yl]phenyl acetate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0170977	5-hydroxy-2-methoxy-4-[(1Z)-prop-1-en-1-yl]phenyl acetate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0170978	1-acetoxy-2-methoxy-4-(3-methyl-oxiranyl)-benzene	C12H14O4	M+NH4	240.1230	0.7
	HMDB0170979	2-methoxy-4-[(1Z)-prop-1-en-1-yl]phenyl 2-hydroxyacetate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0164057	4-(4-hydroxy-3-oxobutyl)phenyl acetate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0164055	4-(3-oxobutyl)phenyl 2-hydroxyacetate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0135904	3-[(3,3-dimethyloxiran-2-yl)methyl]-4-hydroxybenzoic acid	C12H14O4	M+NH4	240.1230	0.7
	HMDB0127824	5-[(3-hydroxy-4-methoxyphenyl)methyl]oxolan-2-one	C12H14O4	M+NH4	240.1230	0.7
	HMDB0131281	2-Hydroxy-3-(4-methoxyphenyl)propenoic acid ethyl ester	C12H14O4	M+NH4	240.1230	0.7
	HMDB0131283	ethyl (2E)-3-(2-hydroxy-4-methoxyphenyl)prop-2-enoate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0131285	2-hydroxyethyl (2E)-3-(4-methoxyphenyl)prop-2-enoate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0131284	ethyl 3-(4-methoxyphenyl)oxirane-2-carboxylate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0135900	4-hydroxy-3-(4-hydroxy-3-methylbut-2-en-1-yl)benzoic acid	C12H14O4	M+NH4	240.1230	0.7
	HMDB0135902	4-hydroxy-3-(4-hydroxy-3-methylbut-2-en-1-yl)benzoic acid	C12H14O4	M+NH4	240.1230	0.7
	HMDB0094660	Diethyl phthalic acid	C12H14O4	M+NH4	240.1230	0.7
	HMDB0002056	Monoisobutyl phthalic acid	C12H14O4	M+NH4	240.1230	0.7
	HMDB0038563	(Z)-3-(2,4,5-Trimethoxyphenyl)-2-propenal	C12H14O4	M+NH4	240.1230	0.7
	HMDB0041379	2,3-Dihydro-3-hydroxy-6-methoxy-2,2-dimethyl-4H-1-benzopyran-4-one	C12H14O4	M+NH4	240.1230	0.7
	HMDB0033776	Apiole	C12H14O4	M+NH4	240.1230	0.7
	HMDB0031668	Dihydrodeoxy-8-epiaustdiol	C12H14O4	M+NH4	240.1230	0.7
	HMDB0034056	5-(3,4-Methylenedioxyphenyl)pentanoic acid	C12H14O4	M+NH4	240.1230	0.7
	HMDB0037681	Vanillin isobutyrate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0029470	Isodillapiole	C12H14O4	M+NH4	240.1230	0.7
	HMDB0037130	Piperonyl isobutyrate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0030725	Dillapiol	C12H14O4	M+NH4	240.1230	0.7
	HMDB0013247	Monobutylphthalate	C12H14O4	M+NH4	240.1230	0.7
	HMDB0029226	5'-(3'-Methoxy-4'-hydroxyphenyl)-gamma-valerolactone	C12H14O4	M+NH4	240.1230	0.7
	HMDB0035593	Rishitin	C14H22O2	M+NH4	240.1958	-2.5
	HMDB0036790	Kobusone	C14H22O2	M+NH4	240.1958	-2.5

240.1952	HMDB0036791	Isokobusone	C14H22O2	M+NH4	240.1958	-2.5
	HMDB0037820	Acetaldehyde butyl phenethyl acetal	C14H22O2	M+NH4	240.1958	-2.5
	HMDB0040178	2,6-Di-tert-butyl-1,4-benzenediol	C14H22O2	M+NH4	240.1958	-2.5
	HMDB0037605	(betaH,11xi)-11-Hydroxy-13-nor-6-eremophilen-8-one	C14H22O2	M+NH4	240.1958	-2.5
240.2319	HMDB0036197	(-)-alpha-Bisabolol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0041575	Isokessane	C15H26O	M+NH4	240.2322	-1.2
	HMDB0036452	alpha-cadinol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0041629	(3S,6E)-nerolidol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0036646	Cedrelanol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0036445	Bulnesol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0035662	Nerolidol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0036579	Carotol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0035711	Panasinsanol A	C15H26O	M+NH4	240.2322	-1.2
	HMDB0039744	Ginsenosol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0037066	beta-Caryophyllene alcohol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0036679	Faurinone	C15H26O	M+NH4	240.2322	-1.2
	HMDB0059841	Cubenol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0036908	Sesquicineol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0038167	Maaliol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0038213	Humulol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0036447	Guaioxide	C15H26O	M+NH4	240.2322	-1.2
	HMDB0030938	beta-Triticene	C15H26O	M+NH4	240.2322	-1.2
	HMDB0036645	Globulol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0035199	Sesquisabinene hydrate	C15H26O	M+NH4	240.2322	-1.2
	HMDB0036732	Licoagroaurone	C15H26O	M+NH4	240.2322	-1.2
	HMDB0037031	Epicubenol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0033239	Pogostol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0035351	4beta-8-Daucen-4-ol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0037394	p-Hydroxynonanophenone	C15H26O	M+NH4	240.2322	-1.2
	HMDB0036642	Isointermedeol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0036198	(+)-alpha-Bisabolol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0035021	(-)-Pacifigorgiol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0035364	6-Epi-beta-bisabolol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0004305	Farnesol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0039538	(6Z,9Z)-6,9-Pentadecadien-2-one	C15H26O	M+NH4	240.2322	-1.2
	HMDB0059849	(Z)-Farnesol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0035663	(S)-Nerolidol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0036421	(-)-Valeranone	C15H26O	M+NH4	240.2322	-1.2
	HMDB0037234	Koraiol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0034982	-Epijunenol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0040422	Chamomillol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0037067	Zingiberenol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0030939	alpha-Triticene	C15H26O	M+NH4	240.2322	-1.2
	HMDB0035383	Panasinsanol B	C15H26O	M+NH4	240.2322	-1.2
	HMDB0035811	Shyobunol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0034951	Valerianol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0036580	5,8-Epoxydaucane	C15H26O	M+NH4	240.2322	-1.2
	HMDB0035868	Rosifoliol	C15H26O	M+NH4	240.2322	-1.2
	HMDB0036111	beta-Bisabolol	C15H26O	M+NH4	240.2322	-1.2
241.0737	HMDB0032937	Methyl 4-chloro-1H-indole-3-acetate	C11H10ClNO2	M+NH4	241.0738	-0.5
	HMDB0172053	{2-[(3-methylpentanoyl)oxy]ethoxy}sulfonic acid	C8H16O6S	M+H	241.0740	-1.4
	HMDB0172055	[(1-ethoxy-3-methyl-1-oxopentan-2-yl)oxy]sulfonic acid	C8H16O6S	M+H	241.0740	-1.4
	HMDB0172049	[(5-ethoxy-3-methyl-5-oxopentyl)oxy]sulfonic acid	C8H16O6S	M+H	241.0740	-1.4
	HMDB0172051	(4-ethoxy-2-ethyl-4-oxobutoxy)sulfonic acid	C8H16O6S	M+H	241.0740	-1.4
	HMDB0172047	[(5-ethoxy-3-methyl-5-oxopentan-2-yl)oxy]sulfonic acid	C8H16O6S	M+H	241.0740	-1.4
	HMDB0164652	[(6-hydroxy-8-oxooctan-2-yl)oxy]sulfonic acid	C8H16O6S	M+H	241.0740	-1.4
	HMDB0164651	[(7-hydroxy-1-oxooctan-3-yl)oxy]sulfonic acid	C8H16O6S	M+H	241.0740	-1.4
	HMDB0161161	2-(sulfooxy)octanoic acid	C8H16O6S	M+H	241.0740	-1.4
	HMDB0159453	82542-98-1	C8H16O6S	M+H	241.0740	-1.4
	HMDB0032369	L-Menthyl acetoacetate	C14H24O3	M+H	241.1798	-1.7
	HMDB0160292	4-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}butanoic acid	C14H24O3	M+H	241.1798	-1.7
	HMDB0160289	(5Z,8Z)-4-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M+H	241.1798	-1.7

241.1794	HMDB0160291	SCHEMBL8918721	C14H24O3	M+H	241.1798	-1.7
	HMDB0160290	(8Z)--hydroxytetradeca-5,8-dienoic acid	C14H24O3	M+H	241.1798	-1.7
	HMDB0160293	(5Z)-7-(3-pentyloxiran-2-yl)hept-5-enoic acid	C14H24O3	M+H	241.1798	-1.7
	HMDB0160295	(5Z,8Z)-2-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M+H	241.1798	-1.7
	HMDB0160296	(5Z,8Z)-7-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M+H	241.1798	-1.7
	HMDB0160294	(5Z,8Z)-14-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M+H	241.1798	-1.7
	HMDB0160298	(8Z)-5-hydroxytetradeca-6,8-dienoic acid	C14H24O3	M+H	241.1798	-1.7
241.2156	HMDB0160297	(5Z,7E)-9-hydroxytetradeca-5,7-dienoic acid	C14H24O3	M+H	241.1798	-1.7
	HMDB0032347	Isobutyl -undecenoate	C15H28O2	M+H	241.2162	-2.5
	HMDB0037190	Rhodinyl isovalerate	C15H28O2	M+H	241.2162	-2.5
	HMDB0039715	Auberganol	C15H28O2	M+H	241.2162	-2.5
	HMDB0034455	Exaltolide	C15H28O2	M+H	241.2162	-2.5
	HMDB0036426	Butyl undecylenate	C15H28O2	M+H	241.2162	-2.5
	HMDB0038954	Citronellyl isovalerate	C15H28O2	M+H	241.2162	-2.5
	HMDB0037211	Menthyl isovalerate	C15H28O2	M+H	241.2162	-2.5
	HMDB0037229	Citronellyl pentanoate	C15H28O2	M+H	241.2162	-2.5
242.1745	HMDB0040997	15,5-Farnesanolide	C15H28O2	M+H	241.2162	-2.5
	HMDB0029765	9-Pentadecenoic acid	C15H28O2	M+H	241.2162	-2.5
	HMDB0163216	(2E,4E)-6-(3-pentyloxiran-2-yl)hexa-2,4-dienoic acid	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0163215	(2E)-3-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}prop-2-enoic acid	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0163211	(2E,4E,7Z)-13-hydroxytrideca-2,4,7-trienoic acid	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0163213	(2E,4E,7Z)-9-hydroxytrideca-2,4,7-trienoic acid	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0163214	3-[(1E,4Z)-deca-1,4-dien-1-yl]oxirane-2-carboxylic acid	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0163210	(2E,4E,7Z)-12-hydroxytrideca-2,4,7-trienoic acid	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0112084	3-(3-methyl-5-pentylfuran-2-yl)propanoic acid	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0037730	Furfuryl octanoate	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0037726	Octyl 2-furoate	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0036583	Methyl jasmonate	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0032679	Annuionone A	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0037736	3-Methylbutyl 2-furanbutanoate	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0034564	13-Oxo-9,11-tridecadienoic acid	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0032689	Annuionone C	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0029670	Epoxyeremopetasinorol	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0037244	(8alpha,beta,11beta)-3-Hydroxy-4,15-dinor-1(5)-xanthen-12,8-olide	C13H20O3	M+NH4	242.1751	-2.3
	HMDB0038588	Dioscoretine	C13H23NO3	M+H	242.1751	-2.4
242.2110	HMDB0030427	Linalyl butyrate	C14H24O2	M+NH4	242.2115	-1.9
	HMDB0038260	Geranyl 2-methylpropanoate	C14H24O2	M+NH4	242.2115	-1.9
	HMDB0038246	Bornyl butyrate	C14H24O2	M+NH4	242.2115	-1.9
	HMDB0037814	2-Propenyl cyclohexanepentanoate	C14H24O2	M+NH4	242.2115	-1.9
	HMDB0030426	Linalyl isobutyrate	C14H24O2	M+NH4	242.2115	-1.9
	HMDB0031015	Ethyl (2E,6Z)-dodecadienoate	C14H24O2	M+NH4	242.2115	-1.9
	HMDB0038259	Neryl butyrate	C14H24O2	M+NH4	242.2115	-1.9
	HMDB0032524	Terpinyl isobutyrate	C14H24O2	M+NH4	242.2115	-1.9
	HMDB0036424	Allyl undecylenate	C14H24O2	M+NH4	242.2115	-1.9
	HMDB0032053	alpha-Terpineol butanoate	C14H24O2	M+NH4	242.2115	-1.9
	HMDB0032342	Isobornyl isobutyrate	C14H24O2	M+NH4	242.2115	-1.9
	HMDB0000560	Goshuyic acid	C14H24O2	M+NH4	242.2115	-1.9
	HMDB0039129	Goshuyic acid	C14H24O2	M+NH4	242.2115	-1.9
242.2474	HMDB0031111	5,-Pentadecadien-1-ol	C15H28O	M+NH4	242.2478	-1.8
	HMDB0040377	3-Pentadecenal	C15H28O	M+NH4	242.2478	-1.8
	HMDB0032218	(+/-)-Dihydrofarnesol	C15H28O	M+NH4	242.2478	-1.8
244.0929	HMDB0015122	Cytarabine	C9H13N3O5	M+H	244.0928	0.4
	HMDB0155273	Cytarabine	C9H13N3O5	M+H	244.0928	0.4
	HMDB0060478	gamma-Glutamyl-beta-cyanoalanine	C9H13N3O5	M+H	244.0928	0.4
	HMDB0000089	Cytidine	C9H13N3O5	M+H	244.0928	0.4
	HMDB0001904	3-Nitrotyrosine	C9H10N2O5	M+NH4	244.0928	0.4
244.1538	HMDB0059729	3,4-Methylenesecbacic acid	C12H18O4	M+NH4	244.1543	-2.2
	HMDB0040705	Allixin	C12H18O4	M+NH4	244.1543	-2.2
	HMDB0002366	Tiglylcarnitine	C12H21NO4	M+H	244.1543	-2.2
244.1901	HMDB0176430	(9E)-13-oxotridec-9-enoic acid	C13H22O3	M+NH4	244.1907	-2.5
	HMDB0176431	(9E,11E)-13-hydroxytrideca-9,11-dienoic acid	C13H22O3	M+NH4	244.1907	-2.5
	HMDB0037562	Riesling acetal	C13H22O3	M+NH4	244.1907	-2.5

244.1701	HMDB0040615	4,5-Dihydrovomifoliol	C13H22O3	M+NH4	244.1907	-2.5
	HMDB0031740	Methyl dihydrojasmonate	C13H22O3	M+NH4	244.1907	-2.5
	HMDB0013286	N-Undecanoylglycine	C13H25NO3	M+H	244.1907	-2.5
244.2266	HMDB0062248	(9E)-tetradecenoic acid	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0094671	cyclohexyl octanoate	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0062243	cis-tetradec-7-enoic acid	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0000499	5-Tetradecenoic acid	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0040228	1,1-Diethoxy-3,7-dimethyl-2,6-octadiene	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0037633	xi-Tetrahydro-3-nonyl-2H-pyran-2-one	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0031029	Ethyl (E)-2-dodecenoate	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0030921	(R)-14-Methyloxacyclotetradecan-2-one	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0037228	Citronellyl isobutyrate	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0037369	Butyl 2-decenoate	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0037227	Citronellyl butyrate	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0037189	Rhodinyl isobutyrate	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0037188	Rhodinyl butyrate	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0031073	12-Methyl-13-tridecanolide	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0034561	Houttuynin	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0010732	trans-Tetra-dec-2-enoic acid	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0032321	2-Hexenyl octanoate	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0000521	5Z-Tetradecenoic acid	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0002000	Myristoleic acid	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0005051	Tsuzuic acid	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0061991	Menthyl butyrate	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0032152	Acetaldehyde di-cis-3-hexenyl acetal	C14H26O2	M+NH4	244.2271	-2.1
	HMDB0038056	delta-Tetradecalactone	C14H26O2	M+NH4	244.2271	-2.1
244.2630	HMDB0031078	Pentadecanal	C15H30O	M+NH4	244.2635	-2.0
	HMDB0061956	Z--Pentadecen-1-ol	C15H30O	M+NH4	244.2635	-2.0
	HMDB0059813	Heptyl ketone	C15H30O	M+NH4	244.2635	-2.0
	HMDB0031081	2-Pentadecanone	C15H30O	M+NH4	244.2635	-2.0
245.0762	HMDB0180914	2,4,6-trihydroxy-7-methoxy-3,4-dihydro-2H-1,4-benzoxazin-3-one	C9H9NO6	M+NH4	245.0768	-2.5
	HMDB0125157	2-{[hydroxy(2,4,6-trihydroxyphenyl)methylidene]amino}acetic acid	C9H9NO6	M+NH4	245.0768	-2.5
	HMDB0126635	2-{[hydroxy(3,4,5-trihydroxyphenyl)methylidene]amino}acetic acid	C9H9NO6	M+NH4	245.0768	-2.5
	HMDB0130466	2-{[hydroxy(2,3,4-trihydroxyphenyl)methylidene]amino}acetic acid	C9H9NO6	M+NH4	245.0768	-2.5
	HMDB0130477	2-{[hydroxy(2,4,5-trihydroxyphenyl)methylidene]amino}acetic acid	C9H9NO6	M+NH4	245.0768	-2.5
	HMDB0155302	[(3,4-dihydroxy-5-methoxyphenyl)(hydroxy)methylidene]carbamic acid	C9H9NO6	M+NH4	245.0768	-2.5
	HMDB0157259	[(2,3-dihydroxy-4-methoxyphenyl)(hydroxy)methylidene]carbamic acid	C9H9NO6	M+NH4	245.0768	-2.5
	HMDB0157260	[(2,5-dihydroxy-4-methoxyphenyl)(hydroxy)methylidene]carbamic acid	C9H9NO6	M+NH4	245.0768	-2.5
	HMDB0166885	[(3,5-dihydroxy-4-methoxyphenyl)(hydroxy)methylidene]carbamic acid	C9H9NO6	M+NH4	245.0768	-2.5
	HMDB0177249	[hydroxy(2,3,4-trihydroxy-6-methylphenyl)methylidene]carbamic acid	C9H9NO6	M+NH4	245.0768	-2.5
	HMDB0006794	5-(2'-Carboxyethyl)-4,6-Dihydroxypicolinate	C9H9NO6	M+NH4	245.0768	-2.5
	HMDB0000296	Uridine	C9H12N2O6	M+H	245.0768	-2.5
	HMDB0156330	Uridine	C9H12N2O6	M+H	245.0768	-2.5
	HMDB0000767	Pseudouridine	C9H12N2O6	M+H	245.0768	-2.5
245.1741	HMDB0002327	1,11-Undecanedicarboxylic acid	C13H24O4	M+H	245.1747	-2.6
	HMDB0037184	1,4-Nonanediol diacetate	C13H24O4	M+H	245.1747	-2.6
	HMDB0036141	Menthyl ethylene glycol carbonate	C13H24O4	M+H	245.1747	-2.6
245.9523	HMDB0040147	2-Bromo-1H-indole-3-carboxaldehyde	C9H6BrNO	M+Na	245.9525	-0.8
	HMDB0181331	{[5-(pyridin-2-yl)pentyl]oxy}sulfonic acid	C10H15NO4S	M+H	246.0795	0.6
	HMDB0181329	{[5-(pyridin-2-yl)pentan-2-yl]oxy}sulfonic acid	C10H15NO4S	M+H	246.0795	0.6
	HMDB0181244	{[1-(pyridin-3-yl)pentyl]oxy}sulfonic acid	C10H15NO4S	M+H	246.0795	0.6

246.0796	HMDB0181242	{[5-(pyridin-3-yl)pentyl]oxy}sulfonic acid	C10H15NO4S	M+H	246.0795	0.6
	HMDB0181240	{[5-(pyridin-3-yl)pentan-2-yl]oxy}sulfonic acid	C10H15NO4S	M+H	246.0795	0.6
	HMDB0133620	{[(2E)-2-methyl-3-phenylprop-2-en-1-yl]oxy}sulfonic acid	C10H12O4S	M+NH4	246.0795	0.6
	HMDB0133731	{[(3E)-4-phenylbut-3-en-2-yl]oxy}sulfonic acid	C10H12O4S	M+NH4	246.0795	0.6
	HMDB0180488	{[2-(4-methylphenyl)prop-2-en-1-yl]oxy}sulfonic acid	C10H12O4S	M+NH4	246.0795	0.6
246.1694	HMDB0164279	2-[2-(4-hydroxypentyl)-3-oxocyclopentyl]acetic acid	C12H20O4	M+NH4	246.1700	-2.4
	HMDB0164282	2-(4-hydroxy-3-oxo-2-pentylcyclopentyl)acetic acid	C12H20O4	M+NH4	246.1700	-2.4
	HMDB0164284	2-(2-hydroxy-3-oxo-2-pentylcyclopentyl)acetic acid	C12H20O4	M+NH4	246.1700	-2.4
	HMDB0164283	2-hydroxy-2-(3-oxo-2-pentylcyclopentyl)acetic acid	C12H20O4	M+NH4	246.1700	-2.4
	HMDB0164280	2-(5-hydroxy-3-oxo-2-pentylcyclopentyl)acetic acid	C12H20O4	M+NH4	246.1700	-2.4
	HMDB0030994	5-Heptyltetrahydro-2-oxo-3-furancarboxylic acid	C12H20O4	M+NH4	246.1700	-2.4
	HMDB0000933	Traumatic acid	C12H20O4	M+NH4	246.1700	-2.4
	HMDB0164281	2-[2-(5-hydroxypentyl)-3-oxocyclopentyl]acetic acid	C12H20O4	M+NH4	246.1700	-2.4
	HMDB0000688	Isovalerylcarnitine	C12H23NO4	M+H	246.1700	-2.4
	HMDB0041993	Pivaloylcarnitine	C12H23NO4	M+H	246.1700	-2.4
	HMDB0000378	2-Methylbutyrylcarnitine	C12H23NO4	M+H	246.1700	-2.4
	HMDB0013128	Valerylcarnitine	C12H24NO4	M+H	246.1700	-2.4
246.2057	HMDB0035881	11-Hydroxy-9-tridecanoic acid	C13H24O3	M+NH4	246.2064	-2.7
	HMDB0040004	Menthone 1,3-glyceryl ketal	C13H24O3	M+NH4	246.2064	-2.7
	HMDB0037212	Menthyl lactate	C13H24O3	M+NH4	246.2064	-2.7
	HMDB0036139	Menthone 1,2-glyceryl ketal	C13H24O3	M+NH4	246.2064	-2.7
246.2422	HMDB0172395	2-hydroxy-tetradecaldehyde	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0176318	1-hydroxytetradecan-3-one	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0172394	SCHEMBL1959824	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0172393	SCHEMBL4937612	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0033788	Ethyl dodecanoate	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0034461	Heptyl heptanoate	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0037495	3-Methylbutyl nonanoate	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0038034	Nonyl isovalerate	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0031072	12-Methyltridecanoic acid	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0037312	Decyl butanoate	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0036216	Hexyl octanoate	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0002221	2,6,-Trimethylundecanoic acid	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0038969	Dodecyl acetate	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0032318	Hexanal octane-1,3-diol acetal	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0032548	Undecanal propyleneglycol acetal	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0061781	-Methyltridecanoic acid	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0059865	Isobutyl decanoate	C14H28O2	M+NH4	246.2428	-2.2
	HMDB0000806	Myristic acid	C14H28O2	M+NH4	246.2428	-2.2
247.1650	HMDB0013126	Butenylcarnitine	C11H19NO4	M+NH4	247.1652	-0.9
247.2050	HMDB0040373	Ginsenoside J	C17H26O	M+H	247.2056	-2.6
	HMDB0165432	(4E,9E)-heptadeca-4,9-dien-6-yn-3-one	C17H26O	M+H	247.2056	-2.6
	HMDB0165433	(9E)-heptadeca-1,9-dien-6-yn-3-one	C17H26O	M+H	247.2056	-2.6
	HMDB0030927	Isoavocadienofuran	C17H26O	M+H	247.2056	-2.6
	HMDB0030933	Avocadynofuran	C17H26O	M+H	247.2056	-2.6
	HMDB0030926	Avocadienofuran	C17H26O	M+H	247.2056	-2.6
248.0522	HMDB0037264	2-Hydroxy-4,7-dimethoxy-2H-1,4-benzoxazin-3(4H)-one	C10H11NO5	M+Na	248.0529	-3.0
	HMDB0150448	2-({(2,4-dihydroxy-6-methylphenyl)(hydroxy)methylidene}amino}acetic acid	C10H11NO5	M+Na	248.0529	-3.0
	HMDB0150500	2-({hydroxy[2-hydroxy-6-(hydroxymethyl)phenyl]methylidene}amino}acetic acid	C10H11NO5	M+Na	248.0529	-3.0
	HMDB0154376	2-({[hydroxy(2-hydroxy-3-methoxyphenyl)methylidene]amino}acetic acid	C10H11NO5	M+Na	248.0529	-3.0
	HMDB0159052	SCHEMBL6993698	C10H11NO5	M+Na	248.0529	-3.0
	HMDB0166888	[(3,5-dimethoxyphenyl)(hydroxy)methylidene]carbamic acid	C10H11NO5	M+Na	248.0529	-3.0
	HMDB0168704	{hydroxy[4-(2-hydroxyethoxy)phenyl]methylidene}carbamic acid	C10H11NO5	M+Na	248.0529	-3.0
	HMDB0168708	[(4-ethoxy-2-hydroxyphenyl)(hydroxy)methylidene]carbamic acid	C10H11NO5	M+Na	248.0529	-3.0

	HMDB0140926	2- {[hydroxy(3-hydroxy-4-methoxyphenyl)methylidene]amino}acetic acid	C10H11NO5	M+Na	248.0529	-3.0
	HMDB0131194	2- {[hydroxy(2-hydroxy-4-methoxyphenyl)methylidene]amino}acetic acid	C10H11NO5	M+Na	248.0529	-3.0
	HMDB0128032	2- {[hydroxy(3-hydroxy-5-methoxyphenyl)methylidene]amino}acetic acid	C10H11NO5	M+Na	248.0529	-3.0
	HMDB0060026	Vanilloylglycine	C10H11NO5	M+Na	248.0529	-3.0
	HMDB0168711	[(4-ethoxy-3-hydroxyphenyl)(hydroxy)methylidene]carbamic acid	C10H11NO5	M+Na	248.0529	-3.0
248.1486	HMDB0062735	(R)-3-hydroxybutyrylcarnitine	C11H21NO5	M+H	248.1492	-2.6
	HMDB0013127	(3S)-3- {[(3R)-3-hydroxybutanoyl]oxy }-4-(trimethylazaniumyl)butanoate	C11H21NO5	M+H	248.1492	-2.6
248.1851	HMDB0000623	Dodecanedioic acid	C12H22O4	M+NH4	248.1856	-2.1
	HMDB0041614	Dipropyl hexanedioate	C12H22O4	M+NH4	248.1856	-2.1
	HMDB0041613	Bis(1-methylethyl) hexanedioate	C12H22O4	M+NH4	248.1856	-2.1
	HMDB0030143	Talaromycin A	C12H22O4	M+NH4	248.1856	-2.1
248.2579	HMDB0038678	1,1-Dihexyloxyethane	C14H30O2	M+NH4	248.2584	-2.0
	HMDB0032246	Dodecanal dimethyl acetal	C14H30O2	M+NH4	248.2584	-2.0
	HMDB0172396	1,13-tetradecandiol	C14H30O2	M+NH4	248.2584	-2.0
	HMDB0172397	1,14-Tetradecandiol	C14H30O2	M+NH4	248.2584	-2.0
249.0910	HMDB0060321	1-Hydroxy-6-methoxypyrene	C17H12O2	M+H	249.0910	0.0
249.1843	HMDB0032228	Dimethylbenzyl carbinyol hexanoate	C16H24O2	M+H	249.1849	-2.4
	HMDB0036221	[2-(Dimethoxymethyl)-1-heptenyl]benzene	C16H24O2	M+H	249.1849	-2.4
	HMDB0037719	2-Phenylethyl octanoate	C16H24O2	M+H	249.1849	-2.4
	HMDB0037713	Octyl phenylacetate	C16H24O2	M+H	249.1849	-2.4
	HMDB0036640	Furanofukinin	C16H24O2	M+H	249.1849	-2.4
249.2207	HMDB0041333	(all-Z)-8,11,14-Heptadecatrienal	C17H28O	M+H	249.2213	-2.4
	HMDB0060512	Sterol	C17H28O	M+H	249.2213	-2.4
	HMDB0030932	Avocadenofuran	C17H28O	M+H	249.2213	-2.4
	HMDB0182305	6-(hydroxymethyl)-2-(3-hydroxyprop-1-en-2-yl)--methylspiro[4.5]dec-6-en-8-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0150689	2,5,5,8a-tetramethyl-6-oxo-1,4,4a,5,6,7,8,8a-octahydronaphthalene-1-carboxylic acid	C15H22O3	M+H	251.1642	-2.3
	HMDB0177633	(1Z)-1-ethylidene-5-hydroxy-7-(2-hydroxypropan-2-yl)-4-methylidene-octahydro-1H-inden-2-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0177635	(1Z)-1-ethylidene-5-hydroxy-7-(1-hydroxypropan-2-yl)-4-methylidene-octahydro-1H-inden-2-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0177634	(1Z)-5-hydroxy-1-(2-hydroxyethylidene)-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0240642	3,5-di-tert-butyl-4-hydroxybenzoic acid	C15H22O3	M+H	251.1642	-2.3
	HMDB0177636	(1Z)-1-ethylidene-3,5-dihydroxy-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0177702	(1E)-5-hydroxy-1-(2-hydroxyethylidene)-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0182900	2,2a-dihydroxy-6,6,7b-trimethyl-1H,2H,2aH,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-3-carbaldehyde	C15H22O3	M+H	251.1642	-2.3
	HMDB0183504	(8aR)-4-hydroxy-7-(3-hydroxyprop-1-en-2-yl)-1,8a-dimethyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0183503	(8aR)-4,7-dihydroxy-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0183502	(8aS)-1,4-dihydroxy-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0183506	(8aR)-4-hydroxy-1,8a-dimethyl-7-(2-methyloxiran-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0184276	(8aS)-4-hydroxy-8a-(hydroxymethyl)-1-methyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0184279	(8aR)-3,4-dihydroxy-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0182310	1-(hydroxymethyl)-3-methyl-3'-(prop-1-en-2-yl)-7-oxaspiro[bicyclo[4.1]heptane-2,1'-cyclopentane]-5-one	C15H22O3	M+H	251.1642	-2.3

251.1636	HMDB0182311	9-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0182309	6-(hydroxymethyl)--methyl-2-(2-methyloxiran-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0177703	(1E)-1-ethylidene-5-hydroxy-7-(1-hydroxypropan-2-yl)-4-methylidene-octahydro-1H-inden-2-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0177701	(1E)-1-ethylidene-5-hydroxy-7-(2-hydroxypropan-2-yl)-4-methylidene-octahydro-1H-inden-2-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0177704	(1E)-1-ethylidene-3,5-dihydroxy-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0182302	6-bis(hydroxymethyl)-2-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0182304	2-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0182306	1-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0182303	-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0182307	2-hydroxy-6-(hydroxymethyl)--methyl-3-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0182308	1-hydroxy-6-(hydroxymethyl)--methyl-3-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+H	251.1642	-2.3
	HMDB0015371	Gemfibrozil	C15H22O3	M+H	251.1642	-2.3
	HMDB0035358	Ketosantallic acid	C15H22O3	M+H	251.1642	-2.3
	HMDB0035137	Heliannuol D	C15H22O3	M+H	251.1642	-2.3
	HMDB0035117	(3beta,6beta)-Furanoeremophilane-3,6-diol	C15H22O3	M+H	251.1642	-2.3
	HMDB0035798	Piperdial	C15H22O3	M+H	251.1642	-2.3
	HMDB0036563	Valerenolic acid	C15H22O3	M+H	251.1642	-2.3
	HMDB0039644	Heliannuol A	C15H22O3	M+H	251.1642	-2.3
	HMDB0036036	6,6-Dimethoxy-2,5,5-trimethyl-2-hexene	C15H22O3	M+H	251.1642	-2.3
	HMDB0035760	3-Hydroxytrichothecene	C15H22O3	M+H	251.1642	-2.3
	HMDB0039635	Absciscic alcohol	C15H22O3	M+H	251.1642	-2.3
	HMDB0039156	3beta-Hydroxycinnamolide	C15H22O3	M+H	251.1642	-2.3
	HMDB0037064	FS4 toxin	C15H22O3	M+H	251.1642	-2.3
	HMDB0036037	13-Hydroxymarasmene	C15H22O3	M+H	251.1642	-2.3
	HMDB0034721	Procurcumadiol	C15H22O3	M+H	251.1642	-2.3
	HMDB0036664	Ketopelenolide a	C15H22O3	M+H	251.1642	-2.3
	HMDB0037559	Cadabacilone	C15H22O3	M+H	251.1642	-2.3
	HMDB0031901	Blennin A	C15H22O3	M+H	251.1642	-2.3
	HMDB0036550	3-Ketopatrictrothecene	C15H22O3	M+H	251.1642	-2.3
	HMDB0040754	(3beta,8beta)-3-Hydroxy-7(11)-eremophilen-12,8-olide	C15H22O3	M+H	251.1642	-2.3
	HMDB0037529	Lactaronecatorin A	C15H22O3	M+H	251.1642	-2.3
	HMDB0035148	(6beta,8alpha)-6-Hydroxy-7(11)-eremophilen-12,8-olide	C15H22O3	M+H	251.1642	-2.3
	HMDB0030917	1-Hydroxyacorenone	C15H22O3	M+H	251.1642	-2.3
	HMDB0061839	Ethylhexyl salicylate	C15H22O3	M+H	251.1642	-2.3
	HMDB0177902	3-hydroxy-7,7a-dimethyl-4'-methylidene-octahydrospiro[indene-2,3'-oxolane]-2'-one	C15H22O3	M+H	251.1642	-2.3
251.1999	HMDB0037712	[2,2-Bis(2-methylpropoxy)ethyl]benzene	C16H26O2	M+H	251.2006	-2.6
	HMDB0159344	(7Z,Z)-hexadeca-7,,15-trienoic acid	C16H26O2	M+H	251.2006	-2.6
	HMDB0240361	(7Z,Z,13Z)-hexadecatrienoate	C16H25O2	M+H	251.2006	-2.6
	HMDB0037631	3-Methyl-alpha-ionyl acetate	C16H26O2	M+H	251.2006	-2.6
	HMDB0035293	Norambreinolide	C16H26O2	M+H	251.2006	-2.6
	HMDB0061952	AC1LBPUV	C16H26O2	M+H	251.2006	-2.6
251.2352	HMDB0013299	Pentadecanol	C15H32O	M+Na	251.2345	2.7
	HMDB0062051	3,7,11-trimethyldodecan-1-ol	C15H32O	M+Na	251.2345	2.7
	HMDB0062728	3,7,11-trimethyldodecan-1-ol	C15H32O	M+Na	251.2345	2.7
252.0973	HMDB0181567	2-{[cyano(4-hydroxyphenyl)methyl]-C-hydroxycarbonimidoyl}acetic acid	C11H10N2O4	M+NH4	252.0979	-2.3
	HMDB0181566	2-{[cyano(2-hydroxyphenyl)methyl]-C-hydroxycarbonimidoyl}acetic acid	C11H10N2O4	M+NH4	252.0979	-2.3
	HMDB0134948	2-{[hydroxy(4-hydroxy-1H-indol-3-yl)methylidene]amino}acetic acid	C11H10N2O4	M+NH4	252.0979	-2.3
	HMDB0134945	2-{[hydroxy(7-hydroxy-1H-indol-3-yl)methylidene]amino}acetic acid	C11H10N2O4	M+NH4	252.0979	-2.3

	HMDB0134942	2-[[hydroxy(6-hydroxy-1H-indol-3-yl)methylidene]amino}acetic acid	C11H10N2O4	M+NH4	252.0979	-2.3
	HMDB0134939	2-[[hydroxy(5-hydroxy-1H-indol-3-yl)methylidene]amino}acetic acid	C11H10N2O4	M+NH4	252.0979	-2.3
	HMDB0181568	2-[[cyano(phenyl)methyl]-C-hydroxycarbonimidoyl]-2-hydroxyacetic acid	C11H10N2O4	M+NH4	252.0979	-2.3
252.1588	HMDB0175190	4-Hydroxybenzoic acid 6-heptenyl ester	C14H18O3	M+NH4	252.1594	-2.4
	HMDB0170852	2-hydroxy-4-(prop-2-en-1-yl)phenyl 3-methylbutanoate	C14H18O3	M+NH4	252.1594	-2.4
	HMDB0154116	CHEMBL56	C14H18O3	M+NH4	252.1594	-2.4
	HMDB0135897	3-[4-hydroxy-3-(3-methylbut-2-en-1-yl)phenyl]propanoic acid	C14H18O3	M+NH4	252.1594	-2.4
	HMDB0133175	2-pentyl-3-phenyloxirane-2-carboxylic acid	C14H18O3	M+NH4	252.1594	-2.4
	HMDB0133176	(2Z)-7-hydroxy-2-(phenylmethylidene)heptanoic acid	C14H18O3	M+NH4	252.1594	-2.4
	HMDB0133174	(2Z)-6-hydroxy-2-(phenylmethylidene)heptanoic acid	C14H18O3	M+NH4	252.1594	-2.4
	HMDB0133177	(2Z)-2-[(2-hydroxyphenyl)methylidene]heptanoic acid	C14H18O3	M+NH4	252.1594	-2.4
	HMDB0133172	(2Z)-2-[(3-hydroxyphenyl)methylidene]heptanoic acid	C14H18O3	M+NH4	252.1594	-2.4
	HMDB0133173	(2Z)-2-[(4-hydroxyphenyl)methylidene]heptanoic acid	C14H18O3	M+NH4	252.1594	-2.4
	HMDB0133171	(2Z)-3-hydroxy-2-(phenylmethylidene)heptanoic acid	C14H18O3	M+NH4	252.1594	-2.4
	HMDB0036607	(S)-Pterosin P	C14H18O3	M+NH4	252.1594	-2.4
	HMDB0030763	(S,11S)-Pterosin C	C14H18O3	M+NH4	252.1594	-2.4
	HMDB0036046	Dehydrooreadone	C14H18O3	M+NH4	252.1594	-2.4
	HMDB0038218	Pterosin N	C14H18O3	M+NH4	252.1594	-2.4
252.1953	HMDB0240643	3,5-di-tert-butyl-4-hydroxybenzaldehyde	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0134131	2-[hydroxy(phenyl)methyl]octanal	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0134132	2-[(3-hydroxyphenyl)methyl]octanal	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0134134	2-benzyl-7-hydroxyoctanal	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0177624	(1Z)-1-ethylidene-5-hydroxy-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0177700	(1E)-1-ethylidene-5-hydroxy-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0183493	(8aR)-4-hydroxy-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0150675	2,5,5,8a-tetramethyl-6-oxo-1,4,4a,5,6,7,8,8a-octahydronaphthalene-1-carbaldehyde	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0134153	2-benzyl-octanoic acid	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0134133	2-[(4-hydroxyphenyl)methyl]octanal	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0134135	2-benzyl-8-hydroxyoctanal	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0134137	2-[(2-hydroxyphenyl)methyl]octanal	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0134136	2-benzyl-2-hydroxyoctanal	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0134139	3-[(1Z)-2-hexyl-3-hydroxyprop-1-en-1-yl]phenol	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0134138	2-(phenylmethylidene)octane-1,3-diol	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0134141	(2Z)-2-(phenylmethylidene)octane-1,7-diol	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0134140	4-[(1Z)-2-hexyl-3-hydroxyprop-1-en-1-yl]phenol	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0134143	(2Z)-2-(phenylmethylidene)octane-1,8-diol	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0134142	(2-hexyl-3-phenyloxiran-2-yl)methanol	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0035408	1,-Epoxygermacrone	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0036466	Zerumbone oxide	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0036647	Isocurcumenol	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0038698	xi-2-Hydroxy-1,3,5-bisabolatrien-9-one	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0037710	4-Methylphenyl octanoate	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0035639	Petasalbin	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0037391	p-Hydroxynonanophenone	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0038190	Rishitinol	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0033252	Curcumanolide A	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0038914	4,6-Decadiyn-1-ol isovalerate	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0039621	beta-Santalal acid	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0034562	9-Pentadecene-12,14-diyne-1,11-diol	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0036449	(1alpha,4beta,5beta)-4-Hydroxy-7(11),(14)-guaia dien-8-one	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0033960	Curcumenol	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0035935	Dihydroisoalantolactone	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0031349	Epiacoronene	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0035413	(4alpha,5alpha)-11-Eremophilene-2,9-dione	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0036392	(Z)-alpha-Bergamotenoic acid	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0034956	Oxysolavetivone	C15H22O2	M+NH4	252.1958	-2.0

	HMDB0035869	alpha-Rotunol	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0038795	7,9-Illudadiene-3,14-diol	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0036390	3-Phenylpropyl hexanoate	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0032081	4,-Longipinanedione	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0036035	Acutissimin A	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0035889	Germacrone 4,5-epoxide	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0037739	7-(1,3-Cyclohexadienyl)-5-hydroxy-2,6-dimethyl-2-hepten-4-one	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0036427	Procurcumenol	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0035794	beta-Costic acid	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0035407	Dehydrocurdione	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0041036	Sugeonol	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0038796	2,7(14)-Illudadiene-,15-diol	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0034742	Saussurea lactone	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0033253	Curcumenone	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0030016	Valerenic acid	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0037640	2-Methyl-4-phenyl-2-butyl 2-methylpropanoate	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0035202	7-Hydroxycostal	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0038198	3,7-Bisaboladiene-2,8-dione	C15H22O2	M+NH4	252.1958	-2.0
	HMDB0037038	Cyclodehydroisolubimin	C15H22O2	M+NH4	252.1958	-2.0
252.2317	HMDB0175562	2-methyl-3-[(3E)-3-methylhexa-3,5-dien-1-yl]-2-(4-methylpent-3-en-1-yl)oxirane	C16H26O	M+NH4	252.2322	-1.9
	HMDB0175554	(6Z,E)-2,6,-trimethyltrideca-2,6,,12-tetraen-5-ol	C16H26O	M+NH4	252.2322	-1.9
	HMDB0175552	(3E,7Z)-4,8,12-trimethyltrideca-1,3,7,11-tetraen-5-ol	C16H26O	M+NH4	252.2322	-1.9
	HMDB0175555	(2E,6E)-6-methyl-2-(4-methylpent-3-en-1-yl)nona-2,6,8-trien-1-ol	C16H26O	M+NH4	252.2322	-1.9
	HMDB0175561	2-[(1E,5Z)-2,6,-trimethylundeca-1,5,9-trien-1-yl]oxirane	C16H26O	M+NH4	252.2322	-1.9
	HMDB0175560	2-[(3Z)-4,8-dimethylnona-3,7-dien-1-yl]-3-ethenyl-2-methyloxirane	C16H26O	M+NH4	252.2322	-1.9
	HMDB0175563	3-[(3Z,7E)-3,7-dimethyldeca-3,7,9-trien-1-yl]-2,2-dimethyloxirane	C16H26O	M+NH4	252.2322	-1.9
	HMDB0175556	(6Z,E)-2,6,-trimethyltrideca-2,6,,12-tetraen-1-ol	C16H26O	M+NH4	252.2322	-1.9
	HMDB0175558	(3E,7Z)-4,8,12-trimethyltrideca-1,3,7,11-tetraen-6-ol	C16H26O	M+NH4	252.2322	-1.9
	HMDB0175559	(6Z,E)-2,6,-trimethyltrideca-2,6,,12-tetraen-4-ol	C16H26O	M+NH4	252.2322	-1.9
	HMDB0175557	(2E,6Z,E)-2,6,-trimethyltrideca-2,6,,12-tetraen-1-ol	C16H26O	M+NH4	252.2322	-1.9
	HMDB0175553	(2Z,5Z)-6,-dimethyl-2-(prop-2-en-1-ylidene)undeca-5,9-dien-1-ol	C16H26O	M+NH4	252.2322	-1.9
	HMDB0040179	2,6-Di-tert-butyl-4-ethylphenol	C16H26O	M+NH4	252.2322	-1.9
	HMDB0030275	Herculin	C16H29NO	M+H	252.2322	-1.9
253.1195	HMDB0134151	(2Z)-2-(phenylmethyldiene)oct-7-enoic acid	C15H18O2	M+Na	253.1199	-1.6
	HMDB0167514	1,5,8-trimethyl-6H,7H,8H,9H-naphtho[2,1-b]furan-9-ol	C15H18O2	M+Na	253.1199	-1.6
	HMDB0036768	Furanodienone	C15H18O2	M+Na	253.1199	-1.6
	HMDB0035425	(2E,8Z)-Decadiene-4,6-diyn-1-yl 3-methylbutanoate	C15H18O2	M+Na	253.1199	-1.6
	HMDB0036155	Curzerenone	C15H18O2	M+Na	253.1199	-1.6
	HMDB0037706	Cyclohexyl cinnamate	C15H18O2	M+Na	253.1199	-1.6
	HMDB0033235	8,12-Epoxy-4(15),7,11-eudesmatrien-1-one	C15H18O2	M+Na	253.1199	-1.6
	HMDB0182317	2-hydroxy-6-(hydroxymethyl)--methyl-3-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+H	253.1798	-2.1
	HMDB0182312	6,-bis(hydroxymethyl)-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+H	253.1798	-2.1
	HMDB0182315	6-(hydroxymethyl)-2-(3-hydroxyprop-1-en-2-yl)--methylspiro[4.5]decan-8-one	C15H24O3	M+H	253.1798	-2.1
	HMDB0182313	6-hydroxy--(hydroxymethyl)-6-methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+H	253.1798	-2.1
	HMDB0182314	2-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+H	253.1798	-2.1
	HMDB0179273	5-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M+H	253.1798	-2.1
	HMDB0179272	7-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M+H	253.1798	-2.1
	HMDB0179271	6-{5-hydroxy-5-methyl-7-oxabicyclo[4.1]heptan-2-yl}-2-methylhept-2-en-4-one	C15H24O3	M+H	253.1798	-2.1

HMDB0179270	1-(3,3-dimethyloxiran-2-yl)-3-(4-hydroxy-4-methylcyclohex-2-en-1-yl)butan-1-one	C15H24O3	M+H	253.1798	-2.1
HMDB0179268	6-(1,4-dihydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M+H	253.1798	-2.1
HMDB0179267	6-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M+H	253.1798	-2.1
HMDB0179269	1-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M+H	253.1798	-2.1
HMDB0179266	6-[4-hydroxy-4-(hydroxymethyl)cyclohex-2-en-1-yl]-2-methylhept-2-en-4-one	C15H24O3	M+H	253.1798	-2.1
HMDB0179258	3,3a-dihydroxy-3,8-dimethyl-5-(propan-2-yl)-1,2,3,3a,4,5,6,8a-octahydroazulen-6-one	C15H24O3	M+H	253.1798	-2.1
HMDB0182316	1-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+H	253.1798	-2.1
HMDB0182319	6-(hydroxymethyl)--methyl-2-(2-methyloxiran-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+H	253.1798	-2.1
HMDB0182318	1-hydroxy-6-(hydroxymethyl)--methyl-3-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+H	253.1798	-2.1
HMDB0184275	(4aR)-4,4a-dimethyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3,7-triol	C15H24O3	M+H	253.1798	-2.1
HMDB0184273	(4aS)-4a-(hydroxymethyl)-4-methyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M+H	253.1798	-2.1
HMDB0183500	(4aR)-4,4a-dimethyl-6-(2-methyloxiran-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M+H	253.1798	-2.1
HMDB0183495	(4aR)-4-(hydroxymethyl)-4a-methyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M+H	253.1798	-2.1
HMDB0183496	(8aS)-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalene-1,2,4-triol	C15H24O3	M+H	253.1798	-2.1
HMDB0183498	(4aR)-6-(3-hydroxyprop-1-en-2-yl)-4,4a-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M+H	253.1798	-2.1
HMDB0182321	7-hydroxy--(hydroxymethyl)-6-methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+H	253.1798	-2.1
HMDB0182320	7-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+H	253.1798	-2.1
HMDB0179257	1,8a-dihydroxy-1,4-dimethyl-7-(propan-2-ylidene)-decahydroazulen-6-one	C15H24O3	M+H	253.1798	-2.1
HMDB0179146	(6Z)-5-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M+H	253.1798	-2.1
HMDB0179147	(6Z)-2-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M+H	253.1798	-2.1
HMDB0179144	1,7-dimethyl-4-(propan-2-yl)-11-oxabicyclo[8.1]undecane-3,6-dione	C15H24O3	M+H	253.1798	-2.1
HMDB0179148	(6Z)-3-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M+H	253.1798	-2.1
HMDB0179145	(6Z)-3-(1-hydroxypropan-2-yl)-6,-dimethylcyclodec-6-ene-1,4-dione	C15H24O3	M+H	253.1798	-2.1
HMDB0179142	(6Z)-3-(2-hydroxypropan-2-yl)-6,-dimethylcyclodec-6-ene-1,4-dione	C15H24O3	M+H	253.1798	-2.1
HMDB0179143	(6Z)-8-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M+H	253.1798	-2.1
HMDB0179141	(6Z)--hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M+H	253.1798	-2.1
HMDB0179140	(6Z)--(hydroxymethyl)-6-methyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M+H	253.1798	-2.1
HMDB0179139	(6E)-6-(hydroxymethyl)--methyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M+H	253.1798	-2.1
HMDB0177221	(4aR,7aS,7bR)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4-diol	C15H24O3	M+H	253.1798	-2.1
HMDB0168751	(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trienal	C15H24O3	M+H	253.1798	-2.1
HMDB0112086	5-(3-methyl-5-pentylfuran-2-yl)-pentanoic acid	C15H24O3	M+H	253.1798	-2.1
HMDB0112094	3-Methyl-5-propyl-2-furanheptanoic acid	C15H24O3	M+H	253.1798	-2.1
HMDB0030918	1-Hydroxyepiacorone	C15H24O3	M+H	253.1798	-2.1
HMDB0035729	Dihydromyoporone	C15H24O3	M+H	253.1798	-2.1

	HMDB0037969	Urodiolenone	C15H24O3	M+H	253.1798	-2.1
	HMDB0032122	3(4->5)-Abeo-4,11:4,12-diepoxy-3-eudesmanol	C15H24O3	M+H	253.1798	-2.1
	HMDB0037063	Toxin FS2	C15H24O3	M+H	253.1798	-2.1
	HMDB0035613	Epioxylubimin	C15H24O3	M+H	253.1798	-2.1
	HMDB0034574	Apotrichodiol	C15H24O3	M+H	253.1798	-2.1
	HMDB0035767	Piperalol	C15H24O3	M+H	253.1798	-2.1
	HMDB0036448	Zedoarondiol	C15H24O3	M+H	253.1798	-2.1
	HMDB0033149	(4R,5S,7R,11R)-11,12-Dihydroxy-1()-spirovetiven-2-one	C15H24O3	M+H	253.1798	-2.1
	HMDB0035309	6alpha-Carissanol	C15H24O3	M+H	253.1798	-2.1
	HMDB0038502	Bisacurone B	C15H24O3	M+H	253.1798	-2.1
	HMDB0036663	Hydroxypelenolide	C15H24O3	M+H	253.1798	-2.1
	HMDB0030919	Acorusdiol	C15H24O3	M+H	253.1798	-2.1
	HMDB0035597	alpha-Carissanol	C15H24O3	M+H	253.1798	-2.1
	HMDB0040685	2,3-Dihydroabscisic alcohol	C15H24O3	M+H	253.1798	-2.1
253.2158	HMDB0166468	(3Z)-hexadeca-3,15-dienoic acid	C16H28O2	M+H	253.2162	-1.6
	HMDB0032340	Isoambrettolide	C16H28O2	M+H	253.2162	-1.6
	HMDB0038255	Geranyl 2-ethylbutyrate	C16H28O2	M+H	253.2162	-1.6
	HMDB0031086	(Z)-7-Hexadecen-1,16-olide	C16H28O2	M+H	253.2162	-1.6
	HMDB0030429	Linalyl hexanoate	C16H28O2	M+H	253.2162	-1.6
	HMDB0029351	Geranyl hexanoate	C16H28O2	M+H	253.2162	-1.6
	HMDB0037805	D6-Ambrettolide	C16H28O2	M+H	253.2162	-1.6
	HMDB0039131	Ethyl (Z,Z)-5,8-tetradecadienoate	C16H28O2	M+H	253.2162	-1.6
	HMDB0000477	7Z,Z-Hexadecadienoic acid	C16H28O2	M+H	253.2162	-1.6
254.1017	HMDB0137293	3-(4,7-dimethoxy-2H-1,3-benzodioxol-5-yl)prop-2-enal	C12H12O5	M+NH4	254.1023	-2.3
	HMDB0169150	7-hydroxy-2,2-dimethyl-4-oxo-chroman-6-carboxylic acid	C12H12O5	M+NH4	254.1023	-2.3
	HMDB0166280	(4Z)-5-(2H-1,3-benzodioxol-5-yl)-3-hydroxypent-4-enoic acid	C12H12O5	M+NH4	254.1023	-2.3
	HMDB0166279	(4Z)-5-(6-hydroxy-2H-1,3-benzodioxol-5-yl)pent-4-enoic acid	C12H12O5	M+NH4	254.1023	-2.3
	HMDB0166281	3-[3-(2H-1,3-benzodioxol-5-yl)oxiran-2-yl]propanoic acid	C12H12O5	M+NH4	254.1023	-2.3
	HMDB0166282	(4Z)-5-(2H-1,3-benzodioxol-5-yl)-2-hydroxypent-4-enoic acid	C12H12O5	M+NH4	254.1023	-2.3
	HMDB0040407	(S)-2,3-Dihydro-7-hydroxy-2-methyl-4-oxo-4H-1-benzopyran-5-acetic acid	C12H12O5	M+NH4	254.1023	-2.3
	HMDB0030858	Austdiol	C12H12O5	M+NH4	254.1023	-2.3
	HMDB0033096	Apional	C12H12O5	M+NH4	254.1023	-2.3
	HMDB0030582	Dillapional	C12H12O5	M+NH4	254.1023	-2.3
	HMDB0128676	3-(6,7-dimethoxy-2H-1,3-benzodioxol-5-yl)prop-2-enal	C12H12O5	M+NH4	254.1023	-2.3
	HMDB0041725	Dihydroferuloylglycine	C12H15NO5	M+H	254.1023	-2.4
	HMDB0011716	N-Acetylvani alanine	C12H15NO5	M+H	254.1023	-2.4
	HMDB0062177	N-Lactoyl-Tyrosine	C12H15NO5	M+H	254.1023	-2.4
254.1745	HMDB0034462	Heptyl 4-hydroxybenzoate	C14H20O3	M+NH4	254.1751	-2.2
	HMDB0040778	Eremopetasidione	C14H20O3	M+NH4	254.1751	-2.2
	HMDB0182083	2-(3-{2,3-dimethyltricyclo[2.2.1]heptan-3-yl}propylidene)propane-1,3-diol	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0166723	396--2	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0137903	6-hydroxy-5,5,8a-trimethyl-2-methylidene-decahydronaphthalene-1-carbaldehyde	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0150688	5-(hydroxymethyl)-1,1,4a,6-tetramethyl-1,2,3,4,4a,5,8,8a-octahydronaphthalen-2-one	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0163044	(2Z)-5-(5-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl)-3-methylpent-2-enal	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0166721	2,4-di-tert-butyl-6-methylbenzene-1,3-diol	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0166722	UNII-7B7Y8CEM7E	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0177916	4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-7-ol	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0177917	2-[(3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl)methylidene]propane-1,3-diol	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0177914	(2E)-3-[3-(hydroxymethyl)-7-methyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl]-2-methylprop-2-en-1-ol	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0177915	(2E)-3-[7-(hydroxymethyl)-3-methyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl]-2-methylprop-2-en-1-ol	C15H24O2	M+NH4	254.2115	-2.2

HMDB0182081	(2Z)-5-[3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-en-1-ol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0182080	(2Z)-5-[2-(hydroxymethyl)-3-methyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-en-1-ol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0182082	(2Z)-5-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-ene-1,5-diol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0182086	[3-(2-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]ethyl)-2-methyloxiran-2-yl]methanol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0182084	(2Z)-5-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-ene-1,4-diol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0182085	7-[(3Z)-5-hydroxy-4-methylpent-3-en-1-yl]-1,7-dimethyltricyclo[2.2.1,heptan-3-ol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0182087	3-[(3Z)-5-hydroxy-4-methylpent-3-en-1-yl]-2,3-dimethyltricyclo[2.2.1,heptan-1-ol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0179231	1,1,4,7-tetramethyl-1H,1aH,2H,3H,5H,6H,7H,7aH,7bH-cyclopropa[e]azulene-7,7b-diol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0179230	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,7a-diol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0177919	4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-1-ol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0177920	[3-(3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl)-2-methyloxiran-2-yl]methanol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0177918	4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-2-ol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0179224	1-(hydroxymethyl)-1,2,5-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-ol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0179225	2-(hydroxymethyl)-1,1,5-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-ol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0179226	5-(hydroxymethyl)-1,1,2-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-ol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0179228	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,6-diol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0179229	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,3-diol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0179227	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,4-diol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0002352	Capsidiol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0035827	Aubergenone	C15H24O2	M+NH4	254.2115	-2.2
HMDB0035040	7-Hydroxycostol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0037393	(3xi,7(11)Z)-7(11)-Copaene-4,12-diol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0035301	4alpha,5alpha-Epoxy-11-eudesmen-3a-ol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0030916	2-Hydroxyacorenone	C15H24O2	M+NH4	254.2115	-2.2
HMDB0032048	2,6-Di-tert-butyl-4-hydroxymethylphenol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0036680	Cyperolone	C15H24O2	M+NH4	254.2115	-2.2
HMDB0035032	Epilubimin	C15H24O2	M+NH4	254.2115	-2.2
HMDB0035127	(-)-Myrtenyl isovalerate	C15H24O2	M+NH4	254.2115	-2.2
HMDB0035648	Isolubimin	C15H24O2	M+NH4	254.2115	-2.2
HMDB0036446	(4alpha,alpha)-1(5),6-Guaiadiene	C15H24O2	M+NH4	254.2115	-2.2
HMDB0032681	alpha-4,5-Seco-11-eudesmene-4,5-dione	C15H24O2	M+NH4	254.2115	-2.2
HMDB0031348	Epiacorenone	C15H24O2	M+NH4	254.2115	-2.2
HMDB0030891	(2E,6E)-1-Hydroxy-2,6,-farnesatrien-9-one	C15H24O2	M+NH4	254.2115	-2.2
HMDB0039688	Tuberonone	C15H24O2	M+NH4	254.2115	-2.2
HMDB0035147	Rishitinone	C15H24O2	M+NH4	254.2115	-2.2
HMDB0030920	Acorusnol	C15H24O2	M+NH4	254.2115	-2.2
HMDB0039525	Isomelitric acid A	C15H24O2	M+NH4	254.2115	-2.2

	HMDB0036668	Humulene-8-hydroperoxide	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0036687	Tanavulgarol	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0038144	Petasitolone	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0032292	Geranyl tiglate	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0038122	5-Methyl-5-hexen-2-one	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0038027	beta-Ionyl acetate	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0034722	3-Hydroxy-1,-bisaboladien-9-one	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0038178	Davanone	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0036549	Apotrichothecene	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0037906	Hernandulcin	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0034714	Curdione	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0033104	Calamensesquiterpinenol	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0033083	(4S)-Dihydrocurcumenone	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0040712	Humulene diepoxide A	C15H24O2	M+NH4	254.2115	-2.2
	HMDB0135795	6-(3-methoxyoxiran-2-yl)-7-methyl-2H-chromen-2-one	C13H12O4	M+Na	255.0628	-2.3
255.0622	HMDB0135796	8-hydroxy-6-[(E)-2-methoxyethenyl]-7-methyl-2H-chromen-2-one	C13H12O4	M+Na	255.0628	-2.3
	HMDB0135797	5-hydroxy-6-[(E)-2-methoxyethenyl]-7-methyl-2H-chromen-2-one	C13H12O4	M+Na	255.0628	-2.3
	HMDB0135798	3-hydroxy-6-[(E)-2-methoxyethenyl]-7-methyl-2H-chromen-2-one	C13H12O4	M+Na	255.0628	-2.3
	HMDB0135794	7-(hydroxymethyl)-6-[(E)-2-methoxyethenyl]-2H-chromen-2-one	C13H12O4	M+Na	255.0628	-2.3
	HMDB0130065	3-(1,2-dihydroxybut-3-en-1-yl)-1H-isochromen-1-one	C13H12O4	M+Na	255.0628	-2.3
	HMDB0130048	5-hydroxy-3-[(1E)-4-hydroxybut-1-en-1-yl]-1H-isochromen-1-one	C13H12O4	M+Na	255.0628	-2.3
	HMDB0130047	3-(3-ethyloxiran-2-yl)-5-hydroxy-1H-isochromen-1-one	C13H12O4	M+Na	255.0628	-2.3
	HMDB0130046	3-[(1E)-but-1-en-1-yl]-5,7-dihydroxy-1H-isochromen-1-one	C13H12O4	M+Na	255.0628	-2.3
	HMDB0130045	3-[(1E)-but-1-en-1-yl]-5,6-dihydroxy-1H-isochromen-1-one	C13H12O4	M+Na	255.0628	-2.3
	HMDB0130044	5-hydroxy-3-[(1E)-3-hydroxybut-1-en-1-yl]-1H-isochromen-1-one	C13H12O4	M+Na	255.0628	-2.3
	HMDB0128959	7-hydroxy-6-(3-oxobutyl)-2H-chromen-2-one	C13H12O4	M+Na	255.0628	-2.3
	HMDB0030813	Cassiachromone	C13H12O4	M+Na	255.0628	-2.3
	HMDB0041325	Salfredin B11	C13H12O4	M+Na	255.0628	-2.3
	HMDB0033330	Dihydrocoriandrin	C13H12O4	M+Na	255.0628	-2.3
	HMDB0177471	1-(1,6,8-trihydroxy-3-methylnaphthalen-2-yl)ethan-1-one	C13H12O4	M+Na	255.0628	-2.3
255.1351	HMDB0038911	(2S,3S,4S)-5,7,9,11-Tridecatetrayne-1,2,3,4-tetrol	C13H12O4	M+Na	255.0628	-2.3
	HMDB0176371	(9E)-11-hydroxypentadec-9-en-12,14-diynal	C15H20O2	M+Na	255.1355	-1.8
	HMDB0134130	(2Z)-2-[(2-hydroxyphenyl)methylidene]octanal	C15H20O2	M+Na	255.1355	-1.8
	HMDB0134128	2-hexyl-3-phenyloxirane-2-carbaldehyde	C15H20O2	M+Na	255.1355	-1.8
	HMDB0134129	(2Z)-8-hydroxy-2-(phenylmethylidene)octanal	C15H20O2	M+Na	255.1355	-1.8
	HMDB0134127	(2Z)-7-hydroxy-2-(phenylmethylidene)octanal	C15H20O2	M+Na	255.1355	-1.8
	HMDB0134126	(2Z)-2-[(4-hydroxyphenyl)methylidene]octanal	C15H20O2	M+Na	255.1355	-1.8
	HMDB0134125	(2Z)-2-[(3-hydroxyphenyl)methylidene]octanal	C15H20O2	M+Na	255.1355	-1.8
	HMDB0134124	3-hydroxy-2-(phenylmethylidene)octanal	C15H20O2	M+Na	255.1355	-1.8
	HMDB0134123	(2Z)-2-(phenylmethylidene)octanoic acid	C15H20O2	M+Na	255.1355	-1.8
	HMDB0035906	Alantolactone	C15H20O2	M+Na	255.1355	-1.8
	HMDB0035934	Isoalantolactone	C15H20O2	M+Na	255.1355	-1.8
	HMDB0039011	1,3,11(13)-Eudesmatrien-12-oic acid	C15H20O2	M+Na	255.1355	-1.8
	HMDB0041038	Collybial	C15H20O2	M+Na	255.1355	-1.8
	HMDB0041062	,11-Epidioxycalamene	C15H20O2	M+Na	255.1355	-1.8
	HMDB0036206	alpha-Amylcinnamyl formate	C15H20O2	M+Na	255.1355	-1.8
	HMDB0040902	(E)-9-(3-Furanyl)-2,6-dimethyl-2,6-nonadien-4-one	C15H20O2	M+Na	255.1355	-1.8
	HMDB0036110	(S)-Bilobanone	C15H20O2	M+Na	255.1355	-1.8
	HMDB0031000	(Z)-8-Decene-4,6-diyn-1-yl 3-methylbutanoate	C15H20O2	M+Na	255.1355	-1.8
	HMDB0035412	1(),11-Eremophiladiene-2,9-dione	C15H20O2	M+Na	255.1355	-1.8
	HMDB0037563	Turneronol B	C15H20O2	M+Na	255.1355	-1.8
	HMDB0040981	(7b,a)-3-Hydroxy-1,3,5-cadinatrien-9-one	C15H20O2	M+Na	255.1355	-1.8
	HMDB0036881	Germacrone-13-al	C15H20O2	M+Na	255.1355	-1.8
	HMDB0036119	Alloalantolactone	C15H20O2	M+Na	255.1355	-1.8
	HMDB0036766	Furanogermenone	C15H20O2	M+Na	255.1355	-1.8
	HMDB0030790	6-[(3,4-Methylenedioxy)phenyl]-3,3-dimethyl-1-	C15H20O2	M+Na	255.1355	-1.8

	HMDB0037608	Turmeronol A	C15H20O2	M+Na	255.1355	-1.8
	HMDB0030761	Pterosin O	C15H20O2	M+Na	255.1355	-1.8
	HMDB0036688	Costunolide	C15H20O2	M+Na	255.1355	-1.8
	HMDB0036148	Furoeremophilone 1	C15H20O2	M+Na	255.1355	-1.8
255.1950	HMDB0179274	2-[4-hydroxy-4-(hydroxymethyl)cyclohex-2-en-1-yl]-6-methylheptan-4-one	C15H26O3	M+H	255.1955	-1.8
	HMDB0179275	2-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylheptan-4-one	C15H26O3	M+H	255.1955	-1.8
	HMDB0179277	2-(1,4-dihydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M+H	255.1955	-1.8
	HMDB0179276	2-hydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M+H	255.1955	-1.8
	HMDB0179281	3-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylheptan-4-one	C15H26O3	M+H	255.1955	-1.8
	HMDB0179278	2-{5-hydroxy-5-methyl-7-oxabicyclo[4.1]heptan-2-yl}-6-methylheptan-4-one	C15H26O3	M+H	255.1955	-1.8
	HMDB0179279	1-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylheptan-4-one	C15H26O3	M+H	255.1955	-1.8
	HMDB0179280	1-hydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M+H	255.1955	-1.8
	HMDB0179282	3-hydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M+H	255.1955	-1.8
	HMDB0036053	(3beta,9beta)-7-Drimene-3,11,12-triol	C15H26O3	M+H	255.1955	-1.8
	HMDB0029604	Lubiminol	C15H26O3	M+H	255.1955	-1.8
	HMDB0036866	7-Drimene-11,12,14-triol	C15H26O3	M+H	255.1955	-1.8
	HMDB0037197	Kessyl glycol	C15H26O3	M+H	255.1955	-1.8
	HMDB0040276	5-Acetoxydihydrotheaespirane	C15H26O3	M+H	255.1955	-1.8
	HMDB0035780	8-Hydroxy-4(6)-lactarene-5,14-diol	C15H26O3	M+H	255.1955	-1.8
255.2313	HMDB0171478	2-hydroxy-3-methylcyclopentadecan-1-one	C16H30O2	M+H	255.2319	-2.2
	HMDB0171479	2-hydroxy-14-methylcyclopentadecan-1-one	C16H30O2	M+H	255.2319	-2.2
	HMDB0171476	3-(hydroxymethyl)cyclopentadecan-1-one	C16H30O2	M+H	255.2319	-2.2
	HMDB0171477	Cyclopentadecanone, 3-hydroxy-3-methyl-	C16H30O2	M+H	255.2319	-2.2
	HMDB0038958	Citronellyl hexanoate	C16H30O2	M+H	255.2319	-2.2
	HMDB0031711	15-Hexadecanolide	C16H30O2	M+H	255.2319	-2.2
	HMDB0031145	5-Dodecyldihydro-2(3H)-furanone	C16H30O2	M+H	255.2319	-2.2
	HMDB0035877	(Z)-13-Hexadecenoic acid	C16H30O2	M+H	255.2319	-2.2
	HMDB0031053	(E)-6-Hexadecenoic acid	C16H30O2	M+H	255.2319	-2.2
	HMDB0032638	(Z)-5-Hexadecenoic acid	C16H30O2	M+H	255.2319	-2.2
	HMDB0041422	(Z)-14-Methyl-6-pentadecenoic acid	C16H30O2	M+H	255.2319	-2.2
	HMDB0037647	(E)-11-Hexadecenoic acid	C16H30O2	M+H	255.2319	-2.2
	HMDB0010735	Trans-Hexa-dec-2-enoic acid	C16H30O2	M+H	255.2319	-2.2
	HMDB0003229	Palmitoleic acid	C16H30O2	M+H	255.2319	-2.2
	HMDB0002186	Hypogeic acid	C16H30O2	M+H	255.2319	-2.2
	HMDB0033791	(E)-3-Hexadecenoic acid	C16H30O2	M+H	255.2319	-2.2
	HMDB0061979	11Z-hexadecenoic acid	C16H30O2	M+H	255.2319	-2.2
	HMDB0012328	Palmitelaidic acid	C16H30O2	M+H	255.2319	-2.2
	HMDB0031040	2-Heptadecanone	C17H34O	M+H	255.2682	-0.6
255.2681	HMDB0031039	Heptadecanal	C17H34O	M+H	255.2682	-0.6
	HMDB0061980	14-methyl-8-hexadecen-1-ol	C17H34O	M+H	255.2682	-0.6
256.1211	HMDB0171051	{[1-(oxiran-2-yl)heptyl]oxy}sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0171048	[(8-hydroxynon-1-en-3-yl)oxy]sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0171054	[(7-hydroxynon-8-en-1-yl)oxy]sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0171055	[(9-hydroxynon-1-en-3-yl)oxy]sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0179179	[(4-oxononyl)oxy]sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0179823	[(8-oxononan-2-yl)oxy]sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0179825	[(8-oxononyl)oxy]sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0179827	[(2-oxononyl)oxy]sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0171047	[(7-hydroxynon-8-en-2-yl)oxy]sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0163507	{[(6Z)-8-hydroxy-7-methyloct-6-en-1-yl]oxy}sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0163492	[(2E)-2-hexylidene-3-hydroxypropoxy]sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0163493	[(2Z)-2-hexylidene-3-hydroxypropoxy]sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0163496	{[(2Z)-4-hydroxy-2-methyloct-2-en-1-yl]oxy}sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9

	HMDB0163497	{[(2Z)-1-hydroxy-2-methyloct-2-en-4-yl]oxy}sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0163500	{[(2Z)-7-hydroxy-2-methyloct-2-en-1-yl]oxy}sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0163501	{[(6Z)-8-hydroxy-7-methyloct-6-en-2-yl]oxy}sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0163504	[(2-methyl-3-pentyloxiran-2-yl)methoxy]sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0163508	{[(2Z)-8-hydroxy-2-methyloct-2-en-1-yl]oxy}sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
	HMDB0179829	[(2-oxononan-3-yl)oxy]sulfonic acid	C9H18O5S	M+NH4	256.1213	-0.9
256.1385	HMDB0033065	(x)-1,2-Propanediol 1-O-b-D-glucopyranoside	C9H18O7	M+NH4	256.1391	-2.2
256.1536	HMDB0150426	4,5-bis(hydroxymethyl)-2-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C13H18O4	M+NH4	256.1543	-2.9
	HMDB0033191	2,2,4,4-Tetramethyl-6-(1-oxopropyl)-1,3,5-cyclohexanetrione	C13H18O4	M+NH4	256.1543	-2.9
	HMDB0034046	1,2,3,4-Tetramethoxy-5-(2-propenyl)benzene	C13H18O4	M+NH4	256.1543	-2.9
	HMDB0164386	4-{4-[(2E)-4-methyl-5-oxooxolan-2-ylidene]butyl}amino)butanoic acid	C13H21NO4	M+H	256.1543	-2.9
256.1901	HMDB0038256	Geranyl acetoacetate	C14H22O3	M+NH4	256.1907	-2.4
	HMDB0112083	3-(3,4-dimethyl-5-pentylfuran-2-yl)-propanoic acid	C14H22O3	M+NH4	256.1907	-2.4
256.2628	HMDB0037544	2-Dodecylcyclobutanone	C16H30O	M+NH4	256.2635	-2.7
	HMDB0034181	3-Methylcyclopentadecanone	C16H30O	M+NH4	256.2635	-2.7
	HMDB0060482	Hexadecenal	C16H30O	M+NH4	256.2635	-2.7
	HMDB0012273	Palmitic amide	C16H33NO	M+H	256.2635	-2.7
257.1745	HMDB0030993	5-Nonyltetrahydro-2-oxo-3-furancarboxylic acid	C14H24O4	M+H	257.1747	-0.9
	HMDB0062363	(6R,8Z)-6-Hydroxy-3-oxotetradecenoic acid	C14H24O4	M+H	257.1747	-0.9
	HMDB0036143	Monomenthyl succinate	C14H24O4	M+H	257.1747	-0.9
	HMDB0062364	(6S,8Z)-6-Hydroxy-3-oxotetradecenoic acid	C14H24O4	M+H	257.1747	-0.9
257.2473	HMDB0000220	Palmitic acid	C16H32O2	M+H	257.2475	-0.8
	HMDB0060083	Palmitic acid	C16H32O2	M+H	257.2475	-0.8
	HMDB0061373	Palmitic acid	C16H32O2	M+H	257.2475	-0.8
	HMDB0002396	Trimethyltridecanoic acid	C16H32O2	M+H	257.2475	-0.8
	HMDB0031068	Isopalmitic acid	C16H32O2	M+H	257.2475	-0.8
	HMDB0034153	Ethyl tetradecanoate	C16H32O2	M+H	257.2475	-0.8
	HMDB0036210	Dodecyl 2-methylpropanoate	C16H32O2	M+H	257.2475	-0.8
	HMDB0032065	Butyl dodecanoate	C16H32O2	M+H	257.2475	-0.8
	HMDB0033166	Octyl octanoate	C16H32O2	M+H	257.2475	-0.8
	HMDB0032249	Dodecyl butyrate	C16H32O2	M+H	257.2475	-0.8
	HMDB0032324	Hexyl decanoate	C16H32O2	M+H	257.2475	-0.8
257.9928	HMDB0166088	{[1-isothiocyano-4-(methylsulfanyl)butan-2-yl]oxy}sulfonic acid	C6H11NO4S3	M+H	257.9923	1.9
	HMDB0166092	{[4-isothiocyano-1-(methylsulfanyl)butan-2-yl]oxy}sulfonic acid	C6H11NO4S3	M+H	257.9923	1.9
258.1003	HMDB0172055	[(1-ethoxy-3-methyl-1-oxopentan-2-yl)oxy]sulfonic acid	C8H16O6S	M+NH4	258.1006	-1.1
	HMDB0172049	[(5-ethoxy-3-methyl-5-oxopentyl)oxy]sulfonic acid	C8H16O6S	M+NH4	258.1006	-1.1
	HMDB0172051	(4-ethoxy-2-ethyl-4-oxobutoxy)sulfonic acid	C8H16O6S	M+NH4	258.1006	-1.1
	HMDB0172047	[(5-ethoxy-3-methyl-5-oxopentan-2-yl)oxy]sulfonic acid	C8H16O6S	M+NH4	258.1006	-1.1
	HMDB0164652	[(6-hydroxy-8-oxooctan-2-yl)oxy]sulfonic acid	C8H16O6S	M+NH4	258.1006	-1.1
	HMDB0164651	[(7-hydroxy-1-oxooctan-3-yl)oxy]sulfonic acid	C8H16O6S	M+NH4	258.1006	-1.1
	HMDB0161161	2-(sulfooxy)octanoic acid	C8H16O6S	M+NH4	258.1006	-1.1
	HMDB0159453	82542-98-1	C8H16O6S	M+NH4	258.1006	-1.1
	HMDB0172053	{2-[(3-methylpentanoyl)oxy]ethoxy}sulfonic acid	C8H16O6S	M+NH4	258.1006	-1.1
258.1095	HMDB0033610	Pandamarilactam 3x	C13H17NO3	M+Na	258.1101	-2.2
	HMDB0139906	3-(4-hydroxyphenyl)-N-(4-oxobutyl)propanimidic acid	C13H17NO3	M+Na	258.1101	-2.2
	HMDB0164387	1-{4-[(2E)-4-methyl-5-oxooxolan-2-ylidene]butyl}-2-oxo-3,4-dihydro-2H-pyrrrol-1-ium	C13H18NO3	M+Na	258.1101	-2.2
	HMDB0000086	Glycerophosphocholine	C8H20NO6P	M+H	258.1101	-2.3
	HMDB0176432	SCHEMBL2554147	C13H20O4	M+NH4	258.1700	-2.3
	HMDB0176436	(9E,11E)-5-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M+NH4	258.1700	-2.3
	HMDB0176435	(9E,11E)-6-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M+NH4	258.1700	-2.3
	HMDB0176434	(9E,11E)-7-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M+NH4	258.1700	-2.3
	HMDB0176439	(9E,11E)-8-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M+NH4	258.1700	-2.3

258.1694	HMDB0176440	(9E)--(3-formyloxiran-2-yl)dec-9-enoic acid	C13H20O4	M+NH4	258.1700	-2.3
	HMDB0176437	(9E,11E)-4-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M+NH4	258.1700	-2.3
	HMDB0176438	(9E,11E)-3-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M+NH4	258.1700	-2.3
	HMDB0176441	8-{3-[(1E)-3-oxoprop-1-en-1-yl]oxiran-2-yl}octanoic acid	C13H20O4	M+NH4	258.1700	-2.3
	HMDB0176442	(9E,11E)-2-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M+NH4	258.1700	-2.3
258.2058	HMDB0013161	2-Hexenoylcarnitine	C13H23NO4	M+H	258.1700	-2.3
	HMDB0032369	L-Menthyl acetoacetate	C14H24O3	M+NH4	258.2064	-2.2
	HMDB0160292	4-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}butanoic acid	C14H24O3	M+NH4	258.2064	-2.2
	HMDB0160290	(8Z)--hydroxytetradeca-5,8-dienoic acid	C14H24O3	M+NH4	258.2064	-2.2
	HMDB0160291	SCHEMBL8918721	C14H24O3	M+NH4	258.2064	-2.2
	HMDB0160289	(5Z,8Z)-4-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M+NH4	258.2064	-2.2
	HMDB0160293	(5Z)-7-(3-pentyloxiran-2-yl)hept-5-enoic acid	C14H24O3	M+NH4	258.2064	-2.2
	HMDB0160295	(5Z,8Z)-2-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M+NH4	258.2064	-2.2
	HMDB0160296	(5Z,8Z)-7-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M+NH4	258.2064	-2.2
	HMDB0160294	(5Z,8Z)-14-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M+NH4	258.2064	-2.2
	HMDB0160298	(8Z)-5-hydroxytetradeca-6,8-dienoic acid	C14H24O3	M+NH4	258.2064	-2.2
	HMDB0160297	(5Z,7E)-9-hydroxytetradeca-5,7-dienoic acid	C14H24O3	M+NH4	258.2064	-2.2
258.2422	HMDB0013272	N-Lauroylglycine	C14H27NO3	M+H	258.2064	-2.2
	HMDB0032347	Isobutyl -undecenoate	C15H28O2	M+NH4	258.2428	-2.1
	HMDB0037190	Rhodinyl isovalerate	C15H28O2	M+NH4	258.2428	-2.1
	HMDB0039715	Auberganol	C15H28O2	M+NH4	258.2428	-2.1
	HMDB0034455	Exaltolide	C15H28O2	M+NH4	258.2428	-2.1
	HMDB0036426	Butyl undecylenate	C15H28O2	M+NH4	258.2428	-2.1
	HMDB0038954	Citronellyl isovalerate	C15H28O2	M+NH4	258.2428	-2.1
	HMDB0037211	Menthyl isovalerate	C15H28O2	M+NH4	258.2428	-2.1
	HMDB0037229	Citronellyl pentanoate	C15H28O2	M+NH4	258.2428	-2.1
	HMDB0040997	15,5-Farnesanolide	C15H28O2	M+NH4	258.2428	-2.1
258.2786	HMDB0029765	9-Pentadecenoic acid	C15H28O2	M+NH4	258.2428	-2.1
	HMDB0001551	Palmitaldehyde	C16H32O	M+NH4	258.2791	-2.1
	HMDB0062168	1-Hexadecenol	C16H32O	M+NH4	258.2791	-2.1
259.1898	HMDB0031052	2-Hexadecanone	C16H32O	M+NH4	258.2791	-2.1
	HMDB0000872	Tetradecanedioic acid	C14H26O4	M+H	259.1904	-2.3
	HMDB0176326	14-hydroxy-3-oxotetradecanoic acid	C14H26O4	M+H	259.1904	-2.3
	HMDB0176325	13-hydroxy-3-oxotetradecanoic acid	C14H26O4	M+H	259.1904	-2.3
	HMDB0176327	SCHEMBL886	C14H26O4	M+H	259.1904	-2.3
	HMDB0041618	Diisobutyl adipate	C14H26O4	M+H	259.1904	-2.3
	HMDB0059946	2-Hydroxypropyl 2-isopropyl-5-methylcyclohexyl carbonate	C14H26O4	M+H	259.1904	-2.3
	HMDB0059947	1-Hydroxypropan-2-yl 2-isopropyl-5-methylcyclohexyl carbonate	C14H26O4	M+H	259.1904	-2.3
	HMDB0040429	Diethyl decanedioate	C14H26O4	M+H	259.1904	-2.3
259.2050	HMDB0176328	4-hydroxy-3-oxotetradecanoic acid	C14H26O4	M+H	259.1904	-2.3
	HMDB0061860	2-Acetyl-3,5,5,6,8,8-hexamethyl-5,6,7,8-tetrahydronaphthalene	C18H26O	M+H	259.2056	-2.5
260.0523	HMDB0001125	Inositol cyclic phosphate	C6H11O8P	M+NH4	260.0530	-2.6
	HMDB0060436	Aminofructose 6-phosphate	C6H14NO8P	M+H	260.0530	-2.6
	HMDB0001109	Glucosamine-1P	C6H14NO8P	M+H	260.0530	-2.6
	HMDB0001254	Glucosamine 6-phosphate	C6H14NO8P	M+H	260.0530	-2.6
	HMDB0038942	Methyl 2,3-dihydro-3,5-dihydroxy-2-oxo-3-indoleacetic acid	C11H11NO5	M+Na	260.0529	-2.5
	HMDB0034251	N-Benzoylaspartic acid	C11H11NO5	M+Na	260.0529	-2.5
	HMDB0176461	(9E,11E)-2,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176450	8-[3-(3-oxopropyl)oxiran-2-yl]octanoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176447	(9E)-3-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176448	(9E)-8-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176446	(9E)-4-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176445	(9E)-5-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176443	(9E)-7-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176444	(9E)-6-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176451	(9E)-12-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176449	(9E)-11-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+NH4	260.1856	-2.4

260.1850	HMDB0176452	(9E)-2-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176460	8-{3-[(1E)-3-hydroxyprop-1-en-1-yl]oxiran-2-yl}octanoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176458	(9E,11E)-8,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176457	(9E,11E)-3,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176459	(9E)--[3-(hydroxymethyl)oxiran-2-yl]dec-9-enoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176456	(9E,11E)-4,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176455	(9E,11E)-5,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176454	(9E,11E)-6,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0176453	(9E,11E)-7,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0030987	2-Carboxy-4-dodecanolide	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0038736	(3S,5R,6R,7E)-3,5,6-Trihydroxy-7-megastigmen-9-one	C13H22O4	M+NH4	260.1856	-2.4
	HMDB0000705	Hexanoylcarnitine	C13H25NO4	M+H	260.1856	-2.4
	HMDB0000826	Pentadecanoic acid	C15H30O2	M+NH4	260.2584	-1.9
260.2579	HMDB0041588	2,6,-Trimethyldecanoic acid	C15H30O2	M+NH4	260.2584	-1.9
	HMDB0032250	Dodecyl propionate	C15H30O2	M+NH4	260.2584	-1.9
	HMDB0032328	Hexyl nonanoate	C15H30O2	M+NH4	260.2584	-1.9
	HMDB0040998	7(14)-Farnesene-9,12-diol	C15H30O2	M+NH4	260.2584	-1.9
	HMDB0036218	Heptyl octanoate	C15H30O2	M+NH4	260.2584	-1.9
	HMDB0038907	3-Methylbutyl decanoate	C15H30O2	M+NH4	260.2584	-1.9
	HMDB0036220	Octyl heptanoate	C15H30O2	M+NH4	260.2584	-1.9
	HMDB0030469	Methyl tetradecanoate	C15H30O2	M+NH4	260.2584	-1.9
	HMDB0037306	Pentyl decanoate	C15H30O2	M+NH4	260.2584	-1.9
	HMDB0059833	Ethyl tridecanoate	C15H30O2	M+NH4	260.2584	-1.9
	HMDB0059820	Isopropyl laurate	C15H30O2	M+NH4	260.2584	-1.9
	HMDB0062084	12-methyltetradecanoic acid	C15H30O2	M+NH4	260.2584	-1.9
	HMDB0061707	13-Methylmyristic acid	C15H30O2	M+NH4	260.2584	-1.9
261.0365	HMDB0039494	Benzoylmalic acid	C11H10O6	M+Na	261.0370	-1.7
	HMDB0137298	3-(7-hydroxy-4-methoxy-2H-1,3-benzodioxol-5-yl)prop-2-enoic acid	C11H10O6	M+Na	261.0370	-1.7
	HMDB0137297	3-(4-hydroxy-7-methoxy-2H-1,3-benzodioxol-5-yl)prop-2-enoic acid	C11H10O6	M+Na	261.0370	-1.7
	HMDB0128680	3-(7-hydroxy-6-methoxy-2H-1,3-benzodioxol-5-yl)prop-2-enoic acid	C11H10O6	M+Na	261.0370	-1.7
	HMDB0128679	3-(6-hydroxy-7-methoxy-2H-1,3-benzodioxol-5-yl)prop-2-enoic acid	C11H10O6	M+Na	261.0370	-1.7
	HMDB0062705	D-Galactopyranose 1-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0000994	Dolichyl phosphate D-mannose	C6H13O9P	M+H	261.0370	-1.9
	HMDB0000213	1D-myo-inositol 1-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0003498	beta-D-Glucose 6-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0002985	Inositol phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0001401	Glucose 6-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0001313	D-myo-Inositol 4-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0001078	Mannose 6-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0001076	Fructose 1-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0006814	D-myo-Inositol 3-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0000124	Fructose 6-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0001586	alpha-D-Glucose 1-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0000645	Galactose 1-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0003971	Beta-D-Fructose 6-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0006328	D-Tagatose 1-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0006797	Sorbose 1-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0006330	D-Mannose 1-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0060467	D-fructose 1-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0006873	D-Tagatose 6-phosphate	C6H13O9P	M+H	261.0370	-1.9
	HMDB0006800	Beta-D-Fructose 2-phosphate	C6H13O9P	M+H	261.0370	-1.9
261.0517	HMDB0141531	7-hydroxy-2-phenyl-4H-chromen-4-one	C15H10O3	M+Na	261.0522	-2.0
	HMDB0141530	6-hydroxy-2-phenyl-4H-chromen-4-one	C15H10O3	M+Na	261.0522	-2.0
	HMDB0141529	2-(2-hydroxyphenyl)-4H-chromen-4-one	C15H10O3	M+Na	261.0522	-2.0
	HMDB0031816	3-Hydroxyflavone	C15H10O3	M+Na	261.0522	-2.0
	HMDB0141532	2-(3-hydroxyphenyl)-4H-chromen-4-one	C15H10O3	M+Na	261.0522	-2.0
	HMDB0141534	5-hydroxy-2-phenyl-4H-chromen-4-one	C15H10O3	M+Na	261.0522	-2.0
	HMDB0130492	7-hydroxy-3-phenyl-4H-chromen-4-one	C15H10O3	M+Na	261.0522	-2.0
	HMDB0141533	2-(4-hydroxyphenyl)-4H-chromen-4-one	C15H10O3	M+Na	261.0522	-2.0

	HMDB0137519	6-hydroxy-2-(phenylmethylidene)-2,3-dihydro-1-benzofuran-3-one	C15H10O3	M+Na	261.0522	-2.0
	HMDB0002399	Cystathionine sulfoxide	C7H14N2O5S	M+Na	261.0516	0.5
261.0718	HMDB0126648	2-{[hydroxy(2,3,4,5-tetrahydroxyphenyl)methylidene]amino}acetic acid	C9H9NO7	M+NH4	261.0717	0.3
	HMDB0130445	2-{[hydroxy(2,3,4,6-tetrahydroxyphenyl)methylidene]amino}acetic acid	C9H9NO7	M+NH4	261.0717	0.3
	HMDB0177296	[hydroxy(2,3,4,5-tetrahydroxy-6-methylphenyl)methylidene]carbamic acid	C9H9NO7	M+NH4	261.0717	0.3
	HMDB0177302	{hydroxy[2,3,4-trihydroxy-6-(hydroxymethyl)phenyl]methylidene}carbamic acid	C9H9NO7	M+NH4	261.0717	0.3
261.0906	HMDB0162080	({7-methyl-5H,6H,7H-cyclopenta[c]pyridin-4-yl)methoxy)sulfonic acid	C10H13NO4S	M+NH4	261.0904	0.9
261.1481	HMDB0137241	(1E,4E)-1-(3,4-dihydroxyphenyl)deca-1,4-dien-3-one	C16H20O3	M+H	261.1485	-1.6
	HMDB0134736	2-(1-hydroxy-4-methylpent-3-en-1-yl)-2-methyl-2H-chromen-8-ol	C16H20O3	M+H	261.1485	-1.6
	HMDB0134734	2-(5-hydroxy-4-methylpent-3-en-1-yl)-2-methyl-2H-chromen-8-ol	C16H20O3	M+H	261.1485	-1.6
	HMDB0134732	2-[(3E)-5-hydroxy-4-methylpent-3-en-1-yl]-2-methyl-2H-chromen-8-ol	C16H20O3	M+H	261.1485	-1.6
	HMDB0134730	2-(2-hydroxy-4-methylpent-3-en-1-yl)-2-methyl-2H-chromen-8-ol	C16H20O3	M+H	261.1485	-1.6
	HMDB0134728	5-methyl-5-(4-methylpent-3-en-1-yl)-3,6-dioxatricyclo[5.4.undeca-1(7),8,-trien-8-ol	C16H20O3	M+H	261.1485	-1.6
	HMDB0134724	2-methyl-2-(4-methylpent-3-en-1-yl)-2H-chromene-7,8-diol	C16H20O3	M+H	261.1485	-1.6
	HMDB0134726	2-[2-(3,3-dimethyloxiran-2-yl)ethyl]-2-methyl-2H-chromen-8-ol	C16H20O3	M+H	261.1485	-1.6
	HMDB0134719	2-(hydroxymethyl)-2-(4-methylpent-3-en-1-yl)-2H-chromen-8-ol	C16H20O3	M+H	261.1485	-1.6
	HMDB0134722	2-methyl-2-(4-methylpent-3-en-1-yl)-2H-chromene-6,8-diol	C16H20O3	M+H	261.1485	-1.6
	HMDB0036456	-Hydroxy-3-methoxy-1,3,5,7-cadinatetraen-9-one	C16H20O3	M+H	261.1485	-1.6
261.1826	HMDB0182767	2-(1-hydroxypropan-2-yl)-4a-methyl-8-methylidene-decahydronaphthalen-1-ol	C15H26O2	M+Na	261.1825	0.4
	HMDB0182764	4a-(hydroxymethyl)-8-methylidene-2-(propan-2-yl)-decahydronaphthalen-1-ol	C15H26O2	M+Na	261.1825	0.4
	HMDB0182219	7-(2-hydroxypropan-2-yl)-1,8a-dimethyl-1,2,3,5,6,7,8,8a-octahydronaphthalen-1-ol	C15H26O2	M+Na	261.1825	0.4
	HMDB0182220	3-(2-hydroxypropan-2-yl)-4a,5-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalen-1-ol	C15H26O2	M+Na	261.1825	0.4
	HMDB0182221	6-(2-hydroxypropan-2-yl)-4,4a-dimethyl-2,3,4,4a,5,6,7,8-octahydronaphthalen-2-ol	C15H26O2	M+Na	261.1825	0.4
	HMDB0182218	2-[8-(hydroxymethyl)-8a-methyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl]propan-2-ol	C15H26O2	M+Na	261.1825	0.4
	HMDB0182217	2-[8a-(hydroxymethyl)-8-methyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl]propan-2-ol	C15H26O2	M+Na	261.1825	0.4
	HMDB0179265	2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O2	M+Na	261.1825	0.4
	HMDB0041589	alpha-Kessyl alcohol	C15H26O2	M+Na	261.1825	0.4
	HMDB0062130	methyl tetradec-13-ynoate	C15H26O2	M+Na	261.1825	0.4
	HMDB0036730	Tricyclohumuladiol	C15H26O2	M+Na	261.1825	0.4
	HMDB0038196	alpha-Bisabolol oxide A	C15H26O2	M+Na	261.1825	0.4
	HMDB0037284	5(1->)-Abeo-1,12-patchoulanediol	C15H26O2	M+Na	261.1825	0.4
	HMDB0036880	1,6,9-Farnesatriene-3,11-diol	C15H26O2	M+Na	261.1825	0.4
	HMDB0037279	2,-Bisaboladiene-1,4-diol	C15H26O2	M+Na	261.1825	0.4
	HMDB0034673	Calamendiol	C15H26O2	M+Na	261.1825	0.4
	HMDB0031383	(3S,4S,6R,7S)-1,-Bisaboladiene-3,4-diol	C15H26O2	M+Na	261.1825	0.4
	HMDB0038250	Isobornyl isovalerate	C15H26O2	M+Na	261.1825	0.4
	HMDB0033228	Guaidiol	C15H26O2	M+Na	261.1825	0.4
	HMDB0036032	3beta-7-Drimene-3,11-diol	C15H26O2	M+Na	261.1825	0.4
	HMDB0031384	beta-Kessyl alcohol	C15H26O2	M+Na	261.1825	0.4
	HMDB0035887	Germacrenone	C15H26O2	M+Na	261.1825	0.4
	HMDB0039130	Methyl (Z,Z)-5,8-tetradecadienoate	C15H26O2	M+Na	261.1825	0.4

	HMDB0038247	Bornyl valerate	C15H26O2	M+Na	261.1825	0.4
	HMDB0040273	Terpenyl isovalerate	C15H26O2	M+Na	261.1825	0.4
	HMDB0032343	Isobornyl 2-methylbutyrate	C15H26O2	M+Na	261.1825	0.4
	HMDB0032209	Citronellyl trans-2-methyl-2-butenate	C15H26O2	M+Na	261.1825	0.4
	HMDB0032291	Geranyl 2-methylbutyrate	C15H26O2	M+Na	261.1825	0.4
	HMDB0035287	Daucol	C15H26O2	M+Na	261.1825	0.4
	HMDB0038136	Curcumadiol	C15H26O2	M+Na	261.1825	0.4
	HMDB0038138	alpha-Bisabolol oxide C	C15H26O2	M+Na	261.1825	0.4
	HMDB0038197	alpha-Bisabolol oxide B	C15H26O2	M+Na	261.1825	0.4
	HMDB0030428	Linalyl isovalerate	C15H26O2	M+Na	261.1825	0.4
	HMDB0037195	2-Propenyl cyclohexanhexanoate	C15H26O2	M+Na	261.1825	0.4
	HMDB0040281	Geranyl valerate	C15H26O2	M+Na	261.1825	0.4
	HMDB0029350	Geranyl 3-methylbutanoate	C15H26O2	M+Na	261.1825	0.4
	HMDB0032054	alpha-Terpinyl pentanoate	C15H26O2	M+Na	261.1825	0.4
	HMDB0038248	Bornyl isovalerate	C15H26O2	M+Na	261.1825	0.4
	HMDB0039745	(2E,6E,9xi)-Farnesol	C15H26O2	M+Na	261.1825	0.4
	HMDB0182766	4a-methyl-8-methylidene-2-(propan-2-yl)-decahydronaphthalene-1,7-diol	C15H26O2	M+Na	261.1825	0.4
	HMDB0182222	2-(8,8a-dimethyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl)propane-1,2-diol	C15H26O2	M+Na	261.1825	0.4
	HMDB0182765	2-(2-hydroxypropan-2-yl)-4a-methyl-8-methylidene-decahydronaphthalen-1-ol	C15H26O2	M+Na	261.1825	0.4
261.1969	HMDB0014413	Ropinirole	C16H24N2O	M+H	261.1961	2.9
	HMDB0015070	Oxymetazoline	C16H24N2O	M+H	261.1961	2.9
	HMDB0033526	Chalciporone	C16H21NO	M+NH4	261.1961	2.9
	HMDB0162739	(8Z)-9-(2-methyl-2H-azepin-7-yl)nona-6,8-dien-3-one	C16H21NO	M+NH4	261.1961	2.9
262.1027	HMDB0000296	Uridine	C9H12N2O6	M+NH4	262.1034	-2.5
	HMDB0156330	Uridine	C9H12N2O6	M+NH4	262.1034	-2.5
	HMDB0000767	Pseudouridine	C9H12N2O6	M+NH4	262.1034	-2.5
	HMDB0028793	Glutaminylaspartic acid	C9H15N3O6	M+H	262.1034	-2.5
	HMDB0029144	gamma-Glutamylasparagine	C9H15N3O6	M+H	262.1034	-2.5
	HMDB0028814	Glutamylasparagine	C9H15N3O6	M+H	262.1034	-2.5
	HMDB0028730	Asparaginylglutamic acid	C9H15N3O6	M+H	262.1034	-2.5
	HMDB0028751	Aspartyl-Glutamine	C9H15N3O6	M+H	262.1034	-2.5
	HMDB0028767	Aspartyl-Gamma-glutamate	C9H15N3O6	M+H	262.1034	-2.5
262.1368	HMDB0240241	Thenyldiamine	C14H19N3S	M+H	262.1372	-1.7
262.1645	HMDB0032472	Polyethylene, oxidized	C12H20O5	M+NH4	262.1649	-1.5
	HMDB0061189	3-Hydroxyisovalerylcarnitine	C12H23NO5	M+H	262.1649	-1.5
	HMDB0062555	Hydroxyisovaleroyl carnitine	C12H23NO5	M+H	262.1649	-1.5
	HMDB0240421	2-Hydroxyisovalerylcarnitine	C12H23NO5	M+H	262.1649	-1.5
262.2007	HMDB0002327	1,11-Undecanedicarboxylic acid	C13H24O4	M+NH4	262.2013	-2.2
	HMDB0037184	1,4-Nonanediol diacetate	C13H24O4	M+NH4	262.2013	-2.2
	HMDB0036141	Menthyl ethylene glycol carbonate	C13H24O4	M+NH4	262.2013	-2.2
262.2371	HMDB0010731	(R)-3-Hydroxy-tetradecanoic acid	C14H28O3	M+NH4	262.2377	-2.2
	HMDB0176324	1,4-dihydroxytetradecan-3-one	C14H28O3	M+NH4	262.2377	-2.2
	HMDB0176322	1,14-dihydroxytetradecan-3-one	C14H28O3	M+NH4	262.2377	-2.2
	HMDB0176321	1,13-dihydroxytetradecan-3-one	C14H28O3	M+NH4	262.2377	-2.2
	HMDB0176323	1,2-dihydroxytetradecan-3-one	C14H28O3	M+NH4	262.2377	-2.2
	HMDB0171056	13-hydroxytetradecanoic acid	C14H28O3	M+NH4	262.2377	-2.2
	HMDB0171057	14-hydroxymyristic acid	C14H28O3	M+NH4	262.2377	-2.2
	HMDB0059850	Ethyl 3-hydroxydodecanoate	C14H28O3	M+NH4	262.2377	-2.2
	HMDB0094672	3-hydroxytetradecanoic acid	C14H28O3	M+NH4	262.2377	-2.2
	HMDB0032417	3-(L-Menthoxo)-2-methylpropane-1,2-diol	C14H28O3	M+NH4	262.2377	-2.2
	HMDB0002261	2-Hydroxymyristic acid	C14H28O3	M+NH4	262.2377	-2.2
	HMDB0061656	(S)-3-hydroxytetradecanoic acid	C14H28O3	M+NH4	262.2377	-2.2
263.1961	HMDB0000378	2-Methylbutyrylcarnitine	C12H23NO4	M+NH4	263.1965	-1.6
	HMDB0000688	Isovalerylcarnitine	C12H23NO4	M+NH4	263.1965	-1.6
	HMDB0041993	Pivaloylcarnitine	C12H23NO4	M+NH4	263.1965	-1.6
	HMDB0013128	Valerylcarnitine	C12H24NO4	M+NH4	263.1965	-1.6
264.0790	HMDB0014584	Gemcitabine	C9H11F2N3O4	M+H	264.0790	-0.1
264.2162	HMDB0072866	MG()	C13H26O4	M+NH4	264.2169	-2.8
	HMDB0072874	MG/)	C13H26O4	M+NH4	264.2169	-2.8
264.2533	HMDB0034557	8,8-Diethoxy-2,6-dimethyl-2-octanol	C14H30O3	M+NH4	264.2533	-0.1
	HMDB0163862	[(oxoundec-1-en-4-yl)oxy]sulfonic acid	C11H20O5S	M+H	265.1104	2.9

265.1112	HMDB0163864	[(-oxoundec-1-en-5-yl)oxy]sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163868	[(2-oxoundec--en-5-yl)oxy]sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163866	[(-oxoundec-1-en-6-yl)oxy]sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163870	[(2-oxoundec--en-4-yl)oxy]sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163872	[(-oxoundec-1-en-3-yl)oxy]sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163875	[(2-oxoundec--en-3-yl)oxy]sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163877	[(2-oxoundec--en-1-yl)oxy]sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0180788	{[(2E)-1-oxoundec-2-en-4-yl]oxy}sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0180791	{[(9E)-11-oxoundec-9-en-2-yl]oxy}sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163295	{[(2E,5Z)-11-hydroxyundeca-2,5-dien-1-yl]oxy}sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163294	{[(6Z,9E)-11-hydroxyundeca-6,9-dien-1-yl]oxy}sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163291	{[(2E)-4-(3-pentyloxiran-2-yl)but-2-en-1-yl]oxy}sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163265	{[(6Z)-11-oxoundec-6-en-5-yl]oxy}sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163267	{[(5Z)-1-oxoundec-5-en-4-yl]oxy}sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163269	{[(6Z)-11-oxoundec-6-en-2-yl]oxy}sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163273	{[(6Z)-11-oxoundec-6-en-1-yl]oxy}sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163275	{[(5Z)-1-oxoundec-5-en-2-yl]oxy}sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163278	{[(2E,5Z)-7-hydroxyundeca-2,5-dien-1-yl]oxy}sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163279	{[(6Z,9E)-11-hydroxyundeca-6,9-dien-5-yl]oxy}sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163282	{[(2E,5Z)--hydroxyundeca-2,5-dien-1-yl]oxy}sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163283	{[(6Z,9E)-11-hydroxyundeca-6,9-dien-2-yl]oxy}sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0163287	(({3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}methoxy)sulfonic acid	C11H20O5S	M+H	265.1104	2.9
	HMDB0180796	{[(9E)-11-oxoundec-9-en-1-yl]oxy}sulfonic acid	C11H20O5S	M+H	265.1104	2.9
265.1795	HMDB0061935	3,5-Bis(1,1-dimethylethyl)-4-hydroxy-benzoic acid ethyl ester	C16H24O3	M+H	265.1798	-1.2
	HMDB0032090	12-Oxo-2,3-dinor-,15-phytodienoic acid	C16H24O3	M+H	265.1798	-1.2
265.2157	HMDB0037224	alpha-Caryophyllene alcohol acetate	C17H28O2	M+H	265.2162	-1.9
	HMDB0240268	2-trans-6-trans-farnesyl acetate	C17H28O2	M+H	265.2162	-1.9
	HMDB0036153	Shyobunyl acetate	C17H28O2	M+H	265.2162	-1.9
	HMDB0037218	Guaiol acetate	C17H28O2	M+H	265.2162	-1.9
	HMDB0039630	Nerolidyl acetate	C17H28O2	M+H	265.2162	-1.9
	HMDB0037273	beta-Caryophyllene alcohol acetate	C17H28O2	M+H	265.2162	-1.9
	HMDB0035910	Cedryl acetate	C17H28O2	M+H	265.2162	-1.9
266.2109	HMDB0036640	Furanofukinin	C16H24O2	M+NH4	266.2115	-2.1
	HMDB0037713	Octyl phenylacetate	C16H24O2	M+NH4	266.2115	-2.1
	HMDB0037719	2-Phenylethyl octanoate	C16H24O2	M+NH4	266.2115	-2.1
	HMDB0036221	[2-(Dimethoxymethyl)-1-heptenyl]benzene	C16H24O2	M+NH4	266.2115	-2.1
266.2472	HMDB0032228	Dimethylbenzyl carbiny hexanoate	C16H24O2	M+NH4	266.2115	-2.1
	HMDB0041333	(all-Z)-8,11,14-Heptadecatrienal	C17H28O	M+NH4	266.2478	-2.4
	HMDB0060512	Sterol	C17H28O	M+NH4	266.2478	-2.4
	HMDB0030932	Avocadenofuran	C17H28O	M+NH4	266.2478	-2.4
267.0985	HMDB0135363	2-(1-hydroxy-3-phenylpropyl)benzene-1,4-diol	C15H16O3	M+Na	267.0992	-2.5
	HMDB0167509	1-(hydroxymethyl)-5,8-dimethyl-6H,7H,8H,9H-naphtho[2,1-b]furan-9-one	C15H16O3	M+Na	267.0992	-2.5
	HMDB0167511	6-hydroxy-1,5,8-trimethyl-6H,7H,8H,9H-naphtho[2,1-b]furan-9-one	C15H16O3	M+Na	267.0992	-2.5
	HMDB0167513	8-hydroxy-1,5,8-trimethyl-6H,7H,8H,9H-naphtho[2,1-b]furan-9-one	C15H16O3	M+Na	267.0992	-2.5
	HMDB0167512	8-(hydroxymethyl)-1,5-dimethyl-6H,7H,8H,9H-naphtho[2,1-b]furan-9-one	C15H16O3	M+Na	267.0992	-2.5
	HMDB0031925	5-Hydroxy-2-(5-methyl-1-oxo-4-hexenyl)benzofuran	C15H16O3	M+Na	267.0992	-2.5
	HMDB0038548	Glandulone B	C15H16O3	M+Na	267.0992	-2.5
	HMDB0030731	3-(1,1-Dimethylallyl)herniarin	C15H16O3	M+Na	267.0992	-2.5
	HMDB0032641	Batatasin IV	C15H16O3	M+Na	267.0992	-2.5
	HMDB0030636	Batatasin III	C15H16O3	M+Na	267.0992	-2.5
	HMDB0034723	Encelin	C15H16O3	M+Na	267.0992	-2.5

	HMDB0167508	5-(hydroxymethyl)-1,8-dimethyl-6H,7H,8H,9H-naphtho[2,1-b]furan-9-one	C15H16O3	M+Na	267.0992	-2.5
267.2314	HMDB0031050	Methyl 2E,4Z-hexadecadienoate	C17H30O2	M+H	267.2319	-1.7
268.1034	HMDB0037842	N-(1-Deoxy-1-fructosyl)serine	C9H17NO8	M+H	268.1027	2.6
	HMDB0000830	Neuraminic acid	C9H17NO8	M+H	268.1027	2.6
	HMDB0186389	3,4,5-trihydroxy-6-[(1-oxopropan-2-yl)oxy]oxane-2-carboxylic acid	C9H14O8	M+NH4	268.1027	2.6
	HMDB0175231	3,4,5-trihydroxy-6-(2-oxopropoxy)oxane-2-carboxylic acid	C9H14O8	M+NH4	268.1027	2.6
	HMDB0145209	3,4,5-trihydroxy-6-(propanoyloxy)oxane-2-carboxylic acid	C9H14O8	M+NH4	268.1027	2.6
	HMDB0187601	3,4,5-trihydroxy-6-(3-oxopropoxy)oxane-2-carboxylic acid	C9H14O8	M+NH4	268.1027	2.6
	HMDB0014340	Vidarabine	C10H13N5O4	M+H	268.1040	-2.3
	HMDB0014638	Zidovudine	C10H13N5O4	M+H	268.1040	-2.3
	HMDB0154951	2-(6-amino-9H-purin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol	C10H13N5O4	M+H	268.1040	-2.3
	HMDB0000050	Adenosine	C10H13N5O4	M+H	268.1040	-2.3
	HMDB0000085	Deoxyguanosine	C10H13N5O4	M+H	268.1040	-2.3
	HMDB0182305	6-(hydroxymethyl)-2-(3-hydroxyprop-1-en-2-yl)--methylspiro[4.5]dec-6-en-8-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0150689	2,5,5,8a-tetramethyl-6-oxo-1,4,4a,5,6,7,8,8a-octahydronaphthalene-1-carboxylic acid	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0177634	(1Z)-5-hydroxy-1-(2-hydroxyethylidene)-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0177633	(1Z)-1-ethylidene-5-hydroxy-7-(2-hydroxypropan-2-yl)-4-methylidene-octahydro-1H-inden-2-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0177635	(1Z)-1-ethylidene-5-hydroxy-7-(1-hydroxypropan-2-yl)-4-methylidene-octahydro-1H-inden-2-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0240642	3,5-di-tert-butyl-4-hydroxybenzoic acid	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0177636	(1Z)-1-ethylidene-3,5-dihydroxy-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0177703	(1E)-1-ethylidene-5-hydroxy-7-(1-hydroxypropan-2-yl)-4-methylidene-octahydro-1H-inden-2-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0182900	2,2a-dihydroxy-6,6,7b-trimethyl-1H,2H,2aH,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-3-carbaldehyde	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0183503	(8aR)-4,7-dihydroxy-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0183504	(8aR)-4-hydroxy-7-(3-hydroxyprop-1-en-2-yl)-1,8a-dimethyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0183502	(8aS)-1,4-dihydroxy-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0183506	(8aR)-4-hydroxy-1,8a-dimethyl-7-(2-methyloxiran-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0184276	(8aS)-4-hydroxy-8a-(hydroxymethyl)-1-methyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0184279	(8aR)-3,4-dihydroxy-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0182311	9-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0182310	1-(hydroxymethyl)-3-methyl-3'-(prop-1-en-2-yl)-7-oxaspiro[bicyclo[4.1]heptane-2,1'-cyclopentane]-5-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0182308	1-hydroxy-6-(hydroxymethyl)--methyl-3-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0177701	(1E)-1-ethylidene-5-hydroxy-7-(2-hydroxypropan-2-yl)-4-methylidene-octahydro-1H-inden-2-one	C15H22O3	M+NH4	268.1907	-2.3

268.1901	HMDB0177702	(1E)-5-hydroxy-1-(2-hydroxyethylidene)-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0177704	(1E)-1-ethylidene-3,5-dihydroxy-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0182302	6,-bis(hydroxymethyl)-2-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0182303	-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0182304	2-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0182307	2-hydroxy-6-(hydroxymethyl)--methyl-3-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0182306	1-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0182309	6-(hydroxymethyl)--methyl-2-(2-methyloxiran-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0035358	Ketosantalac acid	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0035137	Heliannuol D	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0035117	(3beta,6beta)-Furanoeremophilane-3,6-diol	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0035798	Piperdial	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0036563	Valerenolic acid	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0039644	Heliannuol A	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0036036	6,6-Dimethoxy-2,5,5-trimethyl-2-hexene	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0035760	3-Hydroxytrichothecene	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0039156	3beta-Hydroxycinnamolide	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0040754	(3beta,8beta)-3-Hydroxy-7(11)-eremophilen-12,8-olide	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0015371	Gemfibrozil	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0037064	FS4 toxin	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0036037	13-Hydroxymarasmene	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0034721	Procucumadiol	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0036664	Ketopelenolide a	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0037559	Cadabacilone	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0031901	Blennin A	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0036550	3-Ketoapotrithothecene	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0039635	Abscisic alcohol	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0037529	Lactaronecatorin A	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0035148	(6beta,8alpha)-6-Hydroxy-7(11)-eremophilen-12,8-olide	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0030917	1-Hydroxyacorenone	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0061839	Ethylhexyl salicylate	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0177902	3-hydroxy-7,7a-dimethyl-4'-methylidene-octahydrospiro[indene-2,3'-oxolane]-2'-one	C15H22O3	M+NH4	268.1907	-2.3
	HMDB0001932	Metoprolol	C15H25NO3	M+H	268.1907	-2.3
268.2265	HMDB0240361	(7Z,Z,13Z)-hexadecatrienoate	C16H25O2	M+NH4	268.2271	-2.2
	HMDB0159344	(7Z,Z)-hexadeca-7,,15-trienoic acid	C16H26O2	M+NH4	268.2271	-2.2
	HMDB0061952	AC1LBPUV	C16H26O2	M+NH4	268.2271	-2.2
	HMDB0035293	Norambreinolide	C16H26O2	M+NH4	268.2271	-2.2
	HMDB0037631	3-Methyl-alpha-ionyl acetate	C16H26O2	M+NH4	268.2271	-2.2
	HMDB0037712	[2,2-Bis(2-methylpropoxy)ethyl]benzene	C16H26O2	M+NH4	268.2271	-2.2
269.0874	HMDB0000425	3-Deoxy-D-glycero-D-galacto-2-nonulosonic acid	C9H16O9	M+H	269.0867	2.6
	HMDB0000195	Inosine	C10H12N4O5	M+H	269.0880	-2.4
	HMDB0155730	2-(6-hydroxy-9H-purin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol	C10H12N4O5	M+H	269.0880	-2.4
	HMDB0000481	Allopurinol riboside	C10H12N4O5	M+H	269.0880	-2.4
	HMDB0003040	Arabinosylhypoxanthine	C10H12N4O5	M+H	269.0880	-2.4
	HMDB0179332	3,8a-dimethyl-5-methylidene-2H,3H,3aH,4H,4aH,5H,6H,8aH,9H,9aH-naphtho[2,3-b]furan-2,6-dione	C15H18O3	M+Na	269.1148	-2.6
	HMDB0179330	8a-methyl-3,5-dimethylidene-dodecahydronaphtho[2,3-b]furan-2,6-dione	C15H18O3	M+Na	269.1148	-2.6

269.1141	HMDB0170855	2-methoxy-4-(prop-2-en-1-yl)phenyl 3-methylbut-3-enoate	C15H18O3	M+Na	269.1148	-2.6
	HMDB0179331	5,8a-dimethyl-3-methylidene-2H,3H,3aH,4H,4aH,5H,6H,8aH,9H,9aH-naphtho[2,3-b]furan-2,6-dione	C15H18O3	M+Na	269.1148	-2.6
	HMDB0035902	Enokipodin B	C15H18O3	M+Na	269.1148	-2.6
	HMDB0040903	Ipomeabifuran	C15H18O3	M+Na	269.1148	-2.6
	HMDB0038188	Curcolone	C15H18O3	M+Na	269.1148	-2.6
	HMDB0031916	5-Hydroxy-2-(1-hydroxy-5-methyl-4-hexenyl)benzofuran	C15H18O3	M+Na	269.1148	-2.6
	HMDB0037558	3-Oxo-1,4,11(13)-eudesmatrien-12-oic acid	C15H18O3	M+Na	269.1148	-2.6
	HMDB0036473	8-Epixanthatin	C15H18O3	M+Na	269.1148	-2.6
	HMDB0037801	Annuolide A	C15H18O3	M+Na	269.1148	-2.6
	HMDB0030911	2-Oxo-5,11(13)-eudesmadien-12,8-olide	C15H18O3	M+Na	269.1148	-2.6
	HMDB0031900	Methyl (2E,4Z,6E,8E,E)-4,8-dimethyl-12-oxo-2,4,6,8,-dodecapentaenoate	C15H18O3	M+Na	269.1148	-2.6
	HMDB0036488	Annuolide C	C15H18O3	M+Na	269.1148	-2.6
	HMDB0038547	Glandulone A	C15H18O3	M+Na	269.1148	-2.6
	HMDB0036455	Lacinilene C	C15H18O3	M+Na	269.1148	-2.6
	HMDB0036767	Hyacinthin	C15H18O3	M+Na	269.1148	-2.6
	HMDB0038202	Zedoarol	C15H18O3	M+Na	269.1148	-2.6
	HMDB0041920	Loxoprofen	C15H18O3	M+Na	269.1148	-2.6
269.1731	HMDB0072866	MG()	C13H26O4	M+Na	269.1723	2.9
	HMDB0072874	MG/)	C13H26O4	M+Na	269.1723	2.9
269.2468	HMDB0030997	Cyclohexaneundecanoic acid	C17H32O2	M+H	269.2475	-2.6
	HMDB0062437	(9Z)-heptadecenoic acid	C17H32O2	M+H	269.2475	-2.6
	HMDB0040888	2,4-Heptadecanedione	C17H32O2	M+H	269.2475	-2.6
	HMDB0031046	9E-Heptadecenoic acid	C17H32O2	M+H	269.2475	-2.6
	HMDB0060038	Z-Heptadecenoic acid	C17H32O2	M+H	269.2475	-2.6
	HMDB0061858	7-Hexadecenoic acid, methyl ester	C17H32O2	M+H	269.2475	-2.6
270.0908	HMDB0013968	Hydroxyzileuton	C11H12N2O3S	M+NH4	270.0907	0.4
	HMDB0013969	Zileuton sulfoxide	C11H12N2O3S	M+NH4	270.0907	0.4
270.1694	HMDB0175188	7-hydroxyheptyl 4-hydroxybenzoate	C14H20O4	M+NH4	270.1700	-2.2
	HMDB0175187	6-hydroxyheptyl 4-hydroxybenzoate	C14H20O4	M+NH4	270.1700	-2.2
	HMDB0175189	CHEMBL128785	C14H20O4	M+NH4	270.1700	-2.2
	HMDB0162484	2-[(3-hydroxy-5-methoxyphenyl)methyl]-6-methyloxan-4-ol	C14H20O4	M+NH4	270.1700	-2.2
	HMDB0059661	QH(2)	C14H20O4	M+NH4	270.1700	-2.2
	HMDB0036047	3alpha-Hydroxyoreadone	C14H20O4	M+NH4	270.1700	-2.2
	HMDB0033197	2,2,4,4-Tetramethyl-6-(1-oxobutyl)-1,3,5-cyclohexanetrione	C14H20O4	M+NH4	270.1700	-2.2
	HMDB0182319	6-(hydroxymethyl)--methyl-2-(2-methyloxiran-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0182312	6,-bis(hydroxymethyl)-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0182314	2-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0182313	6-hydroxy--(hydroxymethyl)-6-methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0182315	6-(hydroxymethyl)-2-(3-hydroxyprop-1-en-2-yl)--methylspiro[4.5]decan-8-one	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0179270	1-(3,3-dimethyloxiran-2-yl)-3-(4-hydroxy-4-methylcyclohex-2-en-1-yl)butan-1-one	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0179271	6-{5-hydroxy-5-methyl-7-oxabicyclo[4.1]heptan-2-yl}-2-methylhept-2-en-4-one	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0179273	5-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0179272	7-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0179267	6-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0179266	6-[4-hydroxy-4-(hydroxymethyl)cyclohex-2-en-1-yl]-2-methylhept-2-en-4-one	C15H24O3	M+NH4	270.2064	-2.1

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HMDB0179269	1-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M+NH4	270.2064	-2.1
HMDB0179268	6-(1,4-dihydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M+NH4	270.2064	-2.1
HMDB0179258	3,3a-dihydroxy-3,8-dimethyl-5-(propan-2-yl)-1,2,3,3a,4,5,6,8a-octahydroazulen-6-one	C15H24O3	M+NH4	270.2064	-2.1
HMDB0182318	1-hydroxy-6-(hydroxymethyl)--methyl-3-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+NH4	270.2064	-2.1
HMDB0182317	2-hydroxy-6-(hydroxymethyl)--methyl-3-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+NH4	270.2064	-2.1
HMDB0182316	1-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+NH4	270.2064	-2.1
HMDB0184275	(4aR)-4,4a-dimethyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3,7-triol	C15H24O3	M+NH4	270.2064	-2.1
HMDB0184273	(4aS)-4a-(hydroxymethyl)-4-methyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M+NH4	270.2064	-2.1
HMDB0183500	(4aR)-4,4a-dimethyl-6-(2-methyloxiran-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M+NH4	270.2064	-2.1
HMDB0183498	(4aR)-6-(3-hydroxyprop-1-en-2-yl)-4,4a-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M+NH4	270.2064	-2.1
HMDB0183496	(8aS)-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalene-1,2,4-triol	C15H24O3	M+NH4	270.2064	-2.1
HMDB0183495	(4aR)-4-(hydroxymethyl)-4a-methyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M+NH4	270.2064	-2.1
HMDB0182320	7-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+NH4	270.2064	-2.1
HMDB0182321	7-hydroxy--(hydroxymethyl)-6-methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M+NH4	270.2064	-2.1
HMDB0179257	1,8a-dihydroxy-1,4-dimethyl-7-(propan-2-ylidene)-decahydroazulen-6-one	C15H24O3	M+NH4	270.2064	-2.1
HMDB0179147	(6Z)-2-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M+NH4	270.2064	-2.1
HMDB0179146	(6Z)-5-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M+NH4	270.2064	-2.1
HMDB0179144	1,7-dimethyl-4-(propan-2-yl)-11-oxabicyclo[8.1]undecane-3,6-dione	C15H24O3	M+NH4	270.2064	-2.1
HMDB0179145	(6Z)-3-(1-hydroxypropan-2-yl)-6,-dimethylcyclodec-6-ene-1,4-dione	C15H24O3	M+NH4	270.2064	-2.1
HMDB0179148	(6Z)-3-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M+NH4	270.2064	-2.1
HMDB0179142	(6Z)-3-(2-hydroxypropan-2-yl)-6,-dimethylcyclodec-6-ene-1,4-dione	C15H24O3	M+NH4	270.2064	-2.1
HMDB0179143	(6Z)-8-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M+NH4	270.2064	-2.1
HMDB0179141	(6Z)--hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M+NH4	270.2064	-2.1
HMDB0179140	(6Z)--(hydroxymethyl)-6-methyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M+NH4	270.2064	-2.1
HMDB0179139	(6E)-6-(hydroxymethyl)--methyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M+NH4	270.2064	-2.1
HMDB0177221	(4aR,7aS,7bR)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4-diol	C15H24O3	M+NH4	270.2064	-2.1
HMDB0168751	(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trienal	C15H24O3	M+NH4	270.2064	-2.1
HMDB0112086	5-(3-methyl-5-pentylfuran-2-yl)-pentanoic acid	C15H24O3	M+NH4	270.2064	-2.1
HMDB0112094	3-Methyl-5-propyl-2-furanheptanoic acid	C15H24O3	M+NH4	270.2064	-2.1
HMDB0030918	1-Hydroxyepiacorone	C15H24O3	M+NH4	270.2064	-2.1
HMDB0035729	Dihydromyoporone	C15H24O3	M+NH4	270.2064	-2.1
HMDB0037969	Urodiolenone	C15H24O3	M+NH4	270.2064	-2.1
HMDB0032122	3(4->5)-Abeo-4,11:4,12-diepoxy-3-eudesmanol	C15H24O3	M+NH4	270.2064	-2.1
HMDB0037063	Toxin FS2	C15H24O3	M+NH4	270.2064	-2.1
HMDB0035613	Epioxylubimin	C15H24O3	M+NH4	270.2064	-2.1
HMDB0034574	Apotrichodiol	C15H24O3	M+NH4	270.2064	-2.1
HMDB0035767	Piperalol	C15H24O3	M+NH4	270.2064	-2.1

	HMDB0036448	Zedoarondiol	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0033149	(4R,5S,7R,11R)-11,12-Dihydroxy-1()-spirovetiven-2-one	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0035309	6alpha-Carissanol	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0038502	Bisacurone B	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0036663	Hydroxypelenolide	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0030919	Acorusdiol	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0035597	alpha-Carissanol	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0040685	2,3-Dihydroabscisic alcohol	C15H24O3	M+NH4	270.2064	-2.1
	HMDB0032255	N-[(Ethoxycarbonyl)methyl]-p-menthane-3-carboxamide	C15H27NO3	M+H	270.2064	-2.1
270.2422	HMDB0166468	(3Z)-hexadeca-3,15-dienoic acid	C16H28O2	M+NH4	270.2428	-2.0
	HMDB0032340	Isoambrettolide	C16H28O2	M+NH4	270.2428	-2.0
	HMDB0038255	Geranyl 2-ethylbutyrate	C16H28O2	M+NH4	270.2428	-2.0
	HMDB0031086	(Z)-7-Hexadecen-1,16-olide	C16H28O2	M+NH4	270.2428	-2.0
	HMDB0030429	Linalyl hexanoate	C16H28O2	M+NH4	270.2428	-2.0
	HMDB0029351	Geranyl hexanoate	C16H28O2	M+NH4	270.2428	-2.0
	HMDB0037805	D6-Ambrettolide	C16H28O2	M+NH4	270.2428	-2.0
	HMDB0039131	Ethyl (Z,Z)-5,8-tetradecadienoate	C16H28O2	M+NH4	270.2428	-2.0
270.2786	HMDB0000477	7Z,Z-Hexadecadienoic acid	C16H28O2	M+NH4	270.2428	-2.0
	HMDB0041335	8-Heptadecenal	C17H32O	M+NH4	270.2791	-2.0
	HMDB0013813	13-Heptadecyn-1-ol	C17H32O	M+NH4	270.2791	-2.0
	HMDB0040940	Capsiamide	C17H35NO	M+H	270.2791	-2.0
271.0750	HMDB0240217	(2R)-2-amino-3-({2-hydroxy-5-[(1-hydroxyethylidene)amino]phenyl}sulfanyl)propanoic acid	C11H14N2O4S	M+H	271.0747	1.1
	HMDB0166034	[1-(1H-1,3-benzodiazol-2-yl)butoxy]sulfonic acid	C11H14N2O4S	M+H	271.0747	1.1
	HMDB0166037	{[4-(1H-1,3-benzodiazol-2-yl)butan-2-yl]oxy}sulfonic acid	C11H14N2O4S	M+H	271.0747	1.1
	HMDB0166039	[4-(1H-1,3-benzodiazol-2-yl)butoxy]sulfonic acid	C11H14N2O4S	M+H	271.0747	1.1
271.2261	HMDB0010733	3-Oxohexadecanoic acid	C16H30O3	M+H	271.2268	-2.5
	HMDB0160971	(9Z)-11-hydroxyhexadec-9-enoic acid	C16H30O3	M+H	271.2268	-2.5
	HMDB0160975	16-hydroxy-9Z-hexadecenoic acid	C16H30O3	M+H	271.2268	-2.5
	HMDB0160972	8-Hydroxypalmitoleic acid	C16H30O3	M+H	271.2268	-2.5
	HMDB0160974	9-Epoxyhexadecanoic acid	C16H30O3	M+H	271.2268	-2.5
	HMDB0160973	(9Z)-15-hydroxyhexadec-9-enoic acid	C16H30O3	M+H	271.2268	-2.5
	HMDB0160976	hydroxy-palmitoleic acid	C16H30O3	M+H	271.2268	-2.5
	HMDB0166464	2-(3-dodecyloxiran-2-yl)acetic acid	C16H30O3	M+H	271.2268	-2.5
	HMDB0166462	(3Z)-5-hydroxyhexadec-3-enoic acid	C16H30O3	M+H	271.2268	-2.5
	HMDB0166465	(3Z)-16-hydroxyhexadec-3-enoic acid	C16H30O3	M+H	271.2268	-2.5
	HMDB0166463	(3Z)-15-hydroxyhexadec-3-enoic acid	C16H30O3	M+H	271.2268	-2.5
	HMDB0166466	(3Z)-2-hydroxyhexadec-3-enoic acid	C16H30O3	M+H	271.2268	-2.5
	HMDB0030978	11-Oxohexadecanoic acid	C16H30O3	M+H	271.2268	-2.5
	HMDB0030972	8-Oxohexadecanoic acid	C16H30O3	M+H	271.2268	-2.5
	HMDB0030973	9-Oxohexadecanoic acid	C16H30O3	M+H	271.2268	-2.5
	HMDB0166467	4-hydroxy-trans-2-hexadecenoic acid	C16H30O3	M+H	271.2268	-2.5
271.2625	HMDB0002259	Heptadecanoic acid	C17H34O2	M+H	271.2632	-2.4
	HMDB0061709	15-Methylpalmitate	C17H34O2	M+H	271.2632	-2.4
	HMDB0031067	(S)-14-Methylhexadecanoic acid	C17H34O2	M+H	271.2632	-2.4
	HMDB0040598	11-Methylhexadecanoic acid	C17H34O2	M+H	271.2632	-2.4
	HMDB0040392	Isopropyl tetradecanoate	C17H34O2	M+H	271.2632	-2.4
	HMDB0061859	Methyl hexadecanoic acid	C17H34O2	M+H	271.2632	-2.4
	HMDB0037372	3-Methylbutyl dodecanoate	C17H34O2	M+H	271.2632	-2.4
	HMDB0034131	Nonyl octanoate	C17H34O2	M+H	271.2632	-2.4
	HMDB0059870	Ethyl pentadecanoate	C17H34O2	M+H	271.2632	-2.4
	HMDB0061969	Pentadecyl acetate	C17H34O2	M+H	271.2632	-2.4
272.0993	HMDB0159272	3-carbamimidamido-6-(1,2,3-trihydroxypropyl)-3,4-dihydropyrazine-2-carboxylic acid	C9H13N5O5	M+H	272.0989	1.3
	HMDB0179275	2-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylheptan-4-one	C15H26O3	M+NH4	272.2220	-1.9
	HMDB0179276	2-hydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M+NH4	272.2220	-1.9

272.2215	HMDB0179277	2-(1,4-dihydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M+NH4	272.2220	-1.9
	HMDB0179274	2-[4-hydroxy-4-(hydroxymethyl)cyclohex-2-en-1-yl]-6-methylheptan-4-one	C15H26O3	M+NH4	272.2220	-1.9
	HMDB0179278	2-{5-hydroxy-5-methyl-7-oxabicyclo[4.1]heptan-2-yl}-6-methylheptan-4-one	C15H26O3	M+NH4	272.2220	-1.9
	HMDB0179281	3-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylheptan-4-one	C15H26O3	M+NH4	272.2220	-1.9
	HMDB0179279	1-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylheptan-4-one	C15H26O3	M+NH4	272.2220	-1.9
	HMDB0179280	1-hydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M+NH4	272.2220	-1.9
	HMDB0179282	3-hydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M+NH4	272.2220	-1.9
	HMDB0036053	(3beta,9beta)-7-Drimen-3,11,12-triol	C15H26O3	M+NH4	272.2220	-1.9
	HMDB0029604	Lubiminol	C15H26O3	M+NH4	272.2220	-1.9
	HMDB0036866	7-Drimen-11,12,14-triol	C15H26O3	M+NH4	272.2220	-1.9
	HMDB0037197	Kessyl glycol	C15H26O3	M+NH4	272.2220	-1.9
	HMDB0040276	5-Acetoxydihydrotheaespirane	C15H26O3	M+NH4	272.2220	-1.9
	HMDB0035780	8-Hydroxy-4(6)-lactarene-5,14-diol	C15H26O3	M+NH4	272.2220	-1.9
	HMDB0013317	Tridecanoylglycine	C15H29NO3	M+H	272.2220	-1.9
272.2578	HMDB0171478	2-hydroxy-3-methylcyclopentadecan-1-one	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0171479	2-hydroxy-14-methylcyclopentadecan-1-one	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0171476	3-(hydroxymethyl)cyclopentadecan-1-one	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0171477	Cyclopentadecanone, 3-hydroxy-3-methyl-	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0038958	Citronellyl hexanoate	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0031711	15-Hexadecanolide	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0031145	5-Dodecyldihydro-2(3H)-furanone	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0035877	(Z)-13-Hexadecenoic acid	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0031053	(E)-6-Hexadecenoic acid	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0032638	(Z)-5-Hexadecenoic acid	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0041422	(Z)-14-Methyl-6-pentadecenoic acid	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0037647	(E)-11-Hexadecenoic acid	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0010735	Trans-Hexa-dec-2-enoic acid	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0003229	Palmitoleic acid	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0002186	Hypogeic acid	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0033791	(E)-3-Hexadecenoic acid	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0061979	11Z-hexadecenoic acid	C16H30O2	M+NH4	272.2584	-2.2
	HMDB0012328	Palmitelaidic acid	C16H30O2	M+NH4	272.2584	-2.2
272.2942	HMDB0031040	2-Heptadecanone	C17H34O	M+NH4	272.2948	-2.2
	HMDB0031039	Heptadecanal	C17H34O	M+NH4	272.2948	-2.2
	HMDB0061980	14-methyl-8-hexadecen-1-ol	C17H34O	M+NH4	272.2948	-2.2
274.1642	HMDB0176464	(2E,4E)-9-hydroxytrideca-2,4-dienedioic acid	C13H20O5	M+NH4	274.1649	-2.5
	HMDB0176463	(2E,4E)-8-hydroxytrideca-2,4-dienedioic acid	C13H20O5	M+NH4	274.1649	-2.5
	HMDB0176462	(2E,4E)-7-hydroxytrideca-2,4-dienedioic acid	C13H20O5	M+NH4	274.1649	-2.5
	HMDB0176465	(2E,4E)--hydroxytrideca-2,4-dienedioic acid	C13H20O5	M+NH4	274.1649	-2.5
	HMDB0176466	(2E,4E)-11-hydroxytrideca-2,4-dienedioic acid	C13H20O5	M+NH4	274.1649	-2.5
	HMDB0176468	3-[(1E)-9-carboxynon-1-en-1-yl]oxirane-2-carboxylic acid	C13H20O5	M+NH4	274.1649	-2.5
	HMDB0176467	(2E,4E)-6-hydroxytrideca-2,4-dienedioic acid	C13H20O5	M+NH4	274.1649	-2.5
	HMDB0176469	8-{3-[(1E)-2-carboxyeth-1-en-1-yl]oxiran-2-yl}octanoic acid	C13H20O5	M+NH4	274.1649	-2.5
	HMDB0031772	1-Methoxy-1-(2,4,5-trimethoxyphenyl)-2-propanol	C13H20O5	M+NH4	274.1649	-2.5
	HMDB0040352	2-[4-(3-Hydroxypropyl)-2-methoxyphenoxy]-1,3-propanediol	C13H20O5	M+NH4	274.1649	-2.5
	HMDB0176470	(2E,4E)-12-hydroxytrideca-2,4-dienedioic acid	C13H20O5	M+NH4	274.1649	-2.5
274.2005	HMDB0030993	5-Nonyltetrahydro-2-oxo-3-furancarboxylic acid	C14H24O4	M+NH4	274.2013	-2.9
	HMDB0062363	(6R,8Z)-6-Hydroxy-3-oxotetradecenoic acid	C14H24O4	M+NH4	274.2013	-2.9
	HMDB0036143	Monomethyl succinate	C14H24O4	M+NH4	274.2013	-2.9
	HMDB0062364	(6S,8Z)-6-Hydroxy-3-oxotetradecenoic acid	C14H24O4	M+NH4	274.2013	-2.9
	HMDB0013238	Heptanoylcarnitine	C14H27NO4	M+H	274.2013	-2.9
	HMDB0000220	Palmitic acid	C16H32O2	M+NH4	274.2741	-2.0
	HMDB0060083	Palmitic acid	C16H32O2	M+NH4	274.2741	-2.0
	HMDB0061373	Palmitic acid	C16H32O2	M+NH4	274.2741	-2.0
	HMDB0002396	Trimethyltridecanoic acid	C16H32O2	M+NH4	274.2741	-2.0

274.2735	HMDB0031068	Isopalmitic acid	C16H32O2	M+NH4	274.2741	-2.0
	HMDB0034153	Ethyl tetradecanoate	C16H32O2	M+NH4	274.2741	-2.0
	HMDB0036210	Dodecyl 2-methylpropanoate	C16H32O2	M+NH4	274.2741	-2.0
	HMDB0032065	Butyl dodecanoate	C16H32O2	M+NH4	274.2741	-2.0
	HMDB0033166	Octyl octanoate	C16H32O2	M+NH4	274.2741	-2.0
	HMDB0032249	Dodecyl butyrate	C16H32O2	M+NH4	274.2741	-2.0
	HMDB0032324	Hexyl decanoate	C16H32O2	M+NH4	274.2741	-2.0
275.0675	HMDB0015257	Anisindione	C16H12O3	M+Na	275.0679	-1.3
	HMDB0145120	7-Hydroxy-3-methylflavone	C16H12O3	M+Na	275.0679	-1.3
	HMDB0145121	6-hydroxy-3-methyl-2-phenyl-4H-chromen-4-one	C16H12O3	M+Na	275.0679	-1.3
	HMDB0145119	CHEMBL22357	C16H12O3	M+Na	275.0679	-1.3
	HMDB0145122	292-21-7	C16H12O3	M+Na	275.0679	-1.3
	HMDB0145124	2-(4-HYDROXYPHENYL)-3-METHYL-4H-CHROMEN-4-ONE	C16H12O3	M+Na	275.0679	-1.3
	HMDB0145123	2-(3-hydroxyphenyl)-3-methyl-4H-chromen-4-one	C16H12O3	M+Na	275.0679	-1.3
	HMDB0147594	7-methoxy-3-phenyl-4H-chromen-4-one	C16H12O3	M+Na	275.0679	-1.3
	HMDB0033979	7-Hydroxy-2-methylisoflavone	C16H12O3	M+Na	275.0679	-1.3
276.1810	HMDB0013131	Hydroxyhexanoycarnitine	C13H25NO5	M+H	276.1805	1.6
	HMDB0061633	[(2R)-3-carboxy-2-[(3S)-3-hydroxyhexanoyloxy]propyl]trimethylazanium	C13H26NO5	M+H	276.1805	1.6
276.2163	HMDB0000872	Tetradecanedioic acid	C14H26O4	M+NH4	276.2169	-2.3
	HMDB0176325	13-hydroxy-3-oxotetradecanoic acid	C14H26O4	M+NH4	276.2169	-2.3
	HMDB0176327	SCHEMBL886	C14H26O4	M+NH4	276.2169	-2.3
	HMDB0176326	14-hydroxy-3-oxotetradecanoic acid	C14H26O4	M+NH4	276.2169	-2.3
	HMDB0041618	Diisobutyl adipate	C14H26O4	M+NH4	276.2169	-2.3
	HMDB0059946	2-Hydroxypropyl 2-isopropyl-5-methylcyclohexyl carbonate	C14H26O4	M+NH4	276.2169	-2.3
	HMDB0059947	1-Hydroxypropan-2-yl 2-isopropyl-5-methylcyclohexyl carbonate	C14H26O4	M+NH4	276.2169	-2.3
	HMDB0040429	Diethyl decanedioate	C14H26O4	M+NH4	276.2169	-2.3
	HMDB0176328	4-hydroxy-3-oxotetradecanoic acid	C14H26O4	M+NH4	276.2169	-2.3
276.2316	HMDB0061860	2-Acetyl-3,5,5,6,8,8-hexamethyl-5,6,7,8-tetrahydronaphthalene	C18H26O	M+NH4	276.2322	-2.1
277.1275	HMDB0165168	3,4,5-trihydroxy-6-[(3-methylpent-4-en-1-yl)oxy]oxane-2-carboxylic acid	C12H20O7	M+H	277.1282	-2.5
	HMDB0165596	3,4,5-trihydroxy-6-[(2Z)-2-methylpent-2-en-1-yl]oxy]oxane-2-carboxylic acid	C12H20O7	M+H	277.1282	-2.5
	HMDB0174749	6-(cyclohexyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O7	M+H	277.1282	-2.5
	HMDB0176893	6-[(2E)-hex-2-en-1-yloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O7	M+H	277.1282	-2.5
	HMDB0179391	6-[(4E)-hex-4-en-1-yloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O7	M+H	277.1282	-2.5
	HMDB0165166	3,4,5-trihydroxy-6-[(3-methylenepentyl)oxy]oxane-2-carboxylic acid	C12H20O7	M+H	277.1282	-2.5
	HMDB0164628	6-(hex-5-en-1-yloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O7	M+H	277.1282	-2.5
	HMDB0163363	6-[(4Z)-hex-4-en-1-yloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O7	M+H	277.1282	-2.5
	HMDB0034263	Triethyl citrate	C12H20O7	M+H	277.1282	-2.5
	HMDB0029129	Val-His	C11H18N4O3	M+Na	277.1271	1.4
	HMDB0028898	His-Val	C11H18N4O3	M+Na	277.1271	1.4
	HMDB0005767	Homoanserine	C11H18N4O3	M+Na	277.1271	1.4
	HMDB0037180	(S)-Argpyrimidine	C11H18N4O3	M+Na	277.1271	1.4
	HMDB0172482	1-{7-hydroxy-1,2-dimethyl-1H,2H,3H,4H,9H-2H-pyrido[3,4-b]indol-2-yl}ethan-1-one	C15H19N2O2	M+NH4	277.1785	2.6
	HMDB0168364	(8Z)-heptadeca-8,16-dien-11,13-diyne-2,,15-triol	C17H24O3	M+H	277.1798	-2.2
	HMDB0168366	(8Z)-heptadeca-8,16-dien-11,13-diyne-1,,15-triol	C17H24O3	M+H	277.1798	-2.2
	HMDB0168365	(7Z)-1-(oxiran-2-yl)pentadec-7-en-2,4-diyne-1,6-diol	C17H24O3	M+H	277.1798	-2.2
	HMDB0168944	heptadeca-1,9-dien-4,6-diyne-3,9,-triol	C17H24O3	M+H	277.1798	-2.2
	HMDB0171243	(9E)-heptadeca-1,9-dien-4,6-diyne-3,8,11-triol	C17H24O3	M+H	277.1798	-2.2

277.1792	HMDB0171244	(8E)-heptadeca-8,16-dien-11,13-diyne-2,,15-triol	C17H24O3	M+H	277.1798	-2.2
	HMDB0171245	(7E)-1-(oxiran-2-yl)pentadec-7-en-2,4-diyne-1,6-diol	C17H24O3	M+H	277.1798	-2.2
	HMDB0171246	(8E)-heptadeca-8,16-dien-11,13-diyne-1,,15-triol	C17H24O3	M+H	277.1798	-2.2
	HMDB0168363	CHEMBL1719	C17H24O3	M+H	277.1798	-2.2
	HMDB0137250	4-[(1E,4E)-3-hydroxydeca-1,4-dien-1-yl]-2-methoxyphenol	C17H24O3	M+H	277.1798	-2.2
	HMDB0137236	Shogaols	C17H24O3	M+H	277.1798	-2.2
	HMDB0137237	(1E)-1-(4-hydroxy-3-methoxyphenyl)dec-1-en-3-one	C17H24O3	M+H	277.1798	-2.2
	HMDB0015586	Cyclandelate	C17H24O3	M+H	277.1798	-2.2
	HMDB0040375	Ginsenoine K	C17H24O3	M+H	277.1798	-2.2
	HMDB0041201	Panaquinquecol 7	C17H24O3	M+H	277.1798	-2.2
	HMDB0038994	Ginsenoine C	C17H24O3	M+H	277.1798	-2.2
	HMDB0038938	Panaquinquecol 2	C17H24O3	M+H	277.1798	-2.2
	HMDB0031463	[8]-Shogaol	C17H24O3	M+H	277.1798	-2.2
277.9376	HMDB0060361	2,3,5-Trichloromaleylacetate	C6H3Cl3O5	M+NH4	277.9384	-3.0
278.0630	HMDB0131458	2- {[hydroxy(4-hydroxy-3,5-dimethoxyphenyl)methylidene]amino} acetic acid	C11H13NO6	M+Na	278.0635	-1.8
	HMDB0142119	2- {[hydroxy(3-hydroxy-2,4-dimethoxyphenyl)methylidene]amino} acetic acid	C11H13NO6	M+Na	278.0635	-1.8
	HMDB0142123	2- {[hydroxy(2-hydroxy-3,4-dimethoxyphenyl)methylidene]amino} acetic acid	C11H13NO6	M+Na	278.0635	-1.8
	HMDB0142128	2- {[hydroxy(4-hydroxy-2,3-dimethoxyphenyl)methylidene]amino} acetic acid	C11H13NO6	M+Na	278.0635	-1.8
	HMDB0166879	[hydroxy(3,4,5-trimethoxyphenyl)methylidene]carbamic acid	C11H13NO6	M+Na	278.0635	-1.8
	HMDB0062705	D-Galactopyranose 1-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0000213	1D-myo-inositol 1-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0001401	Glucose 6-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0001313	D-myo-Inositol 4-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0001078	Mannose 6-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0001076	Fructose 1-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0000994	Dolichyl phosphate D-mannose	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0006814	D-myo-Inositol 3-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0000124	Fructose 6-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0001586	β-D-Glucose 1-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0000645	Galactose 1-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0002985	Inositol phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0003498	beta-D-Glucose 6-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0006330	D-Mannose 1-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0060467	D-fructose 1-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0006873	D-Tagatose 6-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0006800	Beta-D-Fructose 2-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0006797	Sorbose 1-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0006328	D-Tagatose 1-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
	HMDB0003971	Beta-D-Fructose 6-phosphate	C6H13O9P	M+NH4	278.0635	-1.9
278.0864	HMDB0015139	Ganciclovir	C9H13N5O4	M+Na	278.0860	1.5
	HMDB0158326	3-(N'-hydroxycarbamimidamido)-6-propanoyl-4,5-dihydropyrazine-2-carboxylic acid	C9H13N5O4	M+Na	278.0860	1.5
	HMDB0156014	3-carbamimidamido-6-(2-hydroxypropanoyl)-4,5-dihydropyrazine-2-carboxylic acid	C9H13N5O4	M+Na	278.0860	1.5
	HMDB0002275	7,8-Dihydroneopterin	C9H13N5O4	M+Na	278.0860	1.5
	HMDB0159270	3-carbamimidamido-6-(1,2-dihydroxypropyl)-3,4-dihydropyrazine-2-carboxylic acid	C9H13N5O4	M+Na	278.0860	1.5
	HMDB0165486	6-(1-cyano-2-hydroxy-1-methylethoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H15NO8	M+H	278.0870	-2.3
	HMDB0165485	6-(2-cyano-2-hydroxy-2-methylethoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H15NO8	M+H	278.0870	-2.3
278.1348	HMDB0028820	Glutamyl-Hydroxyproline	C10H16N2O6	M+NH4	278.1347	0.5
	HMDB0029403	Oxypinnatanine	C10H16N2O6	M+NH4	278.1347	0.5
	HMDB0028862	Hydroxypropyl-Glutamate	C10H16N2O6	M+NH4	278.1347	0.5
	HMDB0011161	Glutamylhydroxyproline	C10H16N2O6	M+NH4	278.1347	0.5

	HMDB0029150	欽 煙amma-Glutamylhydroxyproline	C10H16N2O6	M+NH4	278.1347	0.5
278.1824	HMDB0028736	Asparaginy-Lysine	C10H20N4O4	M+NH4	278.1823	0.4
	HMDB0028946	ZINC439628	C10H20N4O4	M+NH4	278.1823	0.4
279.0296	HMDB0132989	{4-[(1E)-3-oxopent-1-en-1-yl]phenyl}oxidanesulfonic acid	C11H12O5S	M+Na	279.0298	-0.6
	HMDB0133689	[(3-methyl-2-oxo-4-phenylbut-3-en-1-yl)oxy]sulfonic acid	C11H12O5S	M+Na	279.0298	-0.6
	HMDB0133691	[3-oxo-2-(phenylmethylidene)butoxy]sulfonic acid	C11H12O5S	M+Na	279.0298	-0.6
	HMDB0133695	[4-(2-methyl-3-oxobut-1-en-1-yl)phenyl]oxidanesulfonic acid	C11H12O5S	M+Na	279.0298	-0.6
	HMDB0133693	[3-(2-methyl-3-oxobut-1-en-1-yl)phenyl]oxidanesulfonic acid	C11H12O5S	M+Na	279.0298	-0.6
279.1584	HMDB0133089	2-(5-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)benzene-1,3,5-triol	C16H22O4	M+H	279.1591	-2.5
	HMDB0133088	2-(4-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)benzene-1,3,5-triol	C16H22O4	M+H	279.1591	-2.5
	HMDB0133086	2-[5-(3,3-dimethyloxiran-2-yl)-3-methylpent-2-en-1-yl]benzene-1,3,5-triol	C16H22O4	M+H	279.1591	-2.5
	HMDB0133087	2-[(2Z)-4-hydroxy-3-(4-methylpent-3-en-1-yl)but-2-en-1-yl]benzene-1,3,5-triol	C16H22O4	M+H	279.1591	-2.5
	HMDB0133090	2-[(6E)-8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl]benzene-1,3,5-triol	C16H22O4	M+H	279.1591	-2.5
	HMDB0133091	2-(8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)benzene-1,3,5-triol	C16H22O4	M+H	279.1591	-2.5
	HMDB0168847	3,4,5-trihydroxy-2,4-bis(3-methylbut-2-en-1-yl)cyclohexa-2,5-dien-1-one	C16H22O4	M+H	279.1591	-2.5
	HMDB0133084	4-(3,7-dimethylocta-2,6-dien-1-yl)benzene-1,2,3,5-tetrol	C16H22O4	M+H	279.1591	-2.5
	HMDB0133085	2-{[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]methyl}benzene-1,3,5-triol	C16H22O4	M+H	279.1591	-2.5
	HMDB0133046	2-(4-hydroxy-3-methylbut-2-en-1-yl)-4-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C16H22O4	M+H	279.1591	-2.5
	HMDB0133045	2-(4-hydroxy-3-methylbut-2-en-1-yl)-4-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C16H22O4	M+H	279.1591	-2.5
	HMDB0133048	2-[(3,3-dimethyloxiran-2-yl)methyl]-4-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C16H22O4	M+H	279.1591	-2.5
	HMDB0133047	bis(3-methylbut-2-en-1-yl)benzene-1,2,3,5-tetrol	C16H22O4	M+H	279.1591	-2.5
	HMDB0001518	alpha-CEHC	C16H22O4	M+H	279.1591	-2.5
	HMDB0033244	Dibutyl phthalate	C16H22O4	M+H	279.1591	-2.5
	HMDB0013835	Diisobutyl phthalate	C16H22O4	M+H	279.1591	-2.5
	HMDB0013248	Monoethylhexyl phthalic acid	C16H22O4	M+H	279.1591	-2.5
279.2320	HMDB0160594	(z,z)-9,12,17-octadecatrienoic acid	C18H30O2	M+H	279.2319	0.5
	HMDB0175412	(5E)-6-methyl-8-[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]oct-5-en-2-one	C18H30O2	M+H	279.2319	0.5
	HMDB0175413	(5E,9Z)-12-(3,3-dimethyloxiran-2-yl)-6,-dimethyldodeca-5,9-dien-2-one	C18H30O2	M+H	279.2319	0.5
	HMDB0175414	(5E,9Z)-1-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+H	279.2319	0.5
	HMDB0175415	(5E,9Z)-3-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+H	279.2319	0.5
	HMDB0175409	(5E,9Z)-8-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+H	279.2319	0.5
	HMDB0175408	(5E,9Z)-4-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+H	279.2319	0.5
	HMDB0175410	(5E,9Z)-12-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+H	279.2319	0.5
	HMDB0173892	(9E,12Z)-octadeca-9,12,17-trienoic acid	C18H30O2	M+H	279.2319	0.5
	HMDB0175402	(5E,9Z)-7-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+H	279.2319	0.5
	HMDB0175403	(5Z,9Z)-6-(hydroxymethyl)-,14-dimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+H	279.2319	0.5

	HMDB0175404	(5E,9Z)-11-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+H	279.2319	0.5
	HMDB0175405	(5E,9E)--(hydroxymethyl)-6,14-dimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+H	279.2319	0.5
	HMDB0175406	(5E,9Z)-15-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+H	279.2319	0.5
	HMDB0175407	(5E,9Z,13E)-15-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+H	279.2319	0.5
	HMDB0175411	4-{3-[(3Z)-4,8-dimethylnona-3,7-dien-1-yl]-3-methyloxiran-2-yl}butan-2-one	C18H30O2	M+H	279.2319	0.5
	HMDB0001388	alpha-Linolenic acid	C18H30O2	M+H	279.2319	0.5
	HMDB0003073	gamma-Linolenic acid	C18H30O2	M+H	279.2319	0.5
	HMDB0030964	Linolenelaidic acid	C18H30O2	M+H	279.2319	0.5
	HMDB0030962	Calendic acid	C18H30O2	M+H	279.2319	0.5
	HMDB0030963	alpha-Eleostearic acid	C18H30O2	M+H	279.2319	0.5
280.0913	HMDB0000086	Glycerophosphocholine	C8H20NO6P	M+Na	280.0920	-2.6
280.2269	HMDB0033957	Crithmumdiol	C17H26O2	M+NH4	280.2271	-0.7
	HMDB0039358	Ginsenyne D	C17H26O2	M+NH4	280.2271	-0.7
	HMDB0038782	1-Heptadecene-4,6-diyne-3,9-diol	C17H26O2	M+NH4	280.2271	-0.7
	HMDB0037209	D-Galactose	C17H26O2	M+NH4	280.2271	-0.7
	HMDB0040374	Ginsenyne I	C17H26O2	M+NH4	280.2271	-0.7
	HMDB0038024	beta-Santalyl acetate	C17H26O2	M+NH4	280.2271	-0.7
	HMDB0032501	Santalyl acetate	C17H26O2	M+NH4	280.2271	-0.7
	HMDB0037832	Vetiveryl acetate	C17H26O2	M+NH4	280.2271	-0.7
	HMDB0062021	1-(3,5-di-tert-butyl-4-hydroxyphenyl)propan-1-one	C17H26O2	M+NH4	280.2271	-0.7
281.1387	HMDB0148677	2-[2,4-dihydroxy-5-methoxy-3-(3-methylbut-2-en-1-yl)phenyl]propanoic acid	C15H20O5	M+H	281.1384	1.2
	HMDB0133288	2-hydroxy-3-[4-hydroxy-3-methoxy-5-(3-methylbut-2-en-1-yl)phenyl]propanoic acid	C15H20O5	M+H	281.1384	1.2
	HMDB0131296	6-[2-(3-hydroxy-4-methoxyphenyl)ethyl]-4-methoxyoxan-2-one	C15H20O5	M+H	281.1384	1.2
	HMDB0036695	Crispolide	C15H20O5	M+H	281.1384	1.2
	HMDB0149837	2-[4,6-dihydroxy-2-methoxy-3-(3-methylbut-2-en-1-yl)phenyl]propanoic acid	C15H20O5	M+H	281.1384	1.2
	HMDB0162521	2-[(3-hydroxy-4,5-dimethoxyphenyl)methyl]-6-methyloxan-4-one	C15H20O5	M+H	281.1384	1.2
	HMDB0175329	4,7,9-trihydroxy--methyl-3,6-dimethylidene-2H,3H,3aH,4H,5H,6H,7H,8H,9H,11aH-cyclodeca[b]furan-2-one	C15H20O5	M+H	281.1384	1.2
	HMDB0165067	1-(furan-3-yl)-4,5-dihydroxy-4,8-dimethylnon-7-ene-1,6-dione	C15H20O5	M+H	281.1384	1.2
	HMDB0165066	1-(furan-3-yl)-4-hydroxy-4-(hydroxymethyl)-8-methylnon-7-ene-1,6-dione	C15H20O5	M+H	281.1384	1.2
	HMDB0165065	1-(3,3-dimethyloxiran-2-yl)-6-(furan-3-yl)-3-hydroxy-3-methylhexane-1,6-dione	C15H20O5	M+H	281.1384	1.2
	HMDB0165064	1-(furan-3-yl)-4,9-dihydroxy-4,8-dimethylnon-7-ene-1,6-dione	C15H20O5	M+H	281.1384	1.2
	HMDB0165063	(7E)-1-(furan-3-yl)-4,9-dihydroxy-4,8-dimethylnon-7-ene-1,6-dione	C15H20O5	M+H	281.1384	1.2
	HMDB0162524	2-[(3-hydroxy-2,5-dimethoxyphenyl)methyl]-6-methyloxan-4-one	C15H20O5	M+H	281.1384	1.2
	HMDB0038545	(1beta,4alpha,5alpha,6beta,8alpha,b)-1,:4,5-Diepox-6-hydroxy-7(11)-germacren-12,8-olide	C15H20O5	M+H	281.1384	1.2
	HMDB0041003	Secobryononic acid	C15H20O5	M+H	281.1384	1.2
	HMDB0036094	Nigelllic acid	C15H20O5	M+H	281.1384	1.2
	HMDB0036095	13-Hydroxyabscisic acid	C15H20O5	M+H	281.1384	1.2
	HMDB0041144	8-Deoxy-11,13-dihydroxygrosheimin	C15H20O5	M+H	281.1384	1.2
	HMDB0035620	Artabsinolide A	C15H20O5	M+H	281.1384	1.2
	HMDB0036051	Dihydromarasmon	C15H20O5	M+H	281.1384	1.2
281.1654	HMDB0038573	Lansiumamide B	C18H17NO	M+NH4	281.1648	2.0
	HMDB0030241	Girinimbine	C18H17NO	M+NH4	281.1648	2.0
	HMDB0030190	(E,E)-Lansamide I	C18H17NO	M+NH4	281.1648	2.0
	HMDB0162717	(8Z)-2-hydroxy-9-(7-methyl-3H-azepin-2-yl)nona-6,8-dien-3-one	C16H21NO2	M+Na	282.1464	-1.6

282.1460	HMDB0162719	1-{3-[(Z)-2-(7-methyl-3H-azepin-2-yl)ethenyl]oxiran-2-yl}pentan-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0162715	(6E,8Z)-9-[7-(hydroxymethyl)-3H-azepin-2-yl]nona-6,8-dien-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0162716	(8Z)-5-hydroxy-9-(7-methyl-3H-azepin-2-yl)nona-6,8-dien-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0162718	(6E)-7-[3-(7-methyl-3H-azepin-2-yl)oxiran-2-yl]hept-6-en-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0162720	(6E,8Z)-9-{5-methyl-8-oxa-4-azabicyclo[5.1]octa-3,5-dien-3-yl}nona-6,8-dien-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0162756	(8Z)-4-hydroxy-9-(2-methyl-2H-azepin-7-yl)nona-6,8-dien-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0162754	(6E,8Z)-9-{4-methyl-8-oxa-3-azabicyclo[5.1]octa-2,5-dien-2-yl}nona-6,8-dien-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0162752	1-{3-[(Z)-2-(2-methyl-2H-azepin-7-yl)ethenyl]oxiran-2-yl}pentan-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0162753	(8Z)-9-{2-methyl-8-oxa-3-azabicyclo[5.1]octa-3,5-dien-4-yl}nona-6,8-dien-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0162755	(8Z)-1-hydroxy-9-(2-methyl-2H-azepin-7-yl)nona-6,8-dien-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0162750	(8Z)-2-hydroxy-9-(2-methyl-2H-azepin-7-yl)nona-6,8-dien-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0162748	(6E,8Z)-9-[2-(hydroxymethyl)-2H-azepin-7-yl]nona-6,8-dien-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0162751	(6E)-7-[3-(2-methyl-2H-azepin-7-yl)oxiran-2-yl]hept-6-en-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0162749	(8Z)-5-hydroxy-9-(2-methyl-2H-azepin-7-yl)nona-6,8-dien-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0162722	(8Z)-4-hydroxy-9-(7-methyl-3H-azepin-2-yl)nona-6,8-dien-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0162721	(8Z)-1-hydroxy-9-(7-methyl-3H-azepin-2-yl)nona-6,8-dien-3-one	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0029829	Norchalciporyl propionate	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0041954	Norcocaine	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0015115	Ramelteon	C16H21NO2	M+Na	282.1464	-1.6
	HMDB0001849	Propranolol	C16H21NO2	M+Na	282.1464	-1.6
282.2051	HMDB0014519	Colestipol	C11H28ClN5O	M+H	282.2055	-1.5
282.2422	HMDB0037224	alpha-Caryophyllene alcohol acetate	C17H28O2	M+NH4	282.2428	-2.0
	HMDB0240268	2-trans-6-trans-farnesyl acetate	C17H28O2	M+NH4	282.2428	-2.0
	HMDB0036153	Shyobunyl acetate	C17H28O2	M+NH4	282.2428	-2.0
	HMDB0037218	Guaiol acetate	C17H28O2	M+NH4	282.2428	-2.0
	HMDB0039630	Nerolidyl acetate	C17H28O2	M+NH4	282.2428	-2.0
	HMDB0037273	beta-Caryophyllene alcohol acetate	C17H28O2	M+NH4	282.2428	-2.0
	HMDB0035910	Cedryl acetate	C17H28O2	M+NH4	282.2428	-2.0
	HMDB0032791	Methyl 15-cyanopentadecanoate	C17H31NO2	M+H	282.2428	-2.0
282.2784	HMDB0037543	(Z)-2-(5-Tetradecenyl)cyclobutanone	C18H32O	M+NH4	282.2791	-2.6
	HMDB0002117	Oleamide	C18H35NO	M+H	282.2791	-2.6
283.1298	HMDB0137241	(1E,4E)-1-(3,4-dihydroxyphenyl)deca-1,4-dien-3-one	C16H20O3	M+Na	283.1305	-2.3
	HMDB0134736	2-(1-hydroxy-4-methylpent-3-en-1-yl)-2-methyl-2H-chromen-8-ol	C16H20O3	M+Na	283.1305	-2.3
	HMDB0134732	2-[(3E)-5-hydroxy-4-methylpent-3-en-1-yl]-2-methyl-2H-chromen-8-ol	C16H20O3	M+Na	283.1305	-2.3
	HMDB0134734	2-(5-hydroxy-4-methylpent-3-en-1-yl)-2-methyl-2H-chromen-8-ol	C16H20O3	M+Na	283.1305	-2.3
	HMDB0134730	2-(2-hydroxy-4-methylpent-3-en-1-yl)-2-methyl-2H-chromen-8-ol	C16H20O3	M+Na	283.1305	-2.3
	HMDB0134728	5-methyl-5-(4-methylpent-3-en-1-yl)-3,6-dioxatricyclo[5.4,undeca-1(7),8,-trien-8-ol	C16H20O3	M+Na	283.1305	-2.3
	HMDB0134724	2-methyl-2-(4-methylpent-3-en-1-yl)-2H-chromene-7,8-diol	C16H20O3	M+Na	283.1305	-2.3
	HMDB0134726	2-[2-(3,3-dimethyloxiran-2-yl)ethyl]-2-methyl-2H-chromen-8-ol	C16H20O3	M+Na	283.1305	-2.3
	HMDB0134719	2-(hydroxymethyl)-2-(4-methylpent-3-en-1-yl)-2H-chromen-8-ol	C16H20O3	M+Na	283.1305	-2.3

	HMDB0134722	2-methyl-2-(4-methylpent-3-en-1-yl)-2H-chromene-6,8-diol	C16H20O3	M+Na	283.1305	-2.3
	HMDB0036456	-Hydroxy-3-methoxy-1,3,5,7-cadinatetraen-9-one	C16H20O3	M+Na	283.1305	-2.3
	HMDB0032437	Monoglyceride citrate	C9H14O9	M+NH4	284.0976	2.8
	HMDB0125085	3-oxo-3-[(3,4,5,6-tetrahydroxyoxan-2-yl)methoxy]propanoic acid	C9H14O9	M+NH4	284.0976	2.8
	HMDB0155753	6-(1-carboxyethoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C9H14O9	M+NH4	284.0976	2.8
	HMDB0155754	3,4,5-trihydroxy-6-[(2-hydroxypropanoyl)oxy]oxane-2-carboxylic acid	C9H14O9	M+NH4	284.0976	2.8
	HMDB0186392	3,4,5-trihydroxy-6-[(1-hydroxy-3-oxopropan-2-yl)oxy]oxane-2-carboxylic acid	C9H14O9	M+NH4	284.0976	2.8
	HMDB0186391	3,4,5-trihydroxy-6-(2-hydroxy-3-oxopropoxy)oxane-2-carboxylic acid	C9H14O9	M+NH4	284.0976	2.8
	HMDB0155237	9-[4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-2-(hydroxyamino)-9H-purin-6-ol	C10H13N5O5	M+H	284.0989	-1.9
	HMDB0000133	Guanosine	C10H13N5O5	M+H	284.0989	-1.9
	HMDB0003333	8-Hydroxy-deoxyguanosine	C10H13N5O5	M+H	284.0989	-1.9
	HMDB0029033	Serylarginine	C9H19N5O4	M+Na	284.1329	1.7
	HMDB0028718	Arginylserine	C9H19N5O4	M+Na	284.1329	1.7
	HMDB0186914	3,4,5-trihydroxy-6-[(3-hydroxybutan-2-yl)oxy]oxane-2-carboxylic acid	C10H18O8	M+NH4	284.1340	-2.1
	HMDB0171208	3,4,5-trihydroxy-6-(3-hydroxy-2-methylpropoxy)oxane-2-carboxylic acid	C10H18O8	M+NH4	284.1340	-2.1
	HMDB0171206	3,4,5-trihydroxy-6-(2-hydroxy-2-methylpropoxy)oxane-2-carboxylic acid	C10H18O8	M+NH4	284.1340	-2.1
	HMDB0171205	3,4,5-trihydroxy-6-[(1-hydroxy-2-methylpropan-2-yl)oxy]oxane-2-carboxylic acid	C10H18O8	M+NH4	284.1340	-2.1
	HMDB0112097	5-Butyl-2-furanooctanoic acid	C16H26O3	M+NH4	284.2220	-2.5
	HMDB0112092	5-Pentyl-2-furanheptanoic acid	C16H26O3	M+NH4	284.2220	-2.5
	HMDB0112088	6-(5-hexylfuran-2-yl)hexanoic acid	C16H26O3	M+NH4	284.2220	-2.5
	HMDB0112085	5-(3,4-dimethyl-5-pentylfuran-2-yl)-pentanoic acid	C16H26O3	M+NH4	284.2220	-2.5
	HMDB0112089	7-(3,4-dimethyl-5-propylfuran-2-yl)heptanoic acid	C16H26O3	M+NH4	284.2220	-2.5
	HMDB0060055	Tetranor 12-HETE	C16H26O3	M+NH4	284.2220	-2.5
	HMDB0033917	4-Hydroxy-3-methoxy-2,-bisaboladien-9-one	C16H26O3	M+NH4	284.2220	-2.5
284.2578	HMDB0031050	Methyl 2E,4Z-hexadecadienoate	C17H30O2	M+NH4	284.2584	-2.1
	HMDB0037517	2-Tetradecylcyclobutanone	C18H34O	M+NH4	284.2948	-1.7
284.2943	HMDB0030965	9-Octadecenal	C18H34O	M+NH4	284.2948	-1.7
	HMDB0034146	Octadecanamide	C18H37NO	M+H	284.2948	-1.7
285.2417	HMDB0035473	Avocadyne	C17H32O3	M+H	285.2424	-2.5
	HMDB0038685	Muricatacin	C17H32O3	M+H	285.2424	-2.5
	HMDB0000827	Stearic acid	C18H36O2	M+H	285.2788	-2.1
	HMDB0183479	17-hydroxyoctadecanal	C18H36O2	M+H	285.2788	-2.1
	HMDB0183480	SCHEMBL8	C18H36O2	M+H	285.2788	-2.1
	HMDB0183481	2-hydroxyoctadecanal	C18H36O2	M+H	285.2788	-2.1
	HMDB0031066	16-Methylheptadecanoic acid	C18H36O2	M+H	285.2788	-2.1
	HMDB0029811	Ethyl hexadecanoate	C18H36O2	M+H	285.2788	-2.1
	HMDB0061946	Hexyl dodecanoate	C18H36O2	M+H	285.2788	-2.1
286.1028	HMDB0005923	N4-Acetylcytidine	C11H15N3O6	M+H	286.1034	-2.0
	HMDB0062438	pentacyclo[.6.2.,.,]icosa-1,3,5,7,9(19),,12(),13,15,17-decaen-4-ol	C20H12O	M+NH4	286.1226	-1.9
	HMDB0060091	Benzo[a]pyrene-4,5-oxide	C20H12O	M+NH4	286.1226	-1.9
	HMDB0060439	Benzo[a]pyrene-7,8-oxide	C20H12O	M+NH4	286.1226	-1.9
	HMDB0060090	Benzo[a]pyrene-9,-oxide	C20H12O	M+NH4	286.1226	-1.9
	HMDB0028992	SCHEMBL135934	C12H16N2O3S	M+NH4	286.1220	0.4
	HMDB0028782	Cysteinyl-Phenylalanine	C12H16N2O3S	M+NH4	286.1220	0.4
286.1884	HMDB0015385	Lisdexamfetamine	C15H25N3O	M+Na	286.1890	-2.0
	HMDB0177233	(7bR)-3,6-bis(hydroxymethyl)-6,7b-dimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4-diol	C15H24O4	M+NH4	286.2013	-1.3

286.2009	HMDB0177232	(7bS)-3,7b-bis(hydroxymethyl)-6,6-dimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4-diol	C15H24O4	M+NH4	286.2013	-1.3
	HMDB0177235	(7bR)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4,5-triol	C15H24O4	M+NH4	286.2013	-1.3
	HMDB0177236	(7bS)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4,7a-triol	C15H24O4	M+NH4	286.2013	-1.3
	HMDB0177237	(7bR)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4,4a-triol	C15H24O4	M+NH4	286.2013	-1.3
	HMDB0177234	(7bR)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4,7-triol	C15H24O4	M+NH4	286.2013	-1.3
	HMDB0240213	Prostaglandin lactone-diol	C15H24O4	M+NH4	286.2013	-1.3
	HMDB0036150	4,11,13,15-Tetrahydroridentin B	C15H24O4	M+NH4	286.2013	-1.3
	HMDB0038503	Bisacurone epoxide	C15H24O4	M+NH4	286.2013	-1.3
	HMDB0038153	1-(3-Furanyl)-6,7-dihydroxy-4,8-dimethyl-1-nonanone	C15H24O4	M+NH4	286.2013	-1.3
	HMDB0038154	3,11,12-Trihydroxy-1()-spirovetiven-2-one	C15H24O4	M+NH4	286.2013	-1.3
	HMDB0038165	Acoric acid	C15H24O4	M+NH4	286.2013	-1.3
	HMDB0060570	Deoxydihydro-artemisinin	C15H24O4	M+NH4	286.2013	-1.3
	HMDB0013324	2-Octenoylcarnitine	C15H27NO4	M+H	286.2013	-1.3
	HMDB0240723	octenoylcarnitine	C15H27NO4	M+H	286.2013	-1.3
286.2371	HMDB0167945	2-(4-hydroxy-5-methoxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C16H28O3	M+NH4	286.2377	-2.0
	HMDB0159335	(7Z,Z)-6-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M+NH4	286.2377	-2.0
	HMDB0159337	(7Z,Z)-9-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M+NH4	286.2377	-2.0
	HMDB0159336	(7Z,Z)-12-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M+NH4	286.2377	-2.0
	HMDB0159341	6-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}hexanoic acid	C16H28O3	M+NH4	286.2377	-2.0
	HMDB0159340	(7Z,Z)-15-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M+NH4	286.2377	-2.0
	HMDB0159338	(7Z,9E)-11-hydroxyhexadeca-7,9-dienoic acid	C16H28O3	M+NH4	286.2377	-2.0
	HMDB0159339	(Z)-7-hydroxyhexadeca-8,-dienoic acid	C16H28O3	M+NH4	286.2377	-2.0
	HMDB0159342	FA(16:1)(Ep,cyclo)	C16H28O3	M+NH4	286.2377	-2.0
	HMDB0159343	(7Z,Z)-16-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M+NH4	286.2377	-2.0
	HMDB0159345	(7Z,Z)-2-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M+NH4	286.2377	-2.0
	HMDB0013250	Myristoylglycine	C16H31NO3	M+H	286.2377	-2.0
286.2734	HMDB0030997	Cyclohexaneundecanoic acid	C17H32O2	M+NH4	286.2741	-2.3
	HMDB0062437	(9Z)-heptadecenoic acid	C17H32O2	M+NH4	286.2741	-2.3
	HMDB0040888	2,4-Heptadecanedione	C17H32O2	M+NH4	286.2741	-2.3
	HMDB0031046	9E-Heptadecenoic acid	C17H32O2	M+NH4	286.2741	-2.3
	HMDB0060038	Z-Heptadecenoic acid	C17H32O2	M+NH4	286.2741	-2.3
	HMDB0061858	7-Hexadecenoic acid, methyl ester	C17H32O2	M+NH4	286.2741	-2.3
286.3098	HMDB0002384	Stearaldehyde	C18H36O	M+NH4	286.3104	-2.2
	HMDB0029632	Oleyl alcohol	C18H36O	M+NH4	286.3104	-2.2
	HMDB0062710	Oleyl alcohol	C18H36O	M+NH4	286.3104	-2.2
287.0191	HMDB0000559	3-Methoxy-4-hydroxyphenylethyleneglycol sulfate	C9H12O7S	M+Na	287.0196	-1.7
	HMDB0003332	3-Methoxy-4-Hydroxyphenylglycol sulfate	C9H12O7S	M+Na	287.0196	-1.7
	HMDB0177609	[2-hydroxy-1-(3-hydroxy-4-methoxyphenyl)ethoxy]sulfonic acid	C9H12O7S	M+Na	287.0196	-1.7
	HMDB0177608	[2-hydroxy-2-(3-hydroxy-4-methoxyphenyl)ethoxy]sulfonic acid	C9H12O7S	M+Na	287.0196	-1.7
	HMDB0177607	[5-(1,2-dihydroxyethyl)-2-methoxyphenyl]oxidanesulfonic acid	C9H12O7S	M+Na	287.0196	-1.7
	HMDB0159577	[2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)ethoxy]sulfonic acid	C9H12O7S	M+Na	287.0196	-1.7
	HMDB0151548	[(4,6-dihydroxy-2-methoxy-3-methylphenyl)methoxy]sulfonic acid	C9H12O7S	M+Na	287.0196	-1.7
	HMDB0131262	[(2-hydroxy-4,6-dimethoxyphenyl)methoxy]sulfonic acid	C9H12O7S	M+Na	287.0196	-1.7
	HMDB0180909	[1-(2,4-dihydroxy-6-methoxyphenyl)ethoxy]sulfonic acid	C9H12O7S	M+Na	287.0196	-1.7
287.1409	HMDB0040893	(E,E)-1,7-Diphenyl-4,6-heptadien-3-ol	C19H20O	M+Na	287.1406	0.9
	HMDB0031873	1,7-Diphenyl-4-hepten-3-one	C19H20O	M+Na	287.1406	0.9
	HMDB0133902	(6E)-1,7-diphenylhept-6-en-3-one	C19H20O	M+Na	287.1406	0.9

287.2210	HMDB0000672	Hexadecanedioic acid	C16H30O4	M+H	287.2217	-2.4
	HMDB0062018	1-[2-(Isobutyryloxy)-1-methylethyl]-2,2-dimethylpropyl 2-methylpropanoate	C16H30O4	M+H	287.2217	-2.4
	HMDB0059777	2,2,4-Trimethyl-1,3-pentadienol diisobutyrate	C16H30O4	M+H	287.2217	-2.4
	HMDB0041287	16-Hydroxy--oxohexadecanoic acid	C16H30O4	M+H	287.2217	-2.4
	HMDB0061936	Isooctanedioldibutyrate	C16H30O4	M+H	287.2217	-2.4
287.2374	HMDB0185229	(8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraen-1-ol	C20H30O	M+H	287.2369	1.6
	HMDB0156414	(4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-4,6,8-trienal	C20H30O	M+H	287.2369	1.6
	HMDB0179599	[1,4a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthren-1-yl]methanol	C20H30O	M+H	287.2369	1.6
	HMDB0036728	Kaur-16-en-18-al	C20H30O	M+H	287.2369	1.6
	HMDB0034735	abietal	C20H30O	M+H	287.2369	1.6
	HMDB0000305	Vitamin A	C20H30O	M+H	287.2369	1.6
	HMDB0006216	11-cis-Retinol	C20H30O	M+H	287.2369	1.6
	HMDB0006217	9-cis-Retinol	C20H30O	M+H	287.2369	1.6
	HMDB0006221	13-cis Retinol	C20H30O	M+H	287.2369	1.6
	HMDB0030403	(x)-p-Menth-1-en-4-yl 5-isopropyl-2-methylphenyl ether	C20H30O	M+H	287.2369	1.6
287.2573	HMDB0036841	ent-19-Trachylobanal	C20H30O	M+H	287.2369	1.6
	HMDB0038709	8,13-Abietadien-18-al	C20H30O	M+H	287.2369	1.6
287.8763	HMDB0031042	Avocadene	C17H34O3	M+H	287.2581	-2.7
	HMDB0061663	12-hydroxyheptadecanoic acid	C17H34O3	M+H	287.2581	-2.7
287.8763	HMDB0181394	3,3-dichloro-4-(dichloromethyl)-4,5-dihydroxy-3,4-dihydro-2H-pyrrol-2-one	C5H3Cl4NO3	M+Na	287.8759	1.3
	HMDB0181395	3,3-dichloro-4-[dichloro(hydroxy)methyl]-5-hydroxy-3,4-dihydro-2H-pyrrol-2-one	C5H3Cl4NO3	M+Na	287.8759	1.3
288.1076	HMDB0137300	3-(6-hydroxy-4,7-dimethoxy-2H-1,3-benzodioxol-5-yl)propanoic acid	C12H14O7	M+NH4	288.1078	-0.6
	HMDB0135168	3,4,5-trihydroxy-6-phenoxyoxane-2-carboxylic acid	C12H14O7	M+NH4	288.1078	-0.6
	HMDB0060014	Phenol glucuronide	C12H14O7	M+NH4	288.1078	-0.6
	HMDB0059806	Phenylglucuronide	C12H14O7	M+NH4	288.1078	-0.6
	HMDB0029914	Tetraphyllin B	C12H17NO7	M+H	288.1078	-0.6
288.1380	HMDB0015256	Tolbutamide	C12H18N2O3S	M+NH4	288.1376	1.3
288.1950	HMDB0000145	Estrone	C18H22O2	M+NH4	288.1958	-2.8
	HMDB0032673	15-Octadecene-9,11,13-triynoic acid	C18H22O2	M+NH4	288.1958	-2.8
	HMDB0041142	N-[2-(4-Prenyloxyphenyl)ethyl]tigllamide	C18H25NO2	M+H	288.1958	-2.8
288.2527	HMDB0010733	3-Oxohexadecanoic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0160971	(9Z)-11-hydroxyhexadec-9-enoic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0160975	16-hydroxy-9Z-hexadecenoic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0160972	8-Hydroxypalmitoleic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0160973	(9Z)-15-hydroxyhexadec-9-enoic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0160974	9,-Epoxyhexadecanoic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0160976	hydroxy-palmitoleic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0166464	2-(3-dodecyloxiran-2-yl)acetic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0166465	(3Z)-16-hydroxyhexadec-3-enoic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0166463	(3Z)-15-hydroxyhexadec-3-enoic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0166462	(3Z)-5-hydroxyhexadec-3-enoic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0166466	(3Z)-2-hydroxyhexadec-3-enoic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0030978	11-Oxohexadecanoic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0030972	8-Oxohexadecanoic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0030973	9-Oxohexadecanoic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0166467	4-hydroxy-trans-2-hexadecenoic acid	C16H30O3	M+NH4	288.2533	-2.1
	HMDB0032358	Lauroyl diethanolamide	C16H33NO3	M+H	288.2533	-2.2
288.2891	HMDB0002259	Heptadecanoic acid	C17H34O2	M+NH4	288.2897	-2.1
	HMDB0061709	15-Methylpalmitate	C17H34O2	M+NH4	288.2897	-2.1
	HMDB0031067	(S)-14-Methylhexadecanoic acid	C17H34O2	M+NH4	288.2897	-2.1
	HMDB0040598	11-Methylhexadecanoic acid	C17H34O2	M+NH4	288.2897	-2.1
	HMDB0040392	Isopropyl tetradecanoate	C17H34O2	M+NH4	288.2897	-2.1
	HMDB0061859	Methyl hexadecanoic acid	C17H34O2	M+NH4	288.2897	-2.1
	HMDB0037372	3-Methylbutyl dodecanoate	C17H34O2	M+NH4	288.2897	-2.1
	HMDB0034131	Nonyl octanoate	C17H34O2	M+NH4	288.2897	-2.1
	HMDB0059870	Ethyl pentadecanoate	C17H34O2	M+NH4	288.2897	-2.1

	HMDB0061969	Pentadecyl acetate	C17H34O2	M+NH4	288.2897	-2.1
289.1192	HMDB0015661	Fospropofol	C13H21O5P	M+H	289.1199	-2.5
	HMDB0015027	Dienestrol	C18H18O2	M+Na	289.1199	-2.4
	HMDB0036387	3-Phenylpropyl cinnamate	C18H18O2	M+Na	289.1199	-2.4
	HMDB0142845	4-[(3Z)-4-(4-hydroxyphenyl)hexa-1,3-dien-3-yl]phenol	C18H18O2	M+Na	289.1199	-2.4
289.1985	HMDB0029011	Prolyl-Arginine	C11H21N5O3	M+NH4	289.1983	0.8
	HMDB0028717	Arginylproline	C11H21N5O3	M+NH4	289.1983	0.8
290.2320	HMDB0035918	7(14)-Bisabolene-2,3,,11-tetrol	C15H28O4	M+NH4	290.2326	-2.0
290.2683	HMDB0062548	2-hydroxyhexadecanoate	C16H31O3	M+NH4	290.2690	-2.3
	HMDB0112187	9-Hydroxypalmitic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0112191	13-hydroxyhexadecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0112184	5-hydroxy-hexadecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0112190	12-hydroxyhexadecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0112192	6-hydroxyhexadecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0184174	4-hydroxy-4,8,12-trimethyltridecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0031057	2s-hydroxypalmitic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0184175	8-hydroxy-4,8,12-trimethyltridecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0184180	2-hydroxy-4,8,12-trimethyltridecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0184177	4-(hydroxymethyl)-8,12-dimethyltridecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0184178	8-(hydroxymethyl)-4,12-dimethyltridecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0184328	13-hydroxy-4,8,12-trimethyltridecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0184176	12-hydroxy-4,8,12-trimethyltridecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0155886	15-hydroxypalmitic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0010734	(R)-3-Hydroxy-hexadecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0006294	16-Hydroxy hexadecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0155887	16-Hydroxy hexadecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0112186	8-hydroxypalmitic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0112189	11-hydroxy palmitic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0112185	7-hydroxyhexadecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0112188	-hydroxyhexadecanoic acid	C16H32O3	M+NH4	290.2690	-2.3
	HMDB0061658	(S)-3-hydroxypalmitic acid	C16H32O3	M+NH4	290.2690	-2.3
291.0696	HMDB0155730	2-(6-hydroxy-9H-purin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol	C10H12N4O5	M+Na	291.0700	-1.3
	HMDB0003040	Arabinosylhypoxanthine	C10H12N4O5	M+Na	291.0700	-1.3
	HMDB0000481	Allopurinol riboside	C10H12N4O5	M+Na	291.0700	-1.3
	HMDB0000195	Inosine	C10H12N4O5	M+Na	291.0700	-1.3
291.1949	HMDB0137383	(4E)-1-(3,4-dihydroxyphenyl)dodec-4-en-3-one	C18H26O3	M+H	291.1955	-2.0
	HMDB0184938	(1S,2R,R,11S,15S)-4,14-dihydroxy-15-methyltetracyclo[8.7,,heptadec-6-en-5-one	C18H26O3	M+H	291.1955	-2.0
	HMDB0184937	(1S,S,11S,15S)-2,14-dihydroxy-15-methyltetracyclo[8.7,,heptadec-6-en-5-one	C18H26O3	M+H	291.1955	-2.0
	HMDB0184939	(1S,2R,R,11S,15S)-6,14-dihydroxy-15-methyltetracyclo[8.7,,heptadec-6-en-5-one	C18H26O3	M+H	291.1955	-2.0
	HMDB0184933	(1S,2R,R,11S,15S)-13,14-dihydroxy-15-methyltetracyclo[8.7,,heptadec-6-en-5-one	C18H26O3	M+H	291.1955	-2.0
	HMDB0184932	(1S,2R,R,11S,15S)-8,14-dihydroxy-15-methyltetracyclo[8.7,,heptadec-6-en-5-one	C18H26O3	M+H	291.1955	-2.0
	HMDB0184934	(1S,2R,R,11S,15S)-14-hydroxy-15-(hydroxymethyl)tetracyclo[8.7,,heptadec-6-en-5-one	C18H26O3	M+H	291.1955	-2.0
	HMDB0184931	(1S,2R,S,11S,15S)-14,17-dihydroxy-15-methyltetracyclo[8.7,,heptadec-6-en-5-one	C18H26O3	M+H	291.1955	-2.0
	HMDB0184808	(15S)-17-hydroxy-15-methyltetracyclo[8.7,,heptadecane-5,14-dione	C18H26O3	M+H	291.1955	-2.0
	HMDB0184804	(15S)-15-(hydroxymethyl)tetracyclo[8.7,,heptadecane-5,14-dione	C18H26O3	M+H	291.1955	-2.0
	HMDB0184803	(15S)-13-hydroxy-15-methyltetracyclo[8.7,,heptadecane-5,14-dione	C18H26O3	M+H	291.1955	-2.0
	HMDB0184802	(15S)-8-hydroxy-15-methyltetracyclo[8.7,,heptadecane-5,14-dione	C18H26O3	M+H	291.1955	-2.0
	HMDB0137392	SCHEMBL19369293	C18H26O3	M+H	291.1955	-2.0

	HMDB0061861	Octyl 4-methoxycinnamic acid	C18H26O3	M+H	291.1955	-2.0
	HMDB0031098	(9Z,11E,13E,15Z)-4-Oxo-9,11,13,15-octadecatetraenoic acid	C18H26O3	M+H	291.1955	-2.0
294.1540	HMDB0174749	6-(cyclohexyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O7	M+NH4	294.1547	-2.5
	HMDB0176893	6-[(2E)-hex-2-en-1-yloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O7	M+NH4	294.1547	-2.5
	HMDB0179391	6-[(4E)-hex-4-en-1-yloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O7	M+NH4	294.1547	-2.5
	HMDB0165168	3,4,5-trihydroxy-6-[(3-methylpent-4-en-1-yl)oxy]oxane-2-carboxylic acid	C12H20O7	M+NH4	294.1547	-2.5
	HMDB0165166	3,4,5-trihydroxy-6-[(3-methylidenepentyl)oxy]oxane-2-carboxylic acid	C12H20O7	M+NH4	294.1547	-2.5
	HMDB0164628	6-(hex-5-en-1-yloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O7	M+NH4	294.1547	-2.5
	HMDB0163363	6-[(4Z)-hex-4-en-1-yloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O7	M+NH4	294.1547	-2.5
	HMDB0165596	3,4,5-trihydroxy-6-[(2Z)-2-methylpent-2-en-1-yl]oxy]oxane-2-carboxylic acid	C12H20O7	M+NH4	294.1547	-2.5
	HMDB0034263	Triethyl citrate	C12H20O7	M+NH4	294.1547	-2.5
	HMDB0039780	N-(1-Deoxy-1-fructosyl)isoleucine	C12H23NO7	M+H	294.1547	-2.5
	HMDB0037840	N-(1-Deoxy-1-fructosyl)leucine	C12H23NO7	M+H	294.1547	-2.5
	HMDB0144664	6-[2-(diethylamino)ethoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H23NO7	M+H	294.1547	-2.5
	HMDB0168732	[(6-carboxy-3,4-dihydroxyoxan-2-yl)oxy]diethyl(2-hydroxyethyl)azanium	C12H24NO7	M+H	294.1547	-2.5
	HMDB0028717	Arginylproline	C11H21N5O3	M+Na	294.1537	1.2
	HMDB0029011	Prolyl-Arginine	C11H21N5O3	M+Na	294.1537	1.2
294.2056	HMDB0168366	(8Z)-heptadeca-8,16-dien-11,13-diyne-1,,15-triol	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0168364	(8Z)-heptadeca-8,16-dien-11,13-diyne-2,,15-triol	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0168365	(7Z)-1-(oxiran-2-yl)pentadec-7-en-2,4-diyne-1,6-diol	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0168944	heptadeca-1,9-dien-4,6-diyne-3,9,-triol	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0171243	(9E)-heptadeca-1,9-dien-4,6-diyne-3,8,11-triol	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0171244	(8E)-heptadeca-8,16-dien-11,13-diyne-2,,15-triol	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0171246	(8E)-heptadeca-8,16-dien-11,13-diyne-1,,15-triol	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0171245	(7E)-1-(oxiran-2-yl)pentadec-7-en-2,4-diyne-1,6-diol	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0168363	CHEMBL1719	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0137250	4-[(1E,4E)-3-hydroxydeca-1,4-dien-1-yl]-2-methoxyphenol	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0137237	(1E)-1-(4-hydroxy-3-methoxyphenyl)dec-1-en-3-one	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0137236	Shogaols	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0015586	Cyclandelate	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0040375	Ginsenoside K	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0041201	Panaquinquecol 7	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0038994	Ginsenoside C	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0038938	Panaquinquecol 2	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0031463	[8]-Shogaol	C17H24O3	M+NH4	294.2064	-2.6
	HMDB0036328	Nordihydrocapsaicin	C17H27NO3	M+H	294.2064	-2.6
	HMDB0029846	Nonivamide	C17H27NO3	M+H	294.2064	-2.6
295.1571	HMDB0171035	[(12-oxotridecyl)oxy]sulfonic acid	C13H26O5S	M+H	295.1574	-0.9
	HMDB0171033	[(12-oxotridecan-2-yl)oxy]sulfonic acid	C13H26O5S	M+H	295.1574	-0.9
	HMDB0171039	[(2-oxotridecan-3-yl)oxy]sulfonic acid	C13H26O5S	M+H	295.1574	-0.9
	HMDB0171037	[(2-oxotridecyl)oxy]sulfonic acid	C13H26O5S	M+H	295.1574	-0.9
295.1878	HMDB0035918	7(14)-Bisabolene-2,3,,11-tetrol	C15H28O4	M+Na	295.1880	-0.6
295.2610	HMDB0040983	1,17-Heptadecanediol	C17H36O2	M+Na	295.2607	0.9
	HMDB0032317	Hexanal hexyl isoamyl acetal	C17H36O2	M+Na	295.2607	0.9
	HMDB0133085	2-{[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]methyl} benzene-1,3,5-triol	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0133087	2-[(2Z)-4-hydroxy-3-(4-methylpent-3-en-1-yl)but-2-en-1-yl]benzene-1,3,5-triol	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0133088	2-(4-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)benzene-1,3,5-triol	C16H22O4	M+NH4	296.1856	-2.1

296.1850	HMDB0133086	2-[5-(3,3-dimethyloxiran-2-yl)-3-methylpent-2-en-1-yl]benzene-1,3,5-triol	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0133089	2-(5-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)benzene-1,3,5-triol	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0133090	2-[(6E)-8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl]benzene-1,3,5-triol	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0133091	2-(8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)benzene-1,3,5-triol	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0168847	3,4,5-trihydroxy-2,4-bis(3-methylbut-2-en-1-yl)cyclohexa-2,5-dien-1-one	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0133084	4-(3,7-dimethylocta-2,6-dien-1-yl)benzene-1,2,3,5-tetrol	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0133048	2-[(3,3-dimethyloxiran-2-yl)methyl]-4-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0133047	bis(3-methylbut-2-en-1-yl)benzene-1,2,3,5-tetrol	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0133046	2-(4-hydroxy-3-methylbut-2-en-1-yl)-4-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0133045	2-(4-hydroxy-3-methylbut-2-en-1-yl)-4-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0001518	alpha-CEHC	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0033244	Dibutyl phthalate	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0013835	Diisobutyl phthalate	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0013248	Monoethylhexyl phthalic acid	C16H22O4	M+NH4	296.1856	-2.1
	HMDB0014333	Esmolol	C16H25NO4	M+H	296.1856	-2.1
296.2216	HMDB0137260	4-[(4E)-3-hydroxydec-4-en-1-yl]-2-methoxyphenol	C17H26O3	M+NH4	296.2220	-1.4
	HMDB0137271	4-[(1E)-3-hydroxydec-1-en-1-yl]-2-methoxyphenol	C17H26O3	M+NH4	296.2220	-1.4
	HMDB0168550	(8E,13E)-heptadeca-8,13,16-trien-11-yne-2,,15-triol	C17H26O3	M+NH4	296.2220	-1.4
	HMDB0168551	(2E,7E)-1-(oxiran-2-yl)pentadeca-2,7-dien-4-yne-1,6-diol	C17H26O3	M+NH4	296.2220	-1.4
	HMDB0168549	(4E,9E)-heptadeca-1,4,9-trien-6-yne-3,8,11-triol	C17H26O3	M+NH4	296.2220	-1.4
	HMDB0168552	(4E)-1-[3-(1-hydroxyprop-2-en-1-yl)oxiran-2-yl]dodec-4-en-1-yn-3-ol	C17H26O3	M+NH4	296.2220	-1.4
	HMDB0168553	(4E)-1-(3-heptyloxiran-2-yl)octa-4,7-dien-2-yne-1,6-diol	C17H26O3	M+NH4	296.2220	-1.4
	HMDB0168554	(8E,13E)-heptadeca-8,13,16-trien-11-yne-1,,15-triol	C17H26O3	M+NH4	296.2220	-1.4
	HMDB0031928	Panaxytriol	C17H26O3	M+NH4	296.2220	-1.4
	HMDB0030801	[6]-Paradol	C17H26O3	M+NH4	296.2220	-1.4
	HMDB0039251	Panaxacol	C17H26O3	M+NH4	296.2220	-1.4
	HMDB0030974	8-Acetoxy-4-acoren-3-one	C17H26O3	M+NH4	296.2220	-1.4
296.2577	HMDB0160594	(z,z)-9,12,17-octadecatrienoic acid	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0175414	(5E,9Z)-1-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0175415	(5E,9Z)-3-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0175413	(5E,9Z)-12-(3,3-dimethyloxiran-2-yl)-6,-dimethyldodeca-5,9-dien-2-one	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0175412	(5E)-6-methyl-8-[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]oct-5-en-2-one	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0175410	(5E,9Z)-12-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0175411	4-{3-[(3Z)-4,8-dimethylnona-3,7-dien-1-yl]-3-methyloxiran-2-yl}butan-2-one	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0175408	(5E,9Z)-4-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0173892	(9E,12Z)-octadeca-9,12,17-trienoic acid	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0175402	(5E,9Z)-7-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0175403	(5Z,9Z)-6-(hydroxymethyl)-,14-dimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0175404	(5E,9Z)-11-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0175405	(5E,9E)--(hydroxymethyl)-6,14-dimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0175407	(5E,9Z,13E)-15-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+NH4	296.2584	-2.4

	HMDB0175406	(5E,9Z)-15-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0175409	(5E,9Z)-8-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0001388	alpha-Linolenic acid	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0003073	gamma-Linolenic acid	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0030964	Linolenelaidic acid	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0030962	Calendic acid	C18H30O2	M+NH4	296.2584	-2.4
	HMDB0030963	alpha-Eleostearic acid	C18H30O2	M+NH4	296.2584	-2.4
297.0686	HMDB0014576	Trifluridine	C10H11F3N2O5	M+H	297.0693	-2.3
297.0817	HMDB0013925	Ticlopidine S-oxide	C14H14ClNO S	M+NH4	297.0823	-2.0
	HMDB0013921	7-Hydroxyticlopidine	C14H14ClNO S	M+NH4	297.0823	-2.0
	HMDB0060899	Ticlopidine N-oxide	C14H14ClNO S	M+NH4	297.0823	-2.0
	HMDB0013923	2-Oxoticlopidine	C14H14ClNO S	M+NH4	297.0823	-2.0
	HMDB0184681	6-[(4,5-dihydroxyoxolan-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0154802	6-[2-carboxy-2-(hydroxymethyl)ethoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0157262	6-(3-carboxy-2-hydroxypropoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0157261	6-[(1-carboxy-3-hydroxypropan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0157263	6-[(3,4-dihydroxybutanoyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0157671	6-(1-carboxy-3-hydroxypropoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0157672	6-(3-carboxy-3-hydroxypropoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0157673	6-[(2,4-dihydroxybutanoyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0159602	6-(1-carboxy-2-hydroxypropoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0159603	6-[(1-carboxy-1-hydroxypropan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0159604	6-[(2,3-dihydroxybutanoyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0184680	6-[(2,4-dihydroxyoxolan-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0154803	3,4,5-trihydroxy-6-[[3-hydroxy-2-(hydroxymethyl)propanoyl]oxy]oxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0154799	6-(2-carboxy-2-hydroxy-2-methylethoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0154800	6-[(2,3-dihydroxy-2-methylpropanoyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0154798	6-(1-carboxy-2-hydroxy-1-methylethoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C10H16O10	M+H	297.0816	0.3
	HMDB0165260	(4E,9E)-17-hydroxyheptadeca-1,4,9-trien-6-yne-3,8-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0161927	(2Z)-5-hydroxy-3,7-dimethylocta-2,6-dien-1-yl benzoate	C17H22O3	M+Na	297.1461	-1.7
	HMDB0161930	(2Z)-3,7-dimethylocta-2,6-dien-1-yl 3-	C17H22O3	M+Na	297.1461	-1.7
	HMDB0161929	(2Z)-8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl benzoate	C17H22O3	M+Na	297.1461	-1.7
	HMDB0161928	(2Z,6E)-8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl benzoate	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165239	(9E)-11-hydroxyheptadec-9-en-4,6-diyne-3,8-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165240	(9E)-2-hydroxyheptadec-9-en-4,6-diyne-3,8-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0161925	(2E)-4-hydroxy-3-(4-methylpent-3-en-1-yl)but-2-en-1-yl benzoate	C17H22O3	M+Na	297.1461	-1.7

297.1456	HMDB0161926	(2Z)-4-hydroxy-3,7-dimethylocta-2,6-dien-1-yl benzoate	C17H22O3	M+Na	297.1461	-1.7
	HMDB0161924	(2Z)-5-(3,3-dimethyloxiran-2-yl)-3-methylpent-2-en-1-yl benzoate	C17H22O3	M+Na	297.1461	-1.7
	HMDB0161923	[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]methyl benzoate	C17H22O3	M+Na	297.1461	-1.7
	HMDB0161922	(2Z)-3,7-dimethylocta-2,6-dien-1-yl 4-	C17H22O3	M+Na	297.1461	-1.7
	HMDB0161921	(2Z)-3,7-dimethylocta-2,6-dien-1-yl 2-	C17H22O3	M+Na	297.1461	-1.7
	HMDB0137269	(1E)-1-(4-hydroxy-3-methoxyphenyl)deca-1,9-dien-3-one	C17H22O3	M+Na	297.1461	-1.7
	HMDB0137258	(4E)-1-(4-hydroxy-3-methoxyphenyl)deca-4,9-dien-3-one	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165241	(9E)-16-hydroxyheptadec-9-en-4,6-diyne-3,8-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165243	(9E)-1-hydroxyheptadec-9-en-4,6-diyne-3,8-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165257	(2E,7E)-1-(oxiran-2-yl)pentadeca-2,7-dien-4-yne-1,6-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165256	(4E,9E)-16-hydroxyheptadeca-1,4,9-trien-6-yne-3,8-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165258	(4E)-1-[3-(prop-2-enoyl)oxiran-2-yl]dodec-4-en-1-yn-3-one	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165259	(4E)-1-(3-heptyloxiran-2-yl)octa-4,7-dien-2-yne-1,6-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165253	1-(3-heptyloxiran-2-yl)octa-2,7-dien-4-yne-1,6-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165254	(9E)-17-hydroxyheptadeca-1,6,9-trien-4-yne-3,8-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165252	(2E)-1-[3-(3-oxopent-4-en-1-yn-1-yl)oxiran-2-yl]dec-2-en-1-one	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165255	(4E,9E)-11-hydroxyheptadeca-1,4,9-trien-6-yne-3,8-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165249	(9E)-11-hydroxyheptadeca-1,6,9-trien-4-yne-3,8-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165248	9-hydroxyheptadec-1-en-4,6-diyne-3,8-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165251	(7E)-1-(oxiran-2-yl)pentadeca-4,7-dien-2-yne-1,6-	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165250	(9E)-16-hydroxyheptadeca-1,6,9-trien-4-yne-3,8-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165244	(9E)-17-hydroxyheptadec-9-en-4,6-diyne-3,8-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165246	1-(oxiran-2-yl)pentadeca-2,4-diyne-1,6-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165247	17-hydroxyheptadec-1-en-4,6-diyne-3,8-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165245	16-hydroxyheptadec-1-en-4,6-diyne-3,8-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0165242	1-(3-heptyloxiran-2-yl)octa-2,4-diyne-1,6-dione	C17H22O3	M+Na	297.1461	-1.7
	HMDB0060388	4-Hydroxy-3-polyprenylbenzoate	C17H22O3	M+Na	297.1461	-1.7
	HMDB0060354	2-Polyprenyl-6-methoxy-1,4-benzoquinone	C17H22O3	M+Na	297.1461	-1.7
	HMDB0038939	Panaquinquecol 4	C17H22O3	M+Na	297.1461	-1.7
	HMDB0032697	1b-Furanoeudesm-4(15)-en-1-ol acetate	C17H22O3	M+Na	297.1461	-1.7
	HMDB0033090	[6]-Dehydroshogaol	C17H22O3	M+Na	297.1461	-1.7
	HMDB0040926	2-Butyl-5-[2-(4-hydroxy-3-methoxyphenyl)ethyl]furan	C17H22O3	M+Na	297.1461	-1.7
297.1803	HMDB0031802	Metalaxyl	C15H21NO4	M+NH4	297.1809	-2.0
	HMDB0139662	N-(4-aminobutyl)-3-(4-hydroxy-3,5-dimethoxyphenyl)propanimidic acid	C15H24N2O4	M+H	297.1809	-2.0
	HMDB0139700	N-(4-aminobutyl)-3-(3-hydroxy-4,5-dimethoxyphenyl)propanimidic acid	C15H24N2O4	M+H	297.1809	-2.0
297.2418	HMDB0173893	(9E,12Z)-2-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0173890	12,13-epome(9)	C18H32O3	M+H	297.2424	-2.1
	HMDB0173889	(9E,12Z)-17-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0173891	(9E,12Z)-18-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0173887	(9E,12Z)-11-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0173888	alpha-artemismic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0173886	(9E,12Z)-14-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0173885	(9E,12Z)-8-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0160595	alpha-Hydroxylinoleic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0160592	17-hydroxylinoleic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0160591	(12Z)-9-hydroxyoctadeca-,12-dienoic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0160593	18-hydroxylinoleic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0160589	(9Z,12Z)-14-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0160590	11-Hode	C18H32O3	M+H	297.2424	-2.1
	HMDB0160588	8-Hydroxylinoleic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0112194	13-HODE	C18H32O3	M+H	297.2424	-2.1
	HMDB0062652	9-HODE	C18H32O3	M+H	297.2424	-2.1

	HMDB0029796	(Z)-13-Oxo-9-octadecenoic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0029998	12-Hydroxy-8,-octadecadienoic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0029978	Avenoleic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0010223	9-HODE	C18H32O3	M+H	297.2424	-2.1
	HMDB0004701	9,-Epoxyoctadecenoic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0004702	12,13-EpOME	C18H32O3	M+H	297.2424	-2.1
	HMDB0004670	alpha-Dimorphecolic acid	C18H32O3	M+H	297.2424	-2.1
	HMDB0004667	13-HODE	C18H32O3	M+H	297.2424	-2.1
	HMDB0061708	13-HODE	C18H32O3	M+H	297.2424	-2.1
298.0961	HMDB0014802	Sulfametopyrazine	C11H12N4O3 S	M+NH4	298.0968	-2.5
	HMDB0001173	5'-Methylthioadenosine	C11H15N5O3 S	M+H	298.0968	-2.5
298.1491	HMDB0028719	Arginylthreonine	C10H21N5O4	M+Na	298.1486	1.8
	HMDB0029055	Thr-Arg	C10H21N5O4	M+Na	298.1486	1.8
	HMDB0166259	3,4,5-trihydroxy-6-[(1-hydroxy-3-methylbutan-2-yl)oxy]oxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
	HMDB0166263	3,4,5-trihydroxy-6-[(4-hydroxy-3-methylbutan-2-yl)oxy]oxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
	HMDB0166262	3,4,5-trihydroxy-6-(3-hydroxy-2-methylbutoxy)oxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
	HMDB0171217	3,4,5-trihydroxy-6-[(4-hydroxypentyl)oxy]oxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
	HMDB0171216	3,4,5-trihydroxy-6-[(5-hydroxypentan-2-yl)oxy]oxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
	HMDB0171220	3,4,5-trihydroxy-6-[(5-hydroxypentyl)oxy]oxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
	HMDB0171230	6-(2-ethyl-3-hydroxypropoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
	HMDB0166258	3,4,5-trihydroxy-6-(2-hydroxy-3-methylbutoxy)oxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
	HMDB0166224	3,4,5-trihydroxy-6-[(1-hydroxy-2-methylbutan-2-yl)oxy]oxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
	HMDB0164609	3,4,5-trihydroxy-6-[(4-hydroxy-2-methylbutan-2-yl)oxy]oxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
	HMDB0164610	3,4,5-trihydroxy-6-(3-hydroxy-3-methylbutoxy)oxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
	HMDB0164612	3,4,5-trihydroxy-6-(4-hydroxy-2-methylbutoxy)oxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
	HMDB0164613	3,4,5-trihydroxy-6-(4-hydroxy-3-methylbutoxy)oxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
	HMDB0166221	3,4,5-trihydroxy-6-[(3-hydroxy-2-methylbutan-2-yl)oxy]oxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
	HMDB0166220	3,4,5-trihydroxy-6-[(3-hydroxy-3-methylbutan-2-yl)oxy]oxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
	HMDB0166223	3,4,5-trihydroxy-6-(2-hydroxy-2-methylbutoxy)oxane-2-carboxylic acid	C11H20O8	M+NH4	298.1496	-1.8
298.2369	HMDB0112095	7-(3-methyl-5-pentylfuran-2-yl)-heptanoic acid	C17H28O3	M+NH4	298.2377	-2.6
	HMDB0094642	9-(3-methyl-5-propylfuran-2-yl)-nonanoic acid	C17H28O3	M+NH4	298.2377	-2.6
	HMDB0112087	5-(3-methyl-5-heptylfuran-2-yl)-pentanoic acid	C17H28O3	M+NH4	298.2377	-2.6
	HMDB0112098	5-Pentyl-2-furanoctanoic acid	C17H28O3	M+NH4	298.2377	-2.6
	HMDB0032675	Dihydropanaxacol	C17H28O3	M+NH4	298.2377	-2.6
	HMDB0041388	Valeracetate	C17H28O3	M+NH4	298.2377	-2.6
	HMDB0036422	Fauronyl acetate	C17H28O3	M+NH4	298.2377	-2.6
	HMDB0012535	12S-HHT	C17H28O3	M+NH4	298.2377	-2.6
298.2734	HMDB0062238	(6Z,9Z)-octadecadienoic acid	C18H32O2	M+NH4	298.2741	-2.2
	HMDB0061864	Dihomolinoleic acid	C18H32O2	M+NH4	298.2741	-2.2
	HMDB0005048	E,12Z-Octadecadienoic acid	C18H32O2	M+NH4	298.2741	-2.2
	HMDB0062784	Octadecadienoate	C18H32O2	M+NH4	298.2741	-2.2
	HMDB0030430	Linalyl caprylate	C18H32O2	M+NH4	298.2741	-2.2
	HMDB0029800	Mangiferic acid	C18H32O2	M+NH4	298.2741	-2.2
	HMDB0031097	5-Octadecynoic acid	C18H32O2	M+NH4	298.2741	-2.2
	HMDB0031051	Ethyl 2E,4Z-hexadecadienoate	C18H32O2	M+NH4	298.2741	-2.2

	HMDB0006270	Linoelaidic acid	C18H32O2	M+NH4	298.2741	-2.2
	HMDB0005047	9E,11E-Octadecadienoic acid	C18H32O2	M+NH4	298.2741	-2.2
	HMDB0003797	Bovinic acid	C18H32O2	M+NH4	298.2741	-2.2
	HMDB0000673	Linoleic acid	C18H32O2	M+NH4	298.2741	-2.2
	HMDB0173874	Linoleic acid	C18H32O2	M+NH4	298.2741	-2.2
	HMDB0013648	Palmitoleoyl Ethanolamide	C18H35NO2	M+H	298.2741	-2.2
298.3102	HMDB0034496	6,,14-Trimethyl-2-methylenepentadecanal	C19H36O	M+NH4	298.3104	-0.8
	HMDB0031810	Tridemorph	C19H39NO	M+H	298.3104	-0.8
298.3466	HMDB0004659	8-Isoprostane	C20H40	M+NH4	298.3468	-0.8
	HMDB0062069	icos-5-ene	C20H40	M+NH4	298.3468	-0.8
	HMDB0061960	bis(dec-1-ene)	C20H40	M+NH4	298.3468	-0.8
	HMDB0040709	-Eicosene	C20H40	M+NH4	298.3468	-0.8
299.2574	HMDB0155794	2-hydroxyoleic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0155791	8-Hydroxyoleic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0155790	(9Z)-11-hydroxyoctadec-9-enoic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0155792	17-Hydroxyoleic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0155793	18-hydroxyoleic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0160377	11-hydroxy-9-octadecenoic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0187015	2-Hydroxy-cis-vaccensaure	C18H34O3	M+H	299.2581	-2.2
	HMDB0187014	(11Z)-18-hydroxyoctadec-11-enoic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0187013	Oxiranedecanoic acid, 3-hexyl-	C18H34O3	M+H	299.2581	-2.2
	HMDB0187010	(11Z)-13-hydroxyoctadec-11-enoic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0187012	(11Z)-17-hydroxyoctadec-11-enoic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0187011	-hydroxy-cis-vaccenic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0160378	8-home(9)	C18H34O3	M+H	299.2581	-2.2
	HMDB0160380	18-Hydroxy-9-octadecenoic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0160379	17-hydroxy-9-octadecenoic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0160381	SCHEMBL378128	C18H34O3	M+H	299.2581	-2.2
	HMDB0030979	9-Oxoctadecanoic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0034074	5-Oxoctadecanoic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0030980	-Oxoctadecanoic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0031127	5-Hexyltetrahydro-2-furanoctanoic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0034297	Ricinoleic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0030981	11-Oxoctadecanoic acid	C18H34O3	M+H	299.2581	-2.2
	HMDB0010736	3-keto stearic acid	C18H34O3	M+H	299.2581	-2.2
299.2940	HMDB0000772	Nonadecanoic acid	C19H38O2	M+H	299.2945	-1.5
	HMDB0175455	6,,14-trimethyl-2-methylidenepentadecane-1,-diol	C19H38O2	M+H	299.2945	-1.5
	HMDB0175454	6,,14-trimethyl-2-methylidenepentadecane-1,6-diol	C19H38O2	M+H	299.2945	-1.5
	HMDB0175457	6,,14-trimethyl-2-methylidenepentadecane-1,3-diol	C19H38O2	M+H	299.2945	-1.5
	HMDB0175459	2-(4,8-dimethylnonyl)-6-methylideneheptane-1,7-diol	C19H38O2	M+H	299.2945	-1.5
	HMDB0175456	6,,14-trimethyl-2-methylidenepentadecane-1,14-diol	C19H38O2	M+H	299.2945	-1.5
	HMDB0175458	[2-(4,8,12-trimethyltridecyl)oxiran-2-yl]methanol	C19H38O2	M+H	299.2945	-1.5
	HMDB0175460	6-methyl-2-methylidene--(4-methylpentyl)undecane-1,11-diol	C19H38O2	M+H	299.2945	-1.5
	HMDB0000795	Pristanic acid	C19H38O2	M+H	299.2945	-1.5
	HMDB0004085	Tuberculostearic acid	C19H38O2	M+H	299.2945	-1.5
	HMDB0035675	6-Hydroxy-4-nonadecanone	C19H38O2	M+H	299.2945	-1.5
	HMDB0035674	4-Hydroxy-6-nonadecanone	C19H38O2	M+H	299.2945	-1.5
	HMDB0037397	欽?7-Methyloctadecanoic acid	C19H38O2	M+H	299.2945	-1.5
	HMDB0061710	欽?7-Methyloctadecanoic acid	C19H38O2	M+H	299.2945	-1.5
	HMDB0038070	xi-16-Methyloctadecanoic acid	C19H38O2	M+H	299.2945	-1.5
	HMDB0034154	Methyl stearate	C19H38O2	M+H	299.2945	-1.5
	HMDB0035474	Isopropyl hexadecanoate	C19H38O2	M+H	299.2945	-1.5
	HMDB0061964	Heptadecyl acetate	C19H38O2	M+H	299.2945	-1.5
	HMDB0175461	2,6,-trimethyl-14-methylidenepentadecane-1,15-diol	C19H38O2	M+H	299.2945	-1.5
300.2017	HMDB0061822	Hexaethylene glycol	C12H26O7	M+NH4	300.2017	0.1
300.2164	HMDB0033630	Lactapiperanol C	C16H26O4	M+NH4	300.2169	-1.8
	HMDB0062365	(8R,Z)-8-hydroxy-3-oxohexadeca-6,-dienoic acid	C16H26O4	M+NH4	300.2169	-1.8
	HMDB0062366	(6E,8S,Z)-8-hydroxy-3-oxohexadecadienoic acid	C16H26O4	M+NH4	300.2169	-1.8
	HMDB0003231	Vaccenic acid	C18H34O2	M+NH4	300.2897	-2.0
	HMDB0002080	Petroselinic acid	C18H34O2	M+NH4	300.2897	-2.0
	HMDB0062703	octadec-9-enoic acid	C18H34O2	M+NH4	300.2897	-2.0
	HMDB0062242	7z-octadecenoic acid	C18H34O2	M+NH4	300.2897	-2.0
	HMDB0041480	(Z)-13-Octadecenoic acid	C18H34O2	M+NH4	300.2897	-2.0
	HMDB0062218	(Z)-13-Octadecenoic acid	C18H34O2	M+NH4	300.2897	-2.0

300.2891	HMDB0062093	octadec-13-enoic acid	C18H34O2	M+NH4	300.2897	-2.0
	HMDB0059871	Ethyl 9-hexadecenoate	C18H34O2	M+NH4	300.2897	-2.0
	HMDB0000573	Elaidic acid	C18H34O2	M+NH4	300.2897	-2.0
	HMDB0240219	cis-Vaccenic acid	C18H34O2	M+NH4	300.2897	-2.0
	HMDB0000207	Oleic acid	C18H34O2	M+NH4	300.2897	-2.0
	HMDB0002100	Palmitoylethanolamide	C18H37NO2	M+H	300.2897	-2.0
	HMDB0001480	3-Dehydrosphinganine	C18H37NO2	M+H	300.2897	-2.0
	HMDB0171016	18-Hydroxystearamide	C18H37NO2	M+H	300.2897	-2.0
	HMDB0000252	Sphingosine	C18H37NO2	M+H	300.2897	-2.0
	HMDB0171015	17-Hydroxystearamide	C18H37NO2	M+H	300.2897	-2.0
	HMDB0171017	554-87-1	C18H37NO2	M+H	300.2897	-2.0
	HMDB0062571	3-dehydrosphinganium(1+)	C18H38NO2	M+H	300.2897	-2.0
	HMDB0062807	sphingosine(1+)	C18H38NO2	M+H	300.2897	-2.0
300.3254	HMDB0001958	Pristanal	C19H38O	M+NH4	300.3261	-2.3
	HMDB0061982	18-Nonadecen-1-ol	C19H38O	M+NH4	300.3261	-2.3
	HMDB0061862	2-Nonadecanone	C19H38O	M+NH4	300.3261	-2.3
	HMDB0175444	SCHEMBL75976	C19H38O	M+NH4	300.3261	-2.3
301.1404	HMDB0133087	2-[(2Z)-4-hydroxy-3-(4-methylpent-3-en-1-yl)but-2-en-1-yl]benzene-1,3,5-triol	C16H22O4	M+Na	301.1410	-2.1
	HMDB0133088	2-(4-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)benzene-1,3,5-triol	C16H22O4	M+Na	301.1410	-2.1
	HMDB0133086	2-[5-(3,3-dimethyloxiran-2-yl)-3-methylpent-2-en-1-yl]benzene-1,3,5-triol	C16H22O4	M+Na	301.1410	-2.1
	HMDB0133089	2-(5-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)benzene-1,3,5-triol	C16H22O4	M+Na	301.1410	-2.1
	HMDB0133090	2-[(6E)-8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl]benzene-1,3,5-triol	C16H22O4	M+Na	301.1410	-2.1
	HMDB0133091	2-(8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)benzene-1,3,5-triol	C16H22O4	M+Na	301.1410	-2.1
	HMDB0168847	3,4,5-trihydroxy-2,4-bis(3-methylbut-2-en-1-yl)cyclohexa-2,5-dien-1-one	C16H22O4	M+Na	301.1410	-2.1
	HMDB0133085	2-[[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]methyl]benzene-1,3,5-triol	C16H22O4	M+Na	301.1410	-2.1
	HMDB0133084	4-(3,7-dimethylocta-2,6-dien-1-yl)benzene-1,2,3,5-tetrol	C16H22O4	M+Na	301.1410	-2.1
	HMDB0133048	2-[(3,3-dimethyloxiran-2-yl)methyl]-4-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C16H22O4	M+Na	301.1410	-2.1
	HMDB0133046	2-(4-hydroxy-3-methylbut-2-en-1-yl)-4-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C16H22O4	M+Na	301.1410	-2.1
	HMDB0133045	2-(4-hydroxy-3-methylbut-2-en-1-yl)-4-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C16H22O4	M+Na	301.1410	-2.1
	HMDB0133047	bis(3-methylbut-2-en-1-yl)benzene-1,2,3,5-tetrol	C16H22O4	M+Na	301.1410	-2.1
	HMDB0001518	alpha-CEHC	C16H22O4	M+Na	301.1410	-2.1
	HMDB0033244	Dibutyl phthalate	C16H22O4	M+Na	301.1410	-2.1
	HMDB0013835	Diisobutyl phthalate	C16H22O4	M+Na	301.1410	-2.1
	HMDB0013248	Monoethylhexyl phthalic acid	C16H22O4	M+Na	301.1410	-2.1
302.1960	HMDB0060593	Alpha-dihydroartemisinin	C15H24O5	M+NH4	302.1962	-0.7
	HMDB0061088	Fluoxetine glucuronide	C15H24O5	M+NH4	302.1962	-0.7
302.2318	HMDB0013288	Nonanoylcarnitine	C16H31NO4	M+H	302.2326	-2.6
	HMDB0006320	2,6 Dimethylheptanoyl carnitine	C16H31NO4	M+H	302.2326	-2.6
302.2682	HMDB0035473	Avocadyne	C17H32O3	M+NH4	302.2690	-2.5
	HMDB0038685	Muricatacin	C17H32O3	M+NH4	302.2690	-2.5
302.3047	HMDB0000827	Stearic acid	C18H36O2	M+NH4	302.3054	-2.2
	HMDB0183479	17-hydroxyoctadecanal	C18H36O2	M+NH4	302.3054	-2.2
	HMDB0183481	2-hydroxyoctadecanal	C18H36O2	M+NH4	302.3054	-2.2
	HMDB0183480	SCHEMBL8	C18H36O2	M+NH4	302.3054	-2.2
	HMDB0031066	16-Methylheptadecanoic acid	C18H36O2	M+NH4	302.3054	-2.2
	HMDB0029811	Ethyl hexadecanoate	C18H36O2	M+NH4	302.3054	-2.2
	HMDB0061946	Hexyl dodecanoate	C18H36O2	M+NH4	302.3054	-2.2
304.1749	HMDB0000269	Sphinganine	C18H39NO2	M+H	302.3054	-2.2
	HMDB0013328	Pimelylcarnitine	C14H25NO6	M+H	304.1755	-1.9
	HMDB0240666	[(2R)-3-carboxy-2-[[[(3S)-5-carboxy-3-methylpentanoyl]oxy]propyl]trimethylazanium	C14H26NO6	M+H	304.1755	-1.9
	HMDB0000672	Hexadecanedioic acid	C16H30O4	M+NH4	304.2482	-2.4

304.2475	HMDB0062018	1-[2-(Isobutyryloxy)-1-methylethyl]-2,2-dimethylpropyl 2-methylpropanoate	C16H30O4	M+NH4	304.2482	-2.4
	HMDB0059777	2,2,4-Trimethyl-1,3-pentadienol diisobutyrate	C16H30O4	M+NH4	304.2482	-2.4
	HMDB0041287	16-Hydroxy--oxohexadecanoic acid	C16H30O4	M+NH4	304.2482	-2.4
	HMDB0061936	Isooctanedioldibutyrate	C16H30O4	M+NH4	304.2482	-2.4
304.2630	HMDB0185229	(8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraen-1-ol	C20H30O	M+NH4	304.2635	-1.6
	HMDB0156414	(4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-4,6,8-trienal	C20H30O	M+NH4	304.2635	-1.6
	HMDB0179599	[1,4a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthren-1-yl]methanol	C20H30O	M+NH4	304.2635	-1.6
	HMDB0036728	Kaur-16-en-18-al	C20H30O	M+NH4	304.2635	-1.6
	HMDB0034735	abietal	C20H30O	M+NH4	304.2635	-1.6
	HMDB0000305	Vitamin A	C20H30O	M+NH4	304.2635	-1.6
	HMDB0006216	11-cis-Retinol	C20H30O	M+NH4	304.2635	-1.6
	HMDB0006217	9-cis-Retinol	C20H30O	M+NH4	304.2635	-1.6
	HMDB0006221	13-cis Retinol	C20H30O	M+NH4	304.2635	-1.6
	HMDB0030403	(x)-p-Menth-1-en-4-yl 5-isopropyl-2-methylphenyl ether	C20H30O	M+NH4	304.2635	-1.6
	HMDB0036841	ent-19-Trachylobanal	C20H30O	M+NH4	304.2635	-1.6
	HMDB0038709	8,13-Abietadien-18-al	C20H30O	M+NH4	304.2635	-1.6
304.2838	HMDB0037270	(S)-fenpropimorph	C20H33NO	M+H	304.2635	-1.6
	HMDB0031042	Avocadene	C17H34O3	M+NH4	304.2846	-2.7
304.2838	HMDB0061663	12-hydroxyheptadecanoic acid	C17H34O3	M+NH4	304.2846	-2.7
305.0975	HMDB0001067	N-Acetylasparylglutamic acid	C11H16N2O8	M+H	305.0979	-1.4
305.1508	HMDB0134626	2-hydroxy-1,7-diphenylheptan-3-one	C19H22O2	M+Na	305.1512	-1.3
	HMDB0134623	6-hydroxy-1,7-diphenylheptan-3-one	C19H22O2	M+Na	305.1512	-1.3
	HMDB0134625	4-hydroxy-1,7-diphenylheptan-3-one	C19H22O2	M+Na	305.1512	-1.3
	HMDB0134628	1-hydroxy-1,7-diphenylheptan-3-one	C19H22O2	M+Na	305.1512	-1.3
	HMDB0134627	7-hydroxy-1,7-diphenylheptan-3-one	C19H22O2	M+Na	305.1512	-1.3
	HMDB0134630	1-(3-hydroxyphenyl)-7-phenylheptan-3-one	C19H22O2	M+Na	305.1512	-1.3
	HMDB0134629	7-(3-hydroxyphenyl)-1-phenylheptan-3-one	C19H22O2	M+Na	305.1512	-1.3
	HMDB0134634	1-(2-hydroxyphenyl)-7-phenylheptan-3-one	C19H22O2	M+Na	305.1512	-1.3
	HMDB0134632	1-(4-hydroxyphenyl)-7-phenylheptan-3-one	C19H22O2	M+Na	305.1512	-1.3
	HMDB0134633	7-(2-hydroxyphenyl)-1-phenylheptan-3-one	C19H22O2	M+Na	305.1512	-1.3
	HMDB0134631	7-(4-hydroxyphenyl)-1-phenylheptan-3-one	C19H22O2	M+Na	305.1512	-1.3
	HMDB0138211	4-[(3E)-5-hydroxy-7-phenylhept-3-en-1-yl]phenol	C19H22O2	M+Na	305.1512	-1.3
	HMDB0041090	(-)-(E)-1-(4-Hydroxyphenyl)-7-phenyl-6-hepten-3-ol	C19H22O2	M+Na	305.1512	-1.3
	HMDB0035080	Miltirone	C19H22O2	M+Na	305.1512	-1.3
	HMDB0134624	5-hydroxy-1,7-diphenylheptan-3-one	C19H22O2	M+Na	305.1512	-1.3
306.2633	HMDB0037798	(S)-,16-Dihydroxyhexadecanoic acid	C16H32O4	M+NH4	306.2639	-1.9
	HMDB0072861	MG(13)	C16H32O4	M+NH4	306.2639	-1.9
	HMDB0072845	MG(13)	C16H32O4	M+NH4	306.2639	-1.9
	HMDB0072843	MG/a-13)[rac]	C16H32O4	M+NH4	306.2639	-1.9
	HMDB0072841	MG(a-13)[rac]	C16H32O4	M+NH4	306.2639	-1.9
	HMDB0072870	MG/i-13)	C16H32O4	M+NH4	306.2639	-1.9
308.0903	HMDB0000125	Glutathione	C10H17N3O6S	M+H	308.0911	-2.5
	HMDB0062697	gamma-Glutamylcysteinylglycine	C10H17N3O6S	M+H	308.0911	-2.5
	HMDB0015141	Letrozole	C17H11N5	M+Na	308.0907	-1.2
308.2582	HMDB0156088	(1S,2R,11S,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,14-diol	C19H30O2	M+NH4	308.2584	-0.7
	HMDB0062608	5beta-Dihydroepitestosterone	C19H30O2	M+NH4	308.2584	-0.7
	HMDB0155971	(2S,15S)-14-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-one	C19H30O2	M+NH4	308.2584	-0.7
	HMDB0155964	4-Androstene-3,17-diol	C19H30O2	M+NH4	308.2584	-0.7
	HMDB0000031	Androsterone	C19H30O2	M+NH4	308.2584	-0.7
	HMDB0037711	4-Methylphenyl dodecanoate	C19H30O2	M+NH4	308.2584	-0.7
	HMDB0006770	5b-Dihydrotestosterone	C19H30O2	M+NH4	308.2584	-0.7
	HMDB0003818	5-Androstenediol	C19H30O2	M+NH4	308.2584	-0.7
	HMDB0002961	Dihydrotestosterone	C19H30O2	M+NH4	308.2584	-0.7
	HMDB0000546	Epitiocholanolone	C19H30O2	M+NH4	308.2584	-0.7
	HMDB0000365	Epiandrosterone	C19H30O2	M+NH4	308.2584	-0.7

309.0938	HMDB0000490	Etiocholanolone	C19H30O2	M+NH4	308.2584	-0.7
	HMDB0005849	4-Androstenediol	C19H30O2	M+NH4	308.2584	-0.7
	HMDB0003546	Salicin	C13H18O7	M+Na	309.0945	-2.2
	HMDB0034023	Isosalicin	C13H18O7	M+Na	309.0945	-2.2
	HMDB0038331	3-Hydroxybenzyl alcohol glucoside	C13H18O7	M+Na	309.0945	-2.2
309.2419	HMDB0038964	3-Hydroxy-4,6-heptadiyne-1-yl 1-glucoside	C13H18O7	M+Na	309.0945	-2.2
	HMDB0158028	(2S,15S)-15-(hydroxymethyl)-2-methyltetracyclo[8.7,,heptadecane-5,14-diol	C19H32O3	M+H	309.2424	-1.7
	HMDB0158026	(2S,15S)-2,15-dimethyltetracyclo[8.7,,heptadecane-5,13,14-triol	C19H32O3	M+H	309.2424	-1.7
	HMDB0158025	(2R,15S)-2,15-dimethyltetracyclo[8.7,,heptadecane-5,8,14-triol	C19H32O3	M+H	309.2424	-1.7
	HMDB0158027	(2R,15S)-2-(hydroxymethyl)-15-methyltetracyclo[8.7,,heptadecane-5,14-diol	C19H32O3	M+H	309.2424	-1.7
	HMDB0158024	(2S,15S)-2,15-dimethyltetracyclo[8.7,,heptadecane-5,14,17-triol	C19H32O3	M+H	309.2424	-1.7
	HMDB0112090	5-Hexyl-3,4-dimethyl-2-furanheptanoic acid	C19H32O3	M+H	309.2424	-1.7
	HMDB0112096	8-(3,4-dimethyl-5-pentylfuran-2-yl)-octanoic acid	C19H32O3	M+H	309.2424	-1.7
	HMDB0094643	-(3,4-dimethyl-5-propylfuran-2-yl)decanoic acid	C19H32O3	M+H	309.2424	-1.7
	HMDB0112070	5-Ethyl-3,4-dimethyl-2-furanundecanoic acid	C19H32O3	M+H	309.2424	-1.7
	HMDB0112100	9-(3,4-dimethyl-5-butylfuran-2-yl)-nonanoic acid	C19H32O3	M+H	309.2424	-1.7
	HMDB0061646	3-Methyl-5-propyl-2-furanundecanoic acid	C19H32O3	M+H	309.2424	-1.7
	HMDB0030960	Isoobtusilactone A	C19H32O3	M+H	309.2424	-1.7
	HMDB0031379	Annosquamosin B	C19H32O3	M+H	309.2424	-1.7
	HMDB0031091	3-Methyl-5-pentyl-2-furannonanoic acid	C19H32O3	M+H	309.2424	-1.7
310.0863	HMDB0015461	Glycodiazine	C13H15N3O4S	M+H	310.0856	2.2
310.2007	HMDB0137259	(4E)-2-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-4-en-3-one	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0137261	(1Z)-2-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-1-en-3-one	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0137264	(1E)-1-(3,4-dihydroxy-5-methoxyphenyl)dec-1-en-3-one	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0137263	(1E)-1-(2,4-dihydroxy-5-methoxyphenyl)dec-1-en-3-one	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0137265	(1E)-1-(2,4-dihydroxy-3-methoxyphenyl)dec-1-en-3-one	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0137266	(1E)-9-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-1-en-3-one	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0137267	1-[3-(4-hydroxy-3-methoxyphenyl)oxiran-2-yl]octan-1-one	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0137268	(1E)--hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-1-en-3-one	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0137270	(1E)-4-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-1-en-3-one	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0179994	(4-hydroxy-3-methoxyphenyl)methyl 7-methyloct-7-enoate	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0180049	(3,4-dihydroxyphenyl)methyl (6E)-8-methylnon-6-enoate	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0137257	(4E)--hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-4-en-3-one	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0137254	(4E)-1-(3,4-dihydroxy-5-methoxyphenyl)dec-4-en-3-one	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0137256	3-(4-hydroxy-3-methoxyphenyl)-1-(3-pentylloxiran-2-yl)propan-1-one	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0137251	(4Z)-4-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-4-en-3-one	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0137252	(4E)-1-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-4-en-3-one	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0137255	(4E)-9-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-4-en-3-one	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0041249	6-Hydroxyshogaol	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0036693	Acetylbalchanolide	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0034930	(3beta,6beta)-Furanoeremophilane-3,6-diol 6-acetate	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0034738	Isotrichodermin	C17H24O4	M+NH4	310.2013	-1.9

	HMDB0035687	Acetylvalerenolic acid	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0039275	[6]-Gingerdione	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0034658	9-Acetoxyfukinanolide	C17H24O4	M+NH4	310.2013	-1.9
	HMDB0015334	Nadolol	C17H27NO4	M+H	310.2013	-1.9
	HMDB0015345	Metipranolol	C17H27NO4	M+H	310.2013	-1.9
310.2375	HMDB0184952	(15S)-15-methyltetraacyclo[8.7.,heptadec-6-ene-5,14,17-triol	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0184942	(15S)-14-hydroxy-15-(hydroxymethyl)tetraacyclo[8.7.,heptadecan-5-one	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0184941	(15S)-13,14-dihydroxy-15-methyltetraacyclo[8.7.,heptadecan-5-one	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0184940	(15S)-8,14-dihydroxy-15-methyltetraacyclo[8.7.,heptadecan-5-one	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0184800	(1R,2S,R,11S,15S)-5,13-dihydroxy-15-methyltetraacyclo[8.7.,heptadecan-14-one	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0184801	(1R,2S,R,11S,15S)-5-hydroxy-15-(hydroxymethyl)tetraacyclo[8.7.,heptadecan-14-one	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0184799	(1S,2R,R,11S,15S)-5,8-dihydroxy-15-methyltetraacyclo[8.7.,heptadecan-14-one	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0184798	(1R,2S,S,11S,15S)-5,17-dihydroxy-15-methyltetraacyclo[8.7.,heptadecan-14-one	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0173944	(11Z,13E)-18-hydroxyoctadeca-11,13-dien-9-ynoic acid	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0173945	(11Z,13E)-2-hydroxyoctadeca-11,13-dien-9-ynoic acid	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0173940	(11Z,13E)-15-hydroxyoctadeca-11,13-dien-9-ynoic acid	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0173942	-{3-[(1E)-hex-1-en-1-yl]oxiran-2-yl}dec-9-ynoic acid	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0173941	(11Z,13E)-17-hydroxyoctadeca-11,13-dien-9-ynoic acid	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0173943	(11Z)-12-(3-butyloxiran-2-yl)dodec-11-en-9-ynoic acid	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0038035	Panaquinquecol 1	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0030996	(2'E,4'Z,7'Z,8E)-Colnelenic acid	C18H28O3	M+NH4	310.2377	-0.5
	HMDB0040806	[7]-Paradol	C18H28O3	M+NH4	310.2377	-0.5
311.0395	HMDB0031778	Diflubenzuron	C14H9ClF2N2O2	M+H	311.0393	0.5
	HMDB0132861	3-(4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4,6,7-triol	C16H16O5	M+Na	311.0890	2.9
	HMDB0130386	3-(4-hydroxy-3-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4,7-diol	C16H16O5	M+Na	311.0890	2.9
	HMDB0130387	1-(2,4-dihydroxyphenyl)-2-(4-hydroxy-3-methoxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
	HMDB0127762	2-(3-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,5,7-triol	C16H16O5	M+Na	311.0890	2.9
	HMDB0126053	3-(3,4-dihydroxy-2-methoxyphenyl)-1-(3-hydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
	HMDB0132859	3-(4-hydroxyphenyl)-6-methoxy-3,4-dihydro-2H-1-benzopyran-4,7-diol	C16H16O5	M+Na	311.0890	2.9
	HMDB0132862	2-(4-methoxyphenyl)-1-(2,4,5-trihydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
	HMDB0135092	2-(4-hydroxy-3-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,7-diol	C16H16O5	M+Na	311.0890	2.9
	HMDB0134605	5-[(E)-2-(3-hydroxy-2,4-dimethoxyphenyl)ethenyl]benzene-1,3-diol	C16H16O5	M+Na	311.0890	2.9
	HMDB0134596	5-[(E)-2-(3-hydroxy-4-methoxyphenyl)ethenyl]-4-methoxybenzene-1,3-diol	C16H16O5	M+Na	311.0890	2.9
	HMDB0133964	1-(2,3-dihydroxy-4-methoxyphenyl)-3-(4-hydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
	HMDB0133796	3-(2-hydroxy-4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-7,8-diol	C16H16O5	M+Na	311.0890	2.9
	HMDB0133793	2-(7-hydroxy-3,4-dihydro-2H-1-benzopyran-3-yl)-5-methoxybenzene-1,4-diol	C16H16O5	M+Na	311.0890	2.9
	HMDB0133785	3-(2-hydroxy-4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-6,7-diol	C16H16O5	M+Na	311.0890	2.9
	HMDB0133780	1-(2,4-dihydroxyphenyl)-2-(2-hydroxy-4-methoxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9

311.0899

HMDB0132900	1-(2,4-dihydroxy-6-methoxyphenyl)-3-(4-hydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0153690	76172-68-4	C16H16O5	M+Na	311.0890	2.9
HMDB0135915	4-(7-hydroxy-5-methoxy-3,4-dihydro-2H-1-benzopyran-3-yl)benzene-1,3-diol	C16H16O5	M+Na	311.0890	2.9
HMDB0136523	4-[(E)-2-(4-hydroxy-3-methoxyphenyl)ethenyl]-2-methoxybenzene-1,3-diol	C16H16O5	M+Na	311.0890	2.9
HMDB0136526	4-[3-(4-hydroxy-3-methoxyphenyl)oxiran-2-yl]-2-methoxyphenol	C16H16O5	M+Na	311.0890	2.9
HMDB0151879	1-(4,5-dihydroxy-2-methoxyphenyl)-3-(4-hydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0151876	3-hydroxy-1-(4-hydroxy-2-methoxyphenyl)-3-(4-hydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0151878	1-(3,4-dihydroxy-2-methoxyphenyl)-3-(4-hydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0151877	3-(3,4-dihydroxyphenyl)-1-(4-hydroxy-2-methoxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0149638	CHEMBL1289246	C16H16O5	M+Na	311.0890	2.9
HMDB0147632	4-(7-hydroxy-6-methoxy-3,4-dihydro-2H-1-benzopyran-3-yl)benzene-1,3-diol	C16H16O5	M+Na	311.0890	2.9
HMDB0147532	2-(3-methoxyphenyl)-1-(2,4,6-trihydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0146419	3-(3-hydroxyphenyl)-2-methyl-1-(2,4,6-trihydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0151891	3-(3,4-dihydroxy-2-methoxyphenyl)-1-(4-hydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0151889	3-(2,4-dihydroxyphenyl)-1-(4-hydroxy-2-methoxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0166553	3-Hydroxy-2',4',6'-trimethoxybenzophenone	C16H16O5	M+Na	311.0890	2.9
HMDB0166552	SPBio019	C16H16O5	M+Na	311.0890	2.9
HMDB0166549	2-(2,4,6-trimethoxybenzoyl)phenol	C16H16O5	M+Na	311.0890	2.9
HMDB0153954	2-[(2E)-1-hydroxy-3-(4-hydroxyphenyl)prop-2-en-1-yl]-5-methoxybenzene-1,3-diol	C16H16O5	M+Na	311.0890	2.9
HMDB0151904	1-phenyl-3-(3,4,6-trihydroxy-2-methoxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0151901	1-phenyl-3-(3,4,5-trihydroxy-2-methoxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0151899	3-(3,4-dihydroxy-2-methoxyphenyl)-3-hydroxy-1-phenylpropan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0145729		C16H16O5	M+Na	311.0890	2.9
HMDB0145716	2-(3-hydroxyphenyl)-4-methyl-3,4-dihydro-2H-1-benzopyran-3,5,7-triol	C16H16O5	M+Na	311.0890	2.9
HMDB0140888	1-(2,6-dihydroxy-4-methoxyphenyl)-3-(2-hydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0140886	1-(2,6-dihydroxy-4-methoxyphenyl)-3-(3-hydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0140885	1-(2,6-dihydroxy-4-methoxyphenyl)-3-hydroxy-3-phenylpropan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0137620	4-(7-hydroxy-3,4-dihydro-2H-1-benzopyran-3-yl)-2-methoxybenzene-1,3-diol	C16H16O5	M+Na	311.0890	2.9
HMDB0136844	3-(2-hydroxy-4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-5,7-diol	C16H16O5	M+Na	311.0890	2.9
HMDB0136845	3-(2-hydroxy-4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,7-diol	C16H16O5	M+Na	311.0890	2.9
HMDB0136524	4-[(E)-2-(4-hydroxy-3-methoxyphenyl)ethenyl]-6-methoxybenzene-1,3-diol	C16H16O5	M+Na	311.0890	2.9
HMDB0136525	5-[(E)-2-(4-hydroxy-3-methoxyphenyl)ethenyl]-3-methoxybenzene-1,2-diol	C16H16O5	M+Na	311.0890	2.9
HMDB0140887	3-phenyl-1-(2,3,6-trihydroxy-4-methoxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0141223	1-(2,4-dihydroxy-5-methoxyphenyl)-2-(3-hydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
HMDB0141951	2-(4-methoxyphenyl)-1-(2,3,4-trihydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9

	HMDB0141950	3-(4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4,7,8-triol	C16H16O5	M+Na	311.0890	2.9
	HMDB0141225	6-methoxy-3-phenyl-3,4-dihydro-2H-1-benzopyran-4,7,8-triol	C16H16O5	M+Na	311.0890	2.9
	HMDB0141226	2-phenyl-1-(2,3,4-trihydroxy-5-methoxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
	HMDB0141227	2-phenyl-1-(2,4,6-trihydroxy-3-methoxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
	HMDB0141221	4-(7-hydroxy-6-methoxy-3,4-dihydro-2H-1-benzopyran-3-yl)benzene-1,2-diol	C16H16O5	M+Na	311.0890	2.9
	HMDB0141222	3-(3-hydroxyphenyl)-6-methoxy-3,4-dihydro-2H-1-benzopyran-4,7-diol	C16H16O5	M+Na	311.0890	2.9
	HMDB0141224	3-(4-hydroxyphenyl)-6-methoxy-3,4-dihydro-2H-1-benzopyran-7,8-diol	C16H16O5	M+Na	311.0890	2.9
	HMDB0033018	-Methoxyyangonin	C16H16O5	M+Na	311.0890	2.9
	HMDB0133965	1-(2,4-dihydroxy-3-methoxyphenyl)-3-(4-hydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
	HMDB0041686	5'-Methoxy-O-desmethylangolensin	C16H16O5	M+Na	311.0890	2.9
	HMDB0041696	6'-Hydroxyangolensin	C16H16O5	M+Na	311.0890	2.9
	HMDB0030579	C.I. Natural Red	C16H16O5	M+Na	311.0890	2.9
	HMDB0029303	1-(3-Methoxy-4-hydroxy)-phenyl-6,7-dihydroxy-isochroman	C16H16O5	M+Na	311.0890	2.9
	HMDB0030740	11-Methoxyyangonin	C16H16O5	M+Na	311.0890	2.9
	HMDB0132899	1-(2,6-dihydroxy-4-methoxyphenyl)-3-(4-hydroxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
	HMDB0130881	4-(7-hydroxy-3,4-dihydro-2H-1-benzopyran-3-yl)-3-methoxybenzene-1,2-diol	C16H16O5	M+Na	311.0890	2.9
	HMDB0130880	3-(7-hydroxy-3,4-dihydro-2H-1-benzopyran-3-yl)-6-methoxybenzene-1,2-diol	C16H16O5	M+Na	311.0890	2.9
	HMDB0133777	3-(2-hydroxy-4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4,7-diol	C16H16O5	M+Na	311.0890	2.9
	HMDB0130930	3-phenyl-1-(2,4,6-trihydroxy-3-methoxyphenyl)propan-1-one	C16H16O5	M+Na	311.0890	2.9
	HMDB0147516	4-(7-hydroxy-3,4-dihydro-2H-1-benzopyran-3-yl)-6-methoxybenzene-1,3-diol	C16H16O5	M+Na	311.0890	2.9
312.1644	HMDB0031693	Ethyl (S)-3-hydroxybutyrate glucoside	C12H22O8	M+NH4	312.1653	-2.9
	HMDB0165161	6-(3-ethyl-4-hydroxybutoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H22O8	M+NH4	312.1653	-2.9
	HMDB0165160	6-(2-ethyl-4-hydroxybutoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H22O8	M+NH4	312.1653	-2.9
	HMDB0165158	3,4,5-trihydroxy-6-[(3-hydroxy-3-methylpentyl)oxy]oxane-2-carboxylic acid	C12H22O8	M+NH4	312.1653	-2.9
	HMDB0165157	3,4,5-trihydroxy-6-[(1-hydroxy-3-methylpentan-3-yl)oxy]oxane-2-carboxylic acid	C12H22O8	M+NH4	312.1653	-2.9
	HMDB0165154	3,4,5-trihydroxy-6-[(4-hydroxy-3-methylpentyl)oxy]oxane-2-carboxylic acid	C12H22O8	M+NH4	312.1653	-2.9
	HMDB0165153	3,4,5-trihydroxy-6-[(5-hydroxy-3-methylpentan-2-yl)oxy]oxane-2-carboxylic acid	C12H22O8	M+NH4	312.1653	-2.9
	HMDB0164626	3,4,5-trihydroxy-6-[(6-hydroxyhexyl)oxy]oxane-2-carboxylic acid	C12H22O8	M+NH4	312.1653	-2.9
	HMDB0164623	3,4,5-trihydroxy-6-[(5-hydroxyhexyl)oxy]oxane-2-carboxylic acid	C12H22O8	M+NH4	312.1653	-2.9
	HMDB0164622	3,4,5-trihydroxy-6-[(6-hydroxyhexan-2-yl)oxy]oxane-2-carboxylic acid	C12H22O8	M+NH4	312.1653	-2.9
	HMDB0165164	3,4,5-trihydroxy-6-[(5-hydroxy-3-methylpentyl)oxy]oxane-2-carboxylic acid	C12H22O8	M+NH4	312.1653	-2.9
312.1792	HMDB0032221	Dihydro-2,4,6-tris(2-methylpropyl)-4h-1,3,5-dithiazine	C15H31NS2	M+Na	312.1790	0.6
312.2163	HMDB0180101	(3,4-dihydroxyphenyl)methyl 8-methylnonanoate	C17H26O4	M+NH4	312.2169	-2.0
	HMDB0005783	Gingerol	C17H26O4	M+NH4	312.2169	-2.0
	HMDB0040646	Myrsinone	C17H26O4	M+NH4	312.2169	-2.0
	HMDB0035754	Phytuberin	C17H26O4	M+NH4	312.2169	-2.0
	HMDB0035722	Tanacetol A	C17H26O4	M+NH4	312.2169	-2.0
	HMDB0034779	Nordihydrocapsiate	C17H26O4	M+NH4	312.2169	-2.0
	HMDB0013325	2-trans,4-cis-Decadienoylcarnitine	C17H29NO4	M+H	312.2169	-2.0
	HMDB0035654	Phytal	C20H38O	M+NH4	312.3261	-2.5

312.3253	HMDB0172182	(2E)-3,5,7,11-tetramethylhexadeca-2,15-dien-1-ol	C20H38O	M+NH4	312.3261	-2.5
	HMDB0172181	(2E)-3,5,7-trimethyl-11-methylidenehexadec-2-en-1-ol	C20H38O	M+NH4	312.3261	-2.5
	HMDB0172180	(2E)-3,5,11-trimethyl-7-methylidenehexadec-2-en-1-ol	C20H38O	M+NH4	312.3261	-2.5
	HMDB0172179	(2E)-3,7,11-trimethyl-5-methylidenehexadec-2-en-1-ol	C20H38O	M+NH4	312.3261	-2.5
	HMDB0181944	11-Icosenal	C20H38O	M+NH4	312.3261	-2.5
313.1132	HMDB0011677	Galactose-beta-1,4-xylose	C11H20O10	M+H	313.1129	0.9
	HMDB0140855	6-({[3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy}methyl)oxane-2,3,4,5-tetrol	C11H20O10	M+H	313.1129	0.9
	HMDB0167977	3,4,5-trihydroxy-6-[(3,4,5-trihydroxypentyl)oxy]oxane-2-carboxylic acid	C11H20O10	M+H	313.1129	0.9
	HMDB0167974	3,4,5-trihydroxy-6-[(2,3,5-trihydroxypentyl)oxy]oxane-2-carboxylic acid	C11H20O10	M+H	313.1129	0.9
	HMDB0167976	3,4,5-trihydroxy-6-[(1,2,5-trihydroxypentan-3-yl)oxy]oxane-2-carboxylic acid	C11H20O10	M+H	313.1129	0.9
	HMDB0167975	3,4,5-trihydroxy-6-[(1,3,5-trihydroxypentan-2-yl)oxy]oxane-2-carboxylic acid	C11H20O10	M+H	313.1129	0.9
	HMDB0171708	6-({[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]oxy}methyl)oxane-2,3,4,5-tetrol	C11H20O10	M+H	313.1129	0.9
	HMDB0178259	4-{[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]oxy}-6-(hydroxymethyl)oxane-2,3,5-triol	C11H20O10	M+H	313.1129	0.9
	HMDB0029897	Serotonose	C11H20O10	M+H	313.1129	0.9
	HMDB0038863	2-O-b-D-Galactopyranosyl-D-xylose	C11H20O10	M+H	313.1129	0.9
	HMDB0029883	Sambubiose	C11H20O10	M+H	313.1129	0.9
	HMDB0038864	4-O-beta-D-Galactopyranosyl-D-xylose	C11H20O10	M+H	313.1129	0.9
	HMDB0038854	3-O-beta-D-Galactopyranosyl-L-arabinose	C11H20O10	M+H	313.1129	0.9
313.2368	HMDB0062281	(11S)-11-hydroperoxylinoleic acid	C18H32O4	M+H	313.2373	-1.7
	HMDB0062637	13(S)-HPODE	C18H32O4	M+H	313.2373	-1.7
	HMDB0062434	(9S,E,12Z,15Z)-9-hydroperoxy-,12,15-octadecadienoate	C18H32O4	M+H	313.2373	-1.7
	HMDB0040900	(E)-13-Hydroxy--oxo-11-octadecenoic acid	C18H32O4	M+H	313.2373	-1.7
	HMDB0010221	9,-DiHODE	C18H32O4	M+H	313.2373	-1.7
	HMDB0010208	15,16-DiHODE	C18H32O4	M+H	313.2373	-1.7
	HMDB0010201	12,13-DiHODE	C18H32O4	M+H	313.2373	-1.7
	HMDB0006940	9(S)-HPODE	C18H32O4	M+H	313.2373	-1.7
	HMDB0004706	8(R)-Hydroperoxylinoleic acid	C18H32O4	M+H	313.2373	-1.7
	HMDB0003871	13-L-Hydroperoxylinoleic acid	C18H32O4	M+H	313.2373	-1.7
313.2730	HMDB0175463	-hydroxy-6,,14-trimethyl-2-methylidenepentadecanoic acid	C19H36O3	M+H	313.2737	-2.3
	HMDB0175462	6-hydroxy-6,,14-trimethyl-2-methylidenepentadecanoic acid	C19H36O3	M+H	313.2737	-2.3
	HMDB0175465	3-hydroxy-6,,14-trimethyl-2-methylidenepentadecanoic acid	C19H36O3	M+H	313.2737	-2.3
	HMDB0175467	6-(hydroxymethyl)-,14-dimethyl-2-methylidenepentadecanoic acid	C19H36O3	M+H	313.2737	-2.3
	HMDB0175464	14-hydroxy-6,,14-trimethyl-2-methylidenepentadecanoic acid	C19H36O3	M+H	313.2737	-2.3
	HMDB0175466	2-(4,8,12-trimethyltridecyl)oxirane-2-carboxylic acid	C19H36O3	M+H	313.2737	-2.3
	HMDB0175468	-(hydroxymethyl)-6,14-dimethyl-2-methylidenepentadecanoic acid	C19H36O3	M+H	313.2737	-2.3
	HMDB0175469	15-hydroxy-6,,14-trimethyl-2-methylidenepentadecanoic acid	C19H36O3	M+H	313.2737	-2.3
314.2691	HMDB0013034	Palmitoylglycine	C18H35NO3	M+H	314.2690	0.4
	HMDB0160595	alpha-Hydroxylinoleic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0173889	(9E,12Z)-17-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0173891	(9E,12Z)-18-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0173888	alpha-artemismic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0173893	(9E,12Z)-2-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0160593	18-hydroxylinoleic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0160591	(12Z)-9-hydroxyoctadeca-,12-dienoic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0160592	17-hydroxylinoleic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0160589	(9Z,12Z)-14-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0160590	11-Hode	C18H32O3	M+NH4	314.2690	0.4
	HMDB0160588	8-Hydroxylinoleic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0112194	13-HODE	C18H32O3	M+NH4	314.2690	0.4
	HMDB0062652	9-HODE	C18H32O3	M+NH4	314.2690	0.4

	HMDB0173890	12,13-epome(9)	C18H32O3	M+NH4	314.2690	0.4
	HMDB0173886	(9E,12Z)-14-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0173885	(9E,12Z)-8-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0173887	(9E,12Z)-11-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0029796	(Z)-13-Oxo-9-octadecenoic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0029998	12-Hydroxy-8,-octadecadienoic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0029978	Avenoleic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0010223	9-HODE	C18H32O3	M+NH4	314.2690	0.4
	HMDB0004701	9,-Epoxyoctadecenoic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0004702	12,13-EpOME	C18H32O3	M+NH4	314.2690	0.4
	HMDB0004670	alpha-Dimorphecolic acid	C18H32O3	M+NH4	314.2690	0.4
	HMDB0004667	13-HODE	C18H32O3	M+NH4	314.2690	0.4
	HMDB0061708	13-HODE	C18H32O3	M+NH4	314.2690	0.4
314.3049	HMDB0035575	4,6-Nonadecanedione	C19H36O2	M+NH4	314.3054	-1.4
	HMDB0062658	(E)-nonadec--enoate	C19H35O2	M+NH4	314.3054	-1.4
	HMDB0175447	-hydroxy-6,,14-trimethyl-2-methylidenepentadecanal	C19H36O2	M+NH4	314.3054	-1.4
	HMDB0175446	6-hydroxy-6,,14-trimethyl-2-methylidenepentadecanal	C19H36O2	M+NH4	314.3054	-1.4
	HMDB0175445	SCHEMBL7563427	C19H36O2	M+NH4	314.3054	-1.4
	HMDB0175449	3-hydroxy-6,,14-trimethyl-2-methylidenepentadecanal	C19H36O2	M+NH4	314.3054	-1.4
	HMDB0175448	14-hydroxy-6,,14-trimethyl-2-methylidenepentadecanal	C19H36O2	M+NH4	314.3054	-1.4
	HMDB0175451	6-(hydroxymethyl)-,14-dimethyl-2-methylidenepentadecanal	C19H36O2	M+NH4	314.3054	-1.4
	HMDB0175450	2-(4,8,12-trimethyltridecyl)oxirane-2-carbaldehyde	C19H36O2	M+NH4	314.3054	-1.4
	HMDB0175452	-(hydroxymethyl)-6,14-dimethyl-2-methylidenepentadecanal	C19H36O2	M+NH4	314.3054	-1.4
	HMDB0013622	Z-Nonadecenoic acid	C19H36O2	M+NH4	314.3054	-1.4
	HMDB0175453	15-hydroxy-6,,14-trimethyl-2-methylidenepentadecanal	C19H36O2	M+NH4	314.3054	-1.4
314.3413	HMDB0002019	Phytol	C20H40O	M+NH4	314.3417	-1.4
	HMDB0172145	(2E)-3,5,7,11-tetramethylhexadec-2-en-1-ol	C20H40O	M+NH4	314.3417	-1.4
	HMDB0034933	(Z)-11-Eicosen-1-ol	C20H40O	M+NH4	314.3417	-1.4
	HMDB0003208	Thromboxane	C20H40O	M+NH4	314.3417	-1.4
315.0919	HMDB0015667	Sulfaphenazole	C15H14N4O2S	M+H	315.0910	2.8
	HMDB0012197	Canavaninosuccinate	C9H16N4O7	M+Na	315.0911	2.5
316.1387	HMDB0010350	2-Phenylethanol glucuronide	C14H18O7	M+NH4	316.1391	-1.2
	HMDB0124996	6-(3-ethylphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H18O7	M+NH4	316.1391	-1.2
	HMDB0125173	6-(4-ethylphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H18O7	M+NH4	316.1391	-1.2
	HMDB0168419	AC1O52M4	C14H18O7	M+NH4	316.1391	-1.2
	HMDB0240654	(2S,3S,4S,5R,6S)-6-(4-ethylphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H18O7	M+NH4	316.1391	-1.2
316.2839	HMDB0187015	2-Hydroxy-cis-vaccensaure	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0155790	(9Z)-11-hydroxyoctadec-9-enoic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0155794	2-hydroxyoleic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0155792	17-Hydroxyoleic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0155791	8-Hydroxyoleic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0187014	(11Z)-18-hydroxyoctadec-11-enoic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0187013	Oxiranedecanoic acid, 3-hexyl-	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0187011	-hydroxy-cis-vaccenic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0187012	(11Z)-17-hydroxyoctadec-11-enoic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0187010	(11Z)-13-hydroxyoctadec-11-enoic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0160378	8-home(9)	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0160379	17-hydroxy-9-octadecenoic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0160380	18-Hydroxy-9-octadecenoic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0160381	SCHEMBL378128	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0160377	11-hydroxy-9-octadecenoic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0155793	18-hydroxyoleic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0030979	9-Oxoctadecanoic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0034074	5-Oxoctadecanoic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0030980	-Oxoctadecanoic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0031127	5-Hexyltetrahydro-2-furanoctanoic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0034297	Ricinoleic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0030981	11-Oxoctadecanoic acid	C18H34O3	M+NH4	316.2846	-2.3
	HMDB0010736	3-keto stearic acid	C18H34O3	M+NH4	316.2846	-2.3

	HMDB0038057	Dehydrophytosphingosine	C18H37NO3	M+H	316.2846	-2.3
316.3205	HMDB0000772	Nonadecanoic acid	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0175455	6,,14-trimethyl-2-methylidenepentadecane-1,-diol	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0175454	6,,14-trimethyl-2-methylidenepentadecane-1,6-diol	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0175459	2-(4,8-dimethylnonyl)-6-methylideneheptane-1,7-diol	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0175457	6,,14-trimethyl-2-methylidenepentadecane-1,3-diol	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0175458	[2-(4,8,12-trimethyltridecyl)oxiran-2-yl]methanol	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0175456	6,,14-trimethyl-2-methylidenepentadecane-1,14-diol	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0175460	6-methyl-2-methylidene--(4-methylpentyl)undecane-1,11-diol	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0000795	Pristanic acid	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0004085	Tuberculostearic acid	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0035675	6-Hydroxy-4-nonadecanone	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0035674	4-Hydroxy-6-nonadecanone	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0037397	鈇?7-Methyloctadecanoic acid	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0061710	鈇?7-Methyloctadecanoic acid	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0038070	xi-16-Methyloctadecanoic acid	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0034154	Methyl stearate	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0035474	Isopropyl hexadecanoate	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0061964	Heptadecyl acetate	C19H38O2	M+NH4	316.3210	-1.6
	HMDB0175461	2,6,-trimethyl-14-methylidenepentadecane-1,15-diol	C19H38O2	M+NH4	316.3210	-1.6
317.1142	HMDB0147301	2-methoxy-4-[3-methylidene-5-(prop-1-en-1-yl)-2,3-dihydro-1-benzofuran-2-yl]phenol	C19H18O3	M+Na	317.1148	-1.9
	HMDB0141086	(1E)-1-(4-hydroxyphenyl)-7-phenylhept-1-ene-3,5-dione	C19H18O3	M+Na	317.1148	-1.9
	HMDB0141085	7-(4-hydroxyphenyl)-1-phenylhept-1-ene-3,5-dione	C19H18O3	M+Na	317.1148	-1.9
	HMDB0141083	1-(4-hydroxyphenyl)-7-phenylhept-1-ene-3,5-dione	C19H18O3	M+Na	317.1148	-1.9
	HMDB0138688	2-[3-hydroxy-2-(3-methylbut-2-en-1-yl)phenyl]-1-benzofuran-6-ol	C19H18O3	M+Na	317.1148	-1.9
	HMDB0128993	5-[(E)-2-(4-hydroxyphenyl)ethenyl]-2-[(1E)-3-methylbuta-1,3-dien-1-yl]benzene-1,3-diol	C19H18O3	M+Na	317.1148	-1.9
	HMDB0141084	(1E)-7-(4-hydroxyphenyl)-1-phenylhept-1-ene-3,5-dione	C19H18O3	M+Na	317.1148	-1.9
	HMDB0141109	(1Z)-2-hydroxy-1,7-diphenylhept-1-ene-3,5-dione	C19H18O3	M+Na	317.1148	-1.9
	HMDB0141182	(1E)-7-hydroxy-1,7-diphenylhept-1-ene-3,5-dione	C19H18O3	M+Na	317.1148	-1.9
	HMDB0141172	7-hydroxy-1,7-diphenylhept-1-ene-3,5-dione	C19H18O3	M+Na	317.1148	-1.9
	HMDB0141167	(1E)-4-hydroxy-1,7-diphenylhept-1-ene-3,5-dione	C19H18O3	M+Na	317.1148	-1.9
	HMDB0141166	4-hydroxy-1,7-diphenylhept-1-ene-3,5-dione	C19H18O3	M+Na	317.1148	-1.9
	HMDB0141155	(1E)-1-(3-hydroxyphenyl)-7-phenylhept-1-ene-3,5-dione	C19H18O3	M+Na	317.1148	-1.9
	HMDB0141154	7-(3-hydroxyphenyl)-1-phenylhept-1-ene-3,5-dione	C19H18O3	M+Na	317.1148	-1.9
	HMDB0141133	(1E)-7-(3-hydroxyphenyl)-1-phenylhept-1-ene-3,5-dione	C19H18O3	M+Na	317.1148	-1.9
	HMDB0141132	1-(3-hydroxyphenyl)-7-phenylhept-1-ene-3,5-dione	C19H18O3	M+Na	317.1148	-1.9
	HMDB0141123	(1E)-6-hydroxy-1,7-diphenylhept-1-ene-3,5-dione	C19H18O3	M+Na	317.1148	-1.9
	HMDB0141108	6-hydroxy-1,7-diphenylhept-1-ene-3,5-dione	C19H18O3	M+Na	317.1148	-1.9
	HMDB0033331	(E)-1-[4-Hydroxy-3-(3-methyl-1,3-butadienyl)phenyl]-2-(3,5-dihydroxyphenyl)ethylene	C19H18O3	M+Na	317.1148	-1.9
	HMDB0041305	1-Methoxy-4-[5-(4-methoxyphenoxy)-3-penten-1-ynyl]benzene	C19H18O3	M+Na	317.1148	-1.9
318.1176	HMDB0125177	4-{hydroxy[(3,4,5,6-tetrahydroxyoxan-2-yl)methoxy]methylidene}cyclohexa-2,5-dien-1-one	C13H16O8	M+NH4	318.1183	-2.3
	HMDB0135642	3,4,5-trihydroxy-6-(3-methoxyphenoxy)oxane-2-carboxylic acid	C13H16O8	M+NH4	318.1183	-2.3
	HMDB0166073	3,4,5-trihydroxy-6-[4-(hydroxymethyl)phenoxy]oxane-2-carboxylic acid	C13H16O8	M+NH4	318.1183	-2.3
	HMDB0186745	3,4,5-trihydroxy-6-[3-(hydroxymethyl)phenoxy]oxane-2-carboxylic acid	C13H16O8	M+NH4	318.1183	-2.3
	HMDB0166120	3,4,5-trihydroxy-6-[2-(hydroxymethyl)phenoxy]oxane-2-carboxylic acid	C13H16O8	M+NH4	318.1183	-2.3
	HMDB0240460	4-Methylcatechol 2-glucuronide	C13H16O8	M+NH4	318.1183	-2.3
	HMDB0240458	4-Methylcatechol 1-glucuronide	C13H16O8	M+NH4	318.1183	-2.3
	HMDB0167628	3,4,5-trihydroxy-6-(4-methoxyphenoxy)oxane-2-carboxylic acid	C13H16O8	M+NH4	318.1183	-2.3

	HMDB0167627	3,4,5-trihydroxy-6-(2-methoxyphenoxy)oxane-2-carboxylic acid	C13H16O8	M+NH4	318.1183	-2.3
	HMDB0029497	Dimethyl fukiic acid	C13H16O8	M+NH4	318.1183	-2.3
	HMDB0041271	Salicylic acid beta-D-glucoside	C13H16O8	M+NH4	318.1183	-2.3
	HMDB0125107	(3,4,5,6-tetrahydroxyoxan-2-yl)methyl 4-hydroxybenzoate	C13H16O8	M+NH4	318.1183	-2.3
	HMDB0181159	6-[3-(3,4-dihydro-2H-pyrrol-5-yl)-3-oxopropoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H19NO8	M+H	318.1183	-2.3
	HMDB0181157	6-[[1-(3,4-dihydro-2H-pyrrol-5-yl)-1-oxopropan-2-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H19NO8	M+H	318.1183	-2.3
	HMDB0240321	N(6),N(6)-dimethyladenosine	C12H17N5O4	M+Na	318.1173	1.0
318.1905	HMDB0240724	O-suberoylcarnitine	C15H27NO6	M+H	318.1911	-1.9
318.2427	HMDB0156405	(2Z,4E,6E,8E)-2-hydroxy-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraenal	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0156406	3-Hydroxyretinal	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0156404	(2Z,4E,6E,8E)-3-(hydroxymethyl)-7-methyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraenal	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0156407	(2E,4E,6E)-3-methyl-7-[3-(2,6,6-trimethylcyclohex-1-en-1-yl)oxiran-2-yl]octa-2,4,6-trienal	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0156403	(2E,4E,6Z,8E)-7-(hydroxymethyl)-3-methyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraenal	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0156401	4-Hydroxyretinal	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0156402	(2E,4E,6E,8E)-9-[2-(hydroxymethyl)-6,6-dimethylcyclohex-1-en-1-yl]-3,7-dimethylnona-2,4,6,8-tetraenal	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0156408	(2E,4E)-3-methyl-5-{3-methyl-3-[(E)-2-(2,6,6-trimethylcyclohex-1-en-1-yl)ethenyl]oxiran-2-yl}penta-2,4-dienal	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0156411	5,6-Epoxyretinal	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0061925	Dehydroabietic acid	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0183805	(4E,6Z)-7-methyl-3-methylidene-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-4,6,8-trienoic acid	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0156418	(4E,6E,8E)-3,7-dimethyl-2-oxo-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-4,6,8-trienal	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0156413	(2E,4E,6E,8E)-9-[6-(hydroxymethyl)-2,6-dimethylcyclohex-1-en-1-yl]-3,7-dimethylnona-2,4,6,8-tetraenal	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0156409	(2E)-3-{3-[(1E,3E)-2-methyl-4-(2,6,6-trimethylcyclohex-1-en-1-yl)buta-1,3-dien-1-yl]oxiran-2-yl}but-2-enal	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0156410	3-methyl-3-[(1E,3E,5E)-4-methyl-6-(2,6,6-trimethylcyclohex-1-en-1-yl)hexa-1,3,5-trien-1-yl]oxirane-2-carbaldehyde	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0001852	all-trans-Retinoic acid	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0156412	all-trans-Retinoic acid	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0036564	Sugiol	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0036697	ent-6,16-Kauradien-19-oic acid	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0036711	Yucalexin B7	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0038702	Trilobinol	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0012329	4-Oxoretinol	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0006219	13-cis-Retinoic acid	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0036710	Yucalexin B16	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0041925	Metandienone	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0012874	9,13-cis-Retinoic acid	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0012788	4-OH-Retinal	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0002369	9-cis-Retinoic acid	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0179600	1,4a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carboxylic acid	C20H28O2	M+NH4	318.2428	-0.2
	HMDB0062549	(S)-2-hydroxyoctadecanoic acid	C18H36O3	M+NH4	318.3003	-1.8
	HMDB0112181	DI-7-hydroxy stearic acid	C18H36O3	M+NH4	318.3003	-1.8
	HMDB0112180	5-hydroxyoctadecanoic acid	C18H36O3	M+NH4	318.3003	-1.8
	HMDB0112182	DI-8-hydroxy stearic acid	C18H36O3	M+NH4	318.3003	-1.8
	HMDB0112193	DI-6-hydroxy stearic acid	C18H36O3	M+NH4	318.3003	-1.8
	HMDB0240324	-hydroxystearate	C18H35O3	M+NH4	318.3003	-1.8

318.2997	HMDB0240330	3-hydroxystearate	C18H35O3	M+NH4	318.3003	-1.8
	HMDB0112183	DI-11-hydroxy stearic acid	C18H36O3	M+NH4	318.3003	-1.8
	HMDB0171069	18-Hydroxyoctadecanoic acid	C18H36O3	M+NH4	318.3003	-1.8
	HMDB0010737	(R)-3-Hydroxy-Octadecanoic acid	C18H36O3	M+NH4	318.3003	-1.8
	HMDB0037396	xi--Hydroxyoctadecanoic acid	C18H36O3	M+NH4	318.3003	-1.8
	HMDB0061662	13-hydroxyoctadecanoic acid	C18H36O3	M+NH4	318.3003	-1.8
	HMDB0061661	9-hydroxyoctadecanoic acid	C18H36O3	M+NH4	318.3003	-1.8
	HMDB0061706	12-Hydroxystearic acid	C18H36O3	M+NH4	318.3003	-1.8
	HMDB0171068	17-hydroxy stearic acid	C18H36O3	M+NH4	318.3003	-1.8
319.0779	HMDB0004610	Phytosphingosine	C18H39NO3	M+H	318.3003	-1.8
	HMDB0172667	2-acetyl-4,7,8-trihydroxy-6-methoxy-3-methyl-1,2,3,5,8,8a-hexahydronaphthalene-1,5-dione	C14H16O7	M+Na	319.0788	-2.9
	HMDB0172668	2-acetyl-4,7,8-trihydroxy-6-methoxy-3-methyl-1,2,3,5,6,7-hexahydronaphthalene-1,5-dione	C14H16O7	M+Na	319.0788	-2.9
	HMDB0172666	2-acetyl-4,7,8-trihydroxy-6-methoxy-3-methyl-1,2,3,4,4a,5-hexahydronaphthalene-1,5-dione	C14H16O7	M+Na	319.0788	-2.9
	HMDB0172089	6-(2-ethenylphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O7	M+Na	319.0788	-2.9
	HMDB0125168	6-(4-ethenylphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O7	M+Na	319.0788	-2.9
	HMDB0124987	6-(3-ethenylphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O7	M+Na	319.0788	-2.9
	HMDB0159303	6-[(2,4-dihydroxypyrimidin-5-yl)methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C11H14N2O9	M+H	319.0772	2.2
	HMDB0156392	(2Z)-2-[(1E,3E,5E)-4-methyl-6-(2,6,6-trimethylcyclohex-1-en-1-yl)hexa-1,3,5-trien-1-yl]but-2-ene-1,4-diol	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0156399	Hepaxanthin	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0156396	(2E,4E)-3-methyl-5-{3-methyl-3-[(E)-2-(2,6,6-trimethylcyclohex-1-en-1-yl)ethenyl]oxiran-2-yl}penta-2,4-dien-1-ol	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0156398	SCHEMBL8523586	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0156397	(2E)-3-{3-[(1E,3E)-2-methyl-4-(2,6,6-trimethylcyclohex-1-en-1-yl)buta-1,3-dien-1-yl]oxiran-2-yl}but-2-en-1-ol	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0156400	(2E,4E,6E,8E)-9-[6-(hydroxymethyl)-2,6-dimethylcyclohex-1-en-1-yl]-3,7-dimethylnona-2,4,6,8-tetraen-1-ol	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0156416	(2Z,4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraene-1,2-diol	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0156415	(4E,6E,8E)-2-hydroxy-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-4,6,8-trienal	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0179572	4a-(hydroxymethyl)-1-methyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0156393	SCHEMBL3411787	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0156394	3-Hydroxyretinol	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0156389	4-Hydroxyretinol	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0156391	(2Z,4E,6E)-6-methyl-2-[(E)-2-(2,6,6-trimethylcyclohex-1-en-1-yl)ethenyl]octa-2,4,6-triene-1,8-diol	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0156390	(2E,4E,6E,8E)-9-[2-(hydroxymethyl)-6,6-dimethylcyclohex-1-en-1-yl]-3,7-dimethylnona-2,4,6,8-tetraen-1-ol	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0156395	(2E,4E,6E)-3-methyl-7-[3-(2,6,6-trimethylcyclohex-1-en-1-yl)oxiran-2-yl]octa-2,4,6-trien-1-ol	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0179575	6-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0179574	7-(2-hydroxypropan-2-yl)-1,4a-dimethyl-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0183789	17191-5	C20H30O2	M+NH4	320.2584	-1.9

320.2578	HMDB0179581	4-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0179573	1-(hydroxymethyl)-4a-methyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0179576	-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0179577	2,6-dimethyl-13-(propan-2-yl)-12-oxatetracyclo[8.5,,]pentadec-9-ene-6-carbaldehyde	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0179580	4b-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0179578	7-(1-hydroxypropan-2-yl)-1,4a-dimethyl-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0179579	5-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0179583	2-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0179582	3-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0179584	a-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0036811	Isopimaric acid	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0001999	Eicosapentaenoic acid	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0035692	8,15-Isopimaradien-18-oic acid	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0038172	8,13-Abietadien-18-oic acid	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0003598	Retinyl ester	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0036709	Yucalexin B14	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0036703	Siderone	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0039486	ent-8(17),13(16),14-Labdatrien-18-oic acid	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0036775	Yucalexin A16	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0038687	(ent-15beta,16beta)-15,16-Epoxy-3-kauranone	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0036826	Cascarillone	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0036805	8(17),12-Labdadiene-15,16-dial	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0015655	Methyltestosterone	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0041928	Methenolone	C20H30O2	M+NH4	320.2584	-1.9
	HMDB0179571	Resin acid	C20H30O2	M+NH4	320.2584	-1.9
321.0196	HMDB0014332	Lorazepam	C15H10Cl2N2O2	M+H	321.0192	1.2
321.2181	HMDB0033862	3-(8,11,14-Pentadecatrienyl)phenol	C21H30O	M+Na	321.2189	-2.4
321.9482	HMDB0015275	Dichlorphenamide	C6H6Cl2N2O4S2	M+NH4	321.9484	-0.7
322.0762	HMDB0013220	Beta-Citryl-L-glutamic acid	C11H15NO10	M+H	322.0769	-2.1
	HMDB0002044	8-Hydroxyguanosine	C10H13N5O6	M+Na	322.0758	1.2
	HMDB0155333	2-[6-hydroxy-2-(hydroxyamino)-9H-purin-9-yl]-5-(hydroxymethyl)oxolane-3,4-diol	C10H13N5O6	M+Na	322.0758	1.2
	HMDB0187538	9-[4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-2-(hydroxyamino)-9H-purine-6,8-diol	C10H13N5O6	M+Na	322.0758	1.2
	HMDB0179586	[1-(hydroxymethyl)-1-methyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthren-4a-yl]methanol	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0179587	[1-(hydroxymethyl)-4a-methyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthren-1-yl]methanol	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0179589	8-(hydroxymethyl)-4b,8-dimethyl-2-(propan-2-yl)-3,4,4a,4b,5,6,7,8,8a,9-decahydrophenanthren-3-ol	C20H32O2	M+NH4	322.2741	-2.0

322.2734	HMDB0179592	2-[8-(hydroxymethyl)-4b,8-dimethyl-3,4,4a,4b,5,6,7,8,8a,9-decahydrophenanthren-2-yl]propan-1-ol	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0179590	8-(hydroxymethyl)-4b,8-dimethyl-2-(propan-2-yl)-3,4,4a,4b,5,6,7,8,8a,9-decahydrophenanthren-9-ol	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0179591	[2,6-dimethyl-13-(propan-2-yl)-12-oxatetracyclo[8.5.,,]pentadec-9-en-6-yl]methanol	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0185649	(8Z,11Z,14Z)-icosa-8,11,14,19-tetraenoic acid	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0179588	2-[8-(hydroxymethyl)-4b,8-dimethyl-3,4,4a,4b,5,6,7,8,8a,9-decahydrophenanthren-2-yl]propan-2-ol	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0014996	Drostanolone	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0036829	Copalic acid	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0039702	Oryzalexin E	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0036702	Sideridiol	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0039687	Oryzalexin S	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0001043	Arachidonic acid	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0060102	Arachidonic acid	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0002177	Cis-8,11,14,17-Eicosatetraenoic acid	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0006036	Mesterolone	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0036830	Junicedral	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0037824	7,13-Eperudien-15-oic acid	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0036721	ent-17-Hydroxy-16beta-kauran-19-al	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0036754	Yucalexin P21	C20H32O2	M+NH4	322.2741	-2.0
	HMDB0013624	Alpha-Linolenoyl ethanolamide	C20H35NO2	M+H	322.2741	-2.0
	HMDB0060628	Doxepin-N-oxide	C20H35NO2	M+H	322.2741	-2.0
324.0583	HMDB0011640	Uridine 2',3'-cyclic phosphate	C9H11N2O8P	M+NH4	324.0591	-2.5
	HMDB0240312	Cytidine 3'-monophosphate	C9H14N3O8P	M+H	324.0591	-2.6
	HMDB0000095	Cytidine monophosphate	C9H14N3O8P	M+H	324.0591	-2.6
	HMDB0155220	Cytidine monophosphate	C9H14N3O8P	M+H	324.0591	-2.6
	HMDB0011692	Cytidine 2'-phosphate	C9H14N3O8P	M+H	324.0591	-2.6
324.2890	HMDB0174106	{3-methyl-3-[(3E,7E)-4,8,12-trimethyltrideca-3,7,11-trien-1-yl]oxiran-2-yl}methanol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174105	(2Z)-3-Methyl-5-[3-methyl-3-(4,8-dimethyl-3,7-nonadienyl)oxiranyl]-2-pentene-1-ol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174104	(2Z,6E)-3,7-dimethyl-9-[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]nona-2,6-dien-1-ol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174101	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,9-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174100	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,13-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174102	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,5-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174103	147-52-2	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174097	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,8-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174098	(2E)-2-[(3E,7E)-4,8,12-trimethyltrideca-3,7,11-trien-1-yl]but-2-ene-1,4-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174099	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,4-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174096	SCHEMBL116891	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174095	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,12-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174093	(6E,E,14Z)-2,6,,14-tetramethylhexadeca-2,6,,14-tetraene-1,16-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174094	(2Z,6E,Z)-6,-dimethyl-2-(4-methylpent-3-en-1-yl)dodeca-2,6,-triene-1,12-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174150	SCHEMBL8576448	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174152	plaunotol	C20H34O2	M+NH4	324.2897	-2.2

	HMDB0174149	(6E,E,14E)-2,6,,14-tetramethylhexadeca-2,6,,14-tetraene-1,16-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174161	6,7-Epoxygeranylgeraniol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174158	(2E,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,5-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174159	14,15-Epoxygeranylgeraniol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174160	(2E,6E)-3,7-dimethyl-9-[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]nona-2,6-dien-1-ol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174157	May-64	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174156	(2E,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,13-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174155	(2E,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,4-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174154	(2Z)-2-[(3E,7E)-4,8,12-trimethyltrideca-3,7,11-trien-1-yl]but-2-ene-1,4-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174153	(2E,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,8-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0174151	(2E,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,12-diol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0060039	Dihomo-alpha-linolenic acid	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0036835	Sagittariol	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0031058	Sciadonic acid	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0010378	5,8,11-Eicosatrienoic acid	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0002925	Dihomo-gamma-linolenic acid	C20H34O2	M+NH4	324.2897	-2.2
	HMDB0012252	Linoleoyl ethanolamide	C20H37NO2	M+H	324.2897	-2.2
325.0425	HMDB0015380	Olsalazine	C14H10N2O6	M+Na	325.0431	-1.9
	HMDB0156309	286-43-3	C9H13N2O9P	M+H	325.0431	-2.0
	HMDB0060282	Uridine 3'-monophosphate	C9H13N2O9P	M+H	325.0431	-2.0
	HMDB0011641	Uridine 2'-phosphate	C9H13N2O9P	M+H	325.0431	-2.0
	HMDB0001271	Pseudouridine 5'-phosphate	C9H13N2O9P	M+H	325.0431	-2.0
	HMDB0000288	Uridine 5'-monophosphate	C9H13N2O9P	M+H	325.0431	-2.0
325.1770	HMDB0155192	(2S,15S)-2-(hydroxymethyl)-15-methyltetracyclo[8.7,,heptadec-7-ene-5,14-dione	C19H26O3	M+Na	325.1774	-1.3
	HMDB0155191	(2R,15S)-6-hydroxy-2,15-dimethyltetracyclo[8.7,,heptadec-7-ene-5,14-dione	C19H26O3	M+Na	325.1774	-1.3
	HMDB0155189	(2R,15S)-13-hydroxy-2,15-dimethyltetracyclo[8.7,,heptadec-7-ene-5,14-dione	C19H26O3	M+Na	325.1774	-1.3
	HMDB0155193	(2R,15S)-15-(hydroxymethyl)-2-methyltetracyclo[8.7,,heptadec-7-ene-5,14-dione	C19H26O3	M+Na	325.1774	-1.3
	HMDB0155195	(2R,15S)-12-hydroxy-2,15-dimethyltetracyclo[8.7,,heptadec-7-ene-5,14-dione	C19H26O3	M+Na	325.1774	-1.3
	HMDB0155194	(2R,15S)-9-hydroxy-2,15-dimethyltetracyclo[8.7,,heptadec-7-ene-5,14-dione	C19H26O3	M+Na	325.1774	-1.3
	HMDB0156936	(2R,15S)-14-hydroxy-2,15-dimethyltetracyclo[8.7,,heptadec-7-ene-5,13-dione	C19H26O3	M+Na	325.1774	-1.3
	HMDB0158197	SCHEMBL8489736	C19H26O3	M+Na	325.1774	-1.3
	HMDB0158606	SCHEMBL52497	C19H26O3	M+Na	325.1774	-1.3
	HMDB0012782	4-Methoxy-17beta-estradiol	C19H26O3	M+Na	325.1774	-1.3
	HMDB0155190	(2R,15S)-4-hydroxy-2,15-dimethyltetracyclo[8.7,,heptadec-7-ene-5,14-dione	C19H26O3	M+Na	325.1774	-1.3
	HMDB0154995	(2R,15S)-2,15-dimethyltetracyclo[8.7,,heptadecane-5,6,14-trione	C19H26O3	M+Na	325.1774	-1.3
	HMDB0154970	11b-Hydroxyandrost-4-ene-3,17-dione	C19H26O3	M+Na	325.1774	-1.3
	HMDB0137388	(4E)-1-(4-hydroxy-3-methoxyphenyl)dodeca-4,11-dien-3-one	C19H26O3	M+Na	325.1774	-1.3
	HMDB0137399	(1E)-1-(4-hydroxy-3-methoxyphenyl)dodeca-1,11-dien-3-one	C19H26O3	M+Na	325.1774	-1.3
	HMDB0154971	6-Hydroxy-4-androstene-3,17-dione	C19H26O3	M+Na	325.1774	-1.3

	HMDB0154972	(1S,2R,R,11S,15S)-13-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-6-ene-5,14-dione	C19H26O3	M+Na	325.1774	-1.3
	HMDB0154973	7121-	C19H26O3	M+Na	325.1774	-1.3
	HMDB0154976	SCHEMBL2469	C19H26O3	M+Na	325.1774	-1.3
	HMDB0031038	(2Z,8S,9Z)-2,9-Heptadecadiene-8-hydroxy-4,6-diyne-1-yl acetate	C19H26O3	M+Na	325.1774	-1.3
	HMDB0041204	Acetylpanaxydol	C19H26O3	M+Na	325.1774	-1.3
	HMDB0034028	2-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxy-6-methoxyacetophenone	C19H26O3	M+Na	325.1774	-1.3
	HMDB0154977	Formestane	C19H26O3	M+Na	325.1774	-1.3
	HMDB0039568	Ginsenoside H	C19H26O3	M+Na	325.1774	-1.3
	HMDB0034167	Falcarindiol 3-acetate	C19H26O3	M+Na	325.1774	-1.3
	HMDB0040927	2-Hexyl-5-[2-(4-hydroxy-3-methoxyphenyl)ethyl]furan	C19H26O3	M+Na	325.1774	-1.3
	HMDB0000380	2-Methylcitric acid	C19H26O3	M+Na	325.1774	-1.3
	HMDB0000405	2-Methoxyestradiol	C19H26O3	M+Na	325.1774	-1.3
	HMDB0003955	19-Hydroxyandrost-4-ene-3,17-dione	C19H26O3	M+Na	325.1774	-1.3
	HMDB0003959	19-Oxotestosterone	C19H26O3	M+Na	325.1774	-1.3
	HMDB0006774	16a-Hydroxyandrost-4-ene-3,17-dione	C19H26O3	M+Na	325.1774	-1.3
	HMDB0006773	Phenmetrazine	C19H26O3	M+Na	325.1774	-1.3
	HMDB0006771	7a-Hydroxyandrost-4-ene-3,17-dione	C19H26O3	M+Na	325.1774	-1.3
	HMDB0033125	[8]-Dehydroshogaol	C19H26O3	M+Na	325.1774	-1.3
	HMDB0036696	Yucalexin B'11	C19H26O3	M+Na	325.1774	-1.3
325.2364	HMDB0031007	1-Acetoxy-2-hydroxy-16-heptadecyn-4-one	C19H32O4	M+H	325.2373	-2.9
	HMDB0164465	1-(4-hydroxy-3-methoxyphenyl)dodecane-3,5-diol	C19H32O4	M+H	325.2373	-2.9
	HMDB0094647	Mono-(2-ethyl-5-carboxypentyl) phthalate	C16H20O6	M+NH4	326.1598	-2.2
326.1591	HMDB0037772	8-Acetylgelelolide	C16H20O6	M+NH4	326.1598	-2.2
	HMDB0034363	Monocrotaline	C16H23NO6	M+H	326.1598	-2.2
	HMDB0181245	1-[(6-carboxy-3,4-dihydroxyoxan-2-yl)oxy]-3-pentylpyridin-1-ium	C16H24NO6	M+H	326.1598	-2.2
	HMDB0175180	3,4,5-trihydroxy-6-[(6-hydroxyheptyl)oxy]oxane-2-carboxylic acid	C13H24O8	M+NH4	326.1809	-0.4
326.1808	HMDB0175179	3,4,5-trihydroxy-6-[(7-hydroxyheptan-2-yl)oxy]oxane-2-carboxylic acid	C13H24O8	M+NH4	326.1809	-0.4
	HMDB0175183	3,4,5-trihydroxy-6-[(7-hydroxyheptyl)oxy]oxane-2-carboxylic acid	C13H24O8	M+NH4	326.1809	-0.4
326.1941	HMDB0061634	3-hydroxyoctanoyl carnitine	C15H29NO5	M+Na	326.1938	0.9
326.2168	HMDB0029362	(R)-1-O-b-D-glucopyranosyl-1,3-octanediol	C14H28O7	M+NH4	326.2173	-1.6
	HMDB0158028	(2S,15S)-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadecane-5,14-diol	C19H32O3	M+NH4	326.2690	-2.0
	HMDB0158027	(2R,15S)-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecane-5,14-diol	C19H32O3	M+NH4	326.2690	-2.0
	HMDB0158025	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadecane-5,8,14-triol	C19H32O3	M+NH4	326.2690	-2.0
	HMDB0158024	(2S,15S)-2,15-dimethyltetracyclo[8.7.,heptadecane-5,14,17-triol	C19H32O3	M+NH4	326.2690	-2.0
326.2683	HMDB0158026	(2S,15S)-2,15-dimethyltetracyclo[8.7.,heptadecane-5,13,14-triol	C19H32O3	M+NH4	326.2690	-2.0
	HMDB0112090	5-Hexyl-3,4-dimethyl-2-furanheptanoic acid	C19H32O3	M+NH4	326.2690	-2.0
	HMDB0112096	8-(3,4-dimethyl-5-pentylfuran-2-yl)-octanoic acid	C19H32O3	M+NH4	326.2690	-2.0
	HMDB0094643	-(3,4-dimethyl-5-propylfuran-2-yl)decanoic acid	C19H32O3	M+NH4	326.2690	-2.0
	HMDB0112070	5-Ethyl-3,4-dimethyl-2-furanundecanoic acid	C19H32O3	M+NH4	326.2690	-2.0
	HMDB0112100	9-(3,4-dimethyl-5-butylfuran-2-yl)-nonanoic acid	C19H32O3	M+NH4	326.2690	-2.0
	HMDB0061646	3-Methyl-5-propyl-2-furanundecanoic acid	C19H32O3	M+NH4	326.2690	-2.0
	HMDB0030960	Isoobtusilactone A	C19H32O3	M+NH4	326.2690	-2.0
	HMDB0031379	Annosquamosin B	C19H32O3	M+NH4	326.2690	-2.0
	HMDB0031091	3-Methyl-5-pentyl-2-furannonanoic acid	C19H32O3	M+NH4	326.2690	-2.0
	HMDB0062432	(8Z,11Z)-icosadienoic acid	C20H36O2	M+NH4	326.3054	-1.7
326.3048	HMDB0036827	Sclareol	C20H36O2	M+NH4	326.3054	-1.7
	HMDB0005060	Eicosadienoic acid	C20H36O2	M+NH4	326.3054	-1.7
	HMDB0002088	N-Oleylethanolamine	C20H39NO2	M+H	326.3054	-1.7
	HMDB0002337	Homophytanic acid	C21H42O2	M+H	327.3258	-1.1
	HMDB0035670	4-Hydroxy-6-heneicosanone	C21H42O2	M+H	327.3258	-1.1
	HMDB0035669	8-Hydroxy-6-heneicosanone	C21H42O2	M+H	327.3258	-1.1
327.3254	HMDB0035671	6-Hydroxy-4-heneicosanone	C21H42O2	M+H	327.3258	-1.1
	HMDB0035668	6-Hydroxy-8-heneicosanone	C21H42O2	M+H	327.3258	-1.1

	HMDB0031319	2,3,7,11,15-Pentamethylhexadecanoic acid	C21H42O2	M+H	327.3258	-1.1
	HMDB0002345	Heneicosanoic acid	C21H42O2	M+H	327.3258	-1.1
328.2117	HMDB0179991	(4-hydroxy-3-methoxyphenyl)methyl 2-hydroxy-7-methyloctanoate	C17H26O5	M+NH4	328.2118	-0.4
	HMDB0179989	(4-hydroxy-3-methoxyphenyl)methyl 7-hydroxy-7-methyloctanoate	C17H26O5	M+NH4	328.2118	-0.4
	HMDB0179990	(4-hydroxy-3-methoxyphenyl)methyl 8-hydroxy-7-methyloctanoate	C17H26O5	M+NH4	328.2118	-0.4
	HMDB0179993	(3,4-dihydroxy-5-methoxyphenyl)methyl 7-methyloctanoate	C17H26O5	M+NH4	328.2118	-0.4
	HMDB0040980	Valdiate	C17H26O5	M+NH4	328.2118	-0.4
	HMDB0040756	3-Hydroxy-6,8-dimethoxy-7(11)-eremophilen-12,8-olide	C17H26O5	M+NH4	328.2118	-0.4
328.3211	HMDB0013645	N,N-Dimethylsphingosine	C20H41NO2	M+H	328.3210	0.3
	HMDB0013078	Stearoylethanolamide	C20H41NO2	M+H	328.3210	0.3
	HMDB0062436	Gadoleic acid	C20H38O2	M+NH4	328.3210	0.3
	HMDB0181955	(11E)-2-hydroxyicos-11-enal	C20H38O2	M+NH4	328.3210	0.3
	HMDB0181951	(11E)--hydroxyicos-11-enal	C20H38O2	M+NH4	328.3210	0.3
	HMDB0181953	-(3-octyloxiran-2-yl)decanal	C20H38O2	M+NH4	328.3210	0.3
	HMDB0181952	(11E)-19-hydroxyicos-11-enal	C20H38O2	M+NH4	328.3210	0.3
	HMDB0181954	(11E)--hydroxyicos-11-enal	C20H38O2	M+NH4	328.3210	0.3
	HMDB0181950	(11E)-13-hydroxyicos-11-enal	C20H38O2	M+NH4	328.3210	0.3
	HMDB0181956	Trans-gondoic acid	C20H38O2	M+NH4	328.3210	0.3
	HMDB0035159	Paullinic acid	C20H38O2	M+NH4	328.3210	0.3
	HMDB0037127	Oleyl acetate	C20H38O2	M+NH4	328.3210	0.3
	HMDB0034451	Ethyl oleate	C20H38O2	M+NH4	328.3210	0.3
	HMDB0035572	6,8-Icosanedione	C20H38O2	M+NH4	328.3210	0.3
	HMDB0035574	4,6-Icosanedione	C20H38O2	M+NH4	328.3210	0.3
	HMDB0035573	5,7-Icosanedione	C20H38O2	M+NH4	328.3210	0.3
	HMDB0002231	11Z-Eicosenoic acid	C20H38O2	M+NH4	328.3210	0.3
	HMDB0034296	11Z-Eicosenoic acid	C20H38O2	M+NH4	328.3210	0.3
330.0609	HMDB0146641	14,16-dihydroxy-5,7,11,19-tetraoxapentacyclo[.8,?, α icosa-1(12),2,4(8),9,13,15,17-heptaen--one	C16H8O7	M+NH4	330.0608	0.2
	HMDB0146640	16,17-dihydroxy-5,7,11,19-tetraoxapentacyclo[.8,?, α icosa-1(12),2,4(8),9,13(18),14,16-heptaen--one	C16H8O7	M+NH4	330.0608	0.2
	HMDB0146639	15,16-dihydroxy-5,7,11,19-tetraoxapentacyclo[.8,?, α icosa-1(12),2,4(8),9,13(18),14,16-heptaen--one	C16H8O7	M+NH4	330.0608	0.2
330.0722	HMDB0000125	Glutathione	C10H17N3O6S	M+Na	330.0730	-2.5
	HMDB0062697	gamma-Glutamylcysteinylglycine	C10H17N3O6S	M+Na	330.0730	-2.5
330.1395	HMDB0011677	Galactose-beta-1,4-xylose	C11H20O10	M+NH4	330.1395	0.1
	HMDB0140855	6-([3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy)methyl)oxane-2,3,4,5-tetrol	C11H20O10	M+NH4	330.1395	0.1
	HMDB0167974	3,4,5-trihydroxy-6-[(2,3,5-trihydroxypentyl)oxy]oxane-2-carboxylic acid	C11H20O10	M+NH4	330.1395	0.1
	HMDB0167975	3,4,5-trihydroxy-6-[(1,3,5-trihydroxypentan-2-yl)oxy]oxane-2-carboxylic acid	C11H20O10	M+NH4	330.1395	0.1
	HMDB0167977	3,4,5-trihydroxy-6-[(3,4,5-trihydroxypentyl)oxy]oxane-2-carboxylic acid	C11H20O10	M+NH4	330.1395	0.1
	HMDB0167976	3,4,5-trihydroxy-6-[(1,2,5-trihydroxypentan-3-yl)oxy]oxane-2-carboxylic acid	C11H20O10	M+NH4	330.1395	0.1
	HMDB0171708	6-([3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]oxy)methyl)oxane-2,3,4,5-tetrol	C11H20O10	M+NH4	330.1395	0.1
	HMDB0029897	Serotonine	C11H20O10	M+NH4	330.1395	0.1
	HMDB0038863	2-O-b-D-Galactopyranosyl-D-xylose	C11H20O10	M+NH4	330.1395	0.1
	HMDB0029883	Sambubiose	C11H20O10	M+NH4	330.1395	0.1
	HMDB0038864	4-O-beta-D-Galactopyranosyl-D-xylose	C11H20O10	M+NH4	330.1395	0.1
	HMDB0038854	3-O-beta-D-Galactopyranosyl-L-arabinose	C11H20O10	M+NH4	330.1395	0.1
	HMDB0178259	4-{[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]oxy}-6-(hydroxymethyl)oxane-2,3,5-triol	C11H20O10	M+NH4	330.1395	0.1
	HMDB0062637	13(S)-HPODE	C18H32O4	M+NH4	330.2639	-2.1
	HMDB0062281	(11S)-11-hydroperoxylinoleic acid	C18H32O4	M+NH4	330.2639	-2.1
	HMDB0062434	(9S,E,12Z,15Z)-9-hydroperoxy-,12,15-octadecadienoate	C18H32O4	M+NH4	330.2639	-2.1

330.2632	HMDB0040900	(E)-13-Hydroxy--oxo-11-octadecenoic acid	C18H32O4	M+NH4	330.2639	-2.1
	HMDB0010221	9,-DiHODE	C18H32O4	M+NH4	330.2639	-2.1
	HMDB0010208	15,16-DiHODE	C18H32O4	M+NH4	330.2639	-2.1
	HMDB0010201	12,13-DiHODE	C18H32O4	M+NH4	330.2639	-2.1
	HMDB0006940	9(S)-HPODE	C18H32O4	M+NH4	330.2639	-2.1
	HMDB0004706	8(R)-Hydroperoxylinoleic acid	C18H32O4	M+NH4	330.2639	-2.1
	HMDB0003871	13-L-Hydroperoxylinoleic acid	C18H32O4	M+NH4	330.2639	-2.1
	HMDB0006202	4,8 Dimethylnonanoyl carnitine	C18H35NO4	M+H	330.2639	-2.1
330.2998	HMDB0013321	Undecanoylcarnitine	C18H35NO4	M+H	330.2639	-2.1
	HMDB0175463	-hydroxy-6,,14-trimethyl-2-methylidenepentadecanoic acid	C19H36O3	M+NH4	330.3003	-1.4
	HMDB0175462	6-hydroxy-6,,14-trimethyl-2-methylidenepentadecanoic acid	C19H36O3	M+NH4	330.3003	-1.4
	HMDB0175464	14-hydroxy-6,,14-trimethyl-2-methylidenepentadecanoic acid	C19H36O3	M+NH4	330.3003	-1.4
	HMDB0175465	3-hydroxy-6,,14-trimethyl-2-methylidenepentadecanoic acid	C19H36O3	M+NH4	330.3003	-1.4
	HMDB0175467	6-(hydroxymethyl)-,14-dimethyl-2-methylidenepentadecanoic acid	C19H36O3	M+NH4	330.3003	-1.4
	HMDB0175466	2-(4,8,12-trimethyltridecyl)oxirane-2-carboxylic acid	C19H36O3	M+NH4	330.3003	-1.4
	HMDB0175468	-(hydroxymethyl)-6,14-dimethyl-2-methylidenepentadecanoic acid	C19H36O3	M+NH4	330.3003	-1.4
	HMDB0175469	15-hydroxy-6,,14-trimethyl-2-methylidenepentadecanoic acid	C19H36O3	M+NH4	330.3003	-1.4
	HMDB0013654	Palmitoyl Serinol	C19H39NO3	M+H	330.3003	-1.4
330.3364	HMDB0006752	Dihydroceramide	C19H39NO3	M+H	330.3003	-1.4
	HMDB0181948	11,12-Epoxyicosan-1-ol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0172170	(2Z)-2-(2,4,8-trimethyltridecyl)but-2-ene-1,4-diol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0172167	(2E)-3,5,7,11-tetramethylhexadec-2-ene-1,7-diol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0172168	(2E)-3,5,7,11-tetramethylhexadec-2-ene-1,11-diol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0172166	(2E)-3,5,7,11-tetramethylhexadec-2-ene-1,5-diol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0172169	(2E)-3,5,7,11-tetramethylhexadec-2-ene-1,4-diol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0172172	[3-methyl-3-(2,4,8-trimethyltridecyl)oxiran-2-yl]methanol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0172171	(2E)-3,5,7,11-tetramethylhexadec-2-ene-1,15-diol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0181949	(9E)-icos-9-ene-1,-diol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0181947	(11E)-icos-11-ene-1,19-diol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0181946	(11E)-icos-11-ene-1,-diol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0181945	(11E)-icos-11-ene-1,13-diol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0172175	(2E)-3,5,7-trimethyl-11-pentylidodec-2-ene-1,12-diol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0172176	(2E)-3,5,7,11-tetramethylhexadec-2-ene-1,16-diol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0172174	(2E)-3,5-dimethyl-7-(4-methylnonyl)oct-2-ene-1,8-diol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0172173	(2E)-5-(2,6-dimethylundecyl)-3-methylhex-2-ene-1,6-diol	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0031318	2,2,6,,14-Pentamethylpentadecanoic acid	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0034156	Ethyl stearate	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0035672	5-Hydroxy-7-eicosanone	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0035673	4-Hydroxy-6-eicosanone	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0002212	Arachidic acid	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0000801	Phytanic acid	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0000553	3L,7D,11D-Phytanic acid	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0062520	Phytanic acid	C20H40O2	M+NH4	330.3367	-0.8
	HMDB0000417	3D,7D,11D-Phytanic acid	C20H40O2	M+NH4	330.3367	-0.8
331.2839	HMDB0011533	MG/16)	C19H38O4	M+H	331.2843	-1.2
	HMDB0011564	MG(16)	C19H38O4	M+H	331.2843	-1.2
	HMDB0031074	Glycerol-1-monopalmitate	C19H38O4	M+H	331.2843	-1.2
	HMDB0072844	MG(i-16)	C19H38O4	M+H	331.2843	-1.2
	HMDB0072873	MG(i-16)	C19H38O4	M+H	331.2843	-1.2
	HMDB0062521	pregn-5-ene-3,-dione	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0156083	(1S,2R,11S,15S)-14-acetyl-2,15-dimethyltetracyclo[8.7,,heptadec-7-en-5-one	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167156	3-[(8E,11E)-5-hydroxypentadeca-8,11,14-trien-1-yl]phenol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167154	3-[(8E,11E)-7-hydroxypentadeca-8,11,14-trien-1-yl]phenol	C21H30O2	M+NH4	332.2584	-1.8

332.2578	HMDB0167157	3-[(8E,11E)-4-hydroxypentadeca-8,11,14-trien-1-yl]phenol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167155	3-[(8E,11E)-6-hydroxypentadeca-8,11,14-trien-1-yl]phenol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167158	3-[(8E,11E)-3-hydroxypentadeca-8,11,14-trien-1-yl]phenol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167159	3-[(8E,11E)-2-hydroxypentadeca-8,11,14-trien-1-yl]phenol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167161	2-[(8E,11E)-pentadeca-8,11,14-trien-1-yl]benzene-1,4-diol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167160	3-[(8E,11E)-1-hydroxypentadeca-8,11,14-trien-1-yl]phenol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0186443	(1S,2R,S,11S,15S)-14-(1-hydroxyethenyl)-2,15-dimethyltetracyclo[8.7.,heptadec-6-en-5-one	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0186461	PREGANE-3,-DIONE	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0173640	NSC224426	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167171	3-(7-{3-[(2E)-hexa-2,5-dien-1-yl]oxiran-2-yl}heptyl)phenol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167170	3-[(8E)--[3-(prop-2-en-1-yl)oxiran-2-yl]dec-8-en-1-yl]phenol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167162	3-[(8E,11E)-13-hydroxypentadeca-8,11,14-trien-1-yl]phenol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167165	3-[(9E,11E)-8-hydroxypentadeca-9,11,14-trien-1-yl]phenol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167163	3-[(8E,11E)--hydroxypentadeca-8,11,14-trien-1-yl]phenol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167164	3-[(8E)-11-hydroxypentadeca-8,12,14-trien-1-yl]phenol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167166	3-[(8E)-12-hydroxypentadeca-8.,14-trien-1-yl]phenol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167168	4-[(8E,11E)-pentadeca-8,11,14-trien-1-yl]benzene-1,2-diol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167169	3-[(8E,11E)-13-(oxiran-2-yl)trideca-8,11-dien-1-yl]phenol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0167167	Triolefinic (urushiol)	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0001830	Progesterone	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0014613	Tetrahydrocannabinol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0013121	7-Dehydropregnenolone	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0031924	4-Nerolidylcatechol	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0038533	Cardoltriene	C21H30O2	M+NH4	332.2584	-1.8
	HMDB0041865	6,6,9-trimethyl-3-pentyl-6H,6aH,7H,8H,aH-benzo[c]isochromen-1-ol	C21H30O2	M+NH4	332.2584	-1.8
332.2791	HMDB0000782	Octadecanedioic acid	C18H34O4	M+NH4	332.2795	-1.3
	HMDB0170226	17-hydroxy-5-oxooctadecanoic acid	C18H34O4	M+NH4	332.2795	-1.3
	HMDB0170229	4-hydroxy-5-oxooctadecanoic acid	C18H34O4	M+NH4	332.2795	-1.3
	HMDB0170228	2-hydroxy-5-oxooctadecanoic acid	C18H34O4	M+NH4	332.2795	-1.3
	HMDB0170227	18-hydroxy-5-oxooctadecanoic acid	C18H34O4	M+NH4	332.2795	-1.3
	HMDB0170230	6-hydroxy-5-oxooctadecanoic acid	C18H34O4	M+NH4	332.2795	-1.3
	HMDB0004704	9,-DHOMÉ	C18H34O4	M+NH4	332.2795	-1.3
	HMDB0004705	12,13-DHOMÉ	C18H34O4	M+NH4	332.2795	-1.3
	HMDB0061650	(9R,S)-9,-epoxy-18-hydroxyoctadecanoic acid	C18H34O4	M+NH4	332.2795	-1.3
	HMDB0031679	(9xi,xi,12xi)-9,-Dihydroxy-12-octadecenoic acid	C18H34O4	M+NH4	332.2795	-1.3
	HMDB0041220	Dibutyl decanedioate	C18H34O4	M+NH4	332.2795	-1.3
333.1176	HMDB0031721	Leonuriside A	C14H20O9	M+H	333.1180	-1.2
	HMDB0159139	3,4,5-trihydroxy-6- {[2-(4-oxocyclohexyl)acetyl]oxy} oxane-2-carboxylic acid	C14H20O9	M+H	333.1180	-1.2
	HMDB0156096	1-[(1S,2R,11S,15S)-5-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]ethan-1-one	C21H32O2	M+NH4	334.2741	0.7
	HMDB0156105	(2R,15S)-14-(1-hydroxyethyl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-one	C21H32O2	M+NH4	334.2741	0.7
	HMDB0156104	Pregnenolone, 99%	C21H32O2	M+NH4	334.2741	0.7
	HMDB0173660	14-(1-hydroxyethyl)-2,15-dimethyltetracyclo[8.7.,heptadec-13-en-5-one	C21H32O2	M+NH4	334.2741	0.7
	HMDB0186442	(1S,2R,S,11S,15S)-14-(1-hydroxyethyl)-2,15-dimethyltetracyclo[8.7.,heptadec-6-en-5-one	C21H32O2	M+NH4	334.2741	0.7

334.2743	HMDB0186450	(2S,15S)-14-(1-hydroxyethenyl)-2,15-dimethyltetracyclo[8.7.,heptadecan-5-one	C21H32O2	M+NH4	334.2741	0.7
	HMDB0006048	Bolasterone	C21H32O2	M+NH4	334.2741	0.7
	HMDB0038534	5-(8,11-Pentadecadienyl)-1,3-benzenediol	C21H32O2	M+NH4	334.2741	0.7
	HMDB0003069	(S)-hydroxypregn-4-en-3-one	C21H32O2	M+NH4	334.2741	0.7
	HMDB0059652	5-alpha-Pregnan-3,-dione	C21H32O2	M+NH4	334.2741	0.7
	HMDB0034369	(3beta,5alpha)-3-Hydroxypregn-16-en--one	C21H32O2	M+NH4	334.2741	0.7
	HMDB0004627	Calusterone	C21H32O2	M+NH4	334.2741	0.7
	HMDB0000253	Pregnenolone	C21H32O2	M+NH4	334.2741	0.7
	HMDB0003759	5a-Pregnane-3,-dione	C21H32O2	M+NH4	334.2741	0.7
	HMDB0006002	Ethyltestosterone	C21H32O2	M+NH4	334.2741	0.7
	HMDB0006026	Norbolethone	C21H32O2	M+NH4	334.2741	0.7
	HMDB0035580	1-Phenyl-1,3-pentadecanedione	C21H32O2	M+NH4	334.2741	0.7
	HMDB0036729	Kaurenic acid methyl ester	C21H32O2	M+NH4	334.2741	0.7
	HMDB0173666	Pregnane-3,-dione	C21H32O2	M+NH4	334.2741	0.7
334.2944	HMDB0011532	MG(15)	C18H36O4	M+NH4	334.2952	-2.3
	HMDB0072865	MG(a-15)[rac]	C18H36O4	M+NH4	334.2952	-2.3
	HMDB0072862	MG(a-15)[rac]	C18H36O4	M+NH4	334.2952	-2.3
	HMDB0072849	MG(i-15)	C18H36O4	M+NH4	334.2952	-2.3
	HMDB0059633	(9S,S)-9,-dihydroxyoctadecanoate	C18H36O4	M+NH4	334.2952	-2.3
	HMDB0031008	(+)-15,16-Dihydroxyoctadecanoic acid	C18H36O4	M+NH4	334.2952	-2.3
	HMDB0011563	MG(15)	C18H36O4	M+NH4	334.2952	-2.3
	HMDB0072878	MG(i-15)	C18H36O4	M+NH4	334.2952	-2.3
334.3097	HMDB0032033	2,4,12-Octadecatrienoic acid isobutylamide	C22H39NO	M+H	334.3104	-2.2
335.0730	HMDB0183406	3,4,5-trihydroxy-6-(2-methylbenzoyloxy)oxane-2-carboxylic acid	C14H16O8	M+Na	335.0737	-2.2
	HMDB0167833	6-(4-acetylphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O8	M+Na	335.0737	-2.2
	HMDB0167831	6-(3-acetylphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O8	M+Na	335.0737	-2.2
	HMDB0140804	3,4,5-trihydroxy-6-[(2-phenylacetyl)oxy]oxane-2-carboxylic acid	C14H16O8	M+Na	335.0737	-2.2
	HMDB0128031	6-(3-ethenyl-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O8	M+Na	335.0737	-2.2
	HMDB0126430	6-(2-ethenyl-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O8	M+Na	335.0737	-2.2
	HMDB0126429	6-(4-ethenyl-3-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O8	M+Na	335.0737	-2.2
	HMDB0124977	6-(5-ethenyl-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O8	M+Na	335.0737	-2.2
	HMDB0124976	6-(4-ethenyl-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O8	M+Na	335.0737	-2.2
	HMDB0011649	Glycerophosphoinositol	C9H19O11P	M+H	335.0738	-2.3
335.1055	HMDB0015186	Penicillin G	C16H18N2O4S	M+H	335.1060	-1.5
335.2214	HMDB0012850	7'-Carboxy-gamma-chromanol	C20H30O4	M+H	335.2217	-0.9
	HMDB0062486	(6E,8E,E,14E,17E)-5,12-dihydroxyicosa-6,8,,14,17-pentaenoic acid	C20H30O4	M+H	335.2217	-0.9
	HMDB0062423	(6E,8Z,12S,14Z)-12-hydroxy-5-oxoicosa-6,8,,14-tetraenoic acid	C20H30O4	M+H	335.2217	-0.9
	HMDB0062298	15-deoxy-delta-12,14-pgd2	C20H30O4	M+H	335.2217	-0.9
	HMDB0036828	Dehydropinifolic acid	C20H30O4	M+H	335.2217	-0.9
	HMDB0036763	(ent-6alpha,7alpha)-6,7-Dihydroxy-16-kauren-19-oic acid	C20H30O4	M+H	335.2217	-0.9
	HMDB0041055	Phytocassane B	C20H30O4	M+H	335.2217	-0.9
	HMDB0035286	Crispanone	C20H30O4	M+H	335.2217	-0.9
	HMDB0036760	Verimol D	C20H30O4	M+H	335.2217	-0.9
	HMDB0035878	8alpha-8-Hydroxy-12-oxo-13-abieten-18-oic acid	C20H30O4	M+H	335.2217	-0.9
	HMDB0005073	Leukotriene B5	C20H30O4	M+H	335.2217	-0.9
	HMDB0004238	Delta-12-Prostaglandin J2	C20H30O4	M+H	335.2217	-0.9
	HMDB0004236	Prostaglandin B2	C20H30O4	M+H	335.2217	-0.9
	HMDB0004234	12-Keto-leukotriene B4	C20H30O4	M+H	335.2217	-0.9
	HMDB0002710	Prostaglandin J2	C20H30O4	M+H	335.2217	-0.9
	HMDB0001244	15-Keto-13,14-dihydroprostaglandin A2	C20H30O4	M+H	335.2217	-0.9
	HMDB0061111	5,6-Epoxytetraene	C20H30O4	M+H	335.2217	-0.9

	HMDB0060095	Prostaglandin-c2	C20H30O4	M+H	335.2217	-0.9
	HMDB0060054	bicyclo-PGE2	C20H30O4	M+H	335.2217	-0.9
	HMDB0060046	15d PGD2	C20H30O4	M+H	335.2217	-0.9
	HMDB0002752	Prostaglandin A2	C20H30O4	M+H	335.2217	-0.9
	HMDB0062524	Prostaglandin A2	C20H30O4	M+H	335.2217	-0.9
	HMDB0012824	5-Oxo-6-trans-leukotriene B4	C20H30O4	M+H	335.2217	-0.9
336.1396	HMDB0000489	Aspartylglycosamine	C12H21N3O8	M+H	336.1401	-1.6
338.2686	HMDB0112068	(E)-11-(3,4-dimethyl-5-propylfuran-2-yl)undec--enoic acid	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0112071	11-{3,4-dimethyl-5-[(1E)-prop-1-en-1-yl]furan-2-yl}undecanoic acid	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0004673	11,12-Epoxyeicosatrienoic acid	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0062433	8-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0062431	(5Z,8Z,14Z)-7-hydroxyicosa-5,8,11,14-tetraenoic acid	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0062302	18-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0062287	(5E,12S,14Z)-12-hydroxyicosa-5,8,,14-tetraenoic acid	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0062294	15(R)-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0002190	5,6-Epoxy-8,11,14-eicosatrienoic acid	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0010409	11,12-EpETrE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0011134	5-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0011136	19(S)-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0036262	Annoglabasin E	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0036810	8alpha,13R-Epoxy-14-labden-19-oic acid	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0036705	8-OCimanyl acetate	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0038688	(ent-2alpha,3beta,15beta,16beta)-15,16-Epoxy-2,3-kauranediol	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0038689	(ent-2alpha,3beta,15beta)-16-Kaurene-2,3,15-triol	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0010222	9-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0006245	18-Hydroxyarachidonic acid	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0002232	8,9-Epoxyeicosatrienoic acid	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0002283	14R,15S-EpETrE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0003876	15-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0004264	14,15-Epoxy-5,8,11-eicosatrienoic acid	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0004680	16(R)-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0004679	8-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0004682	11(R)-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0005998	-Hydroxyeicosatetraenoic acid	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0038520	2-Hydroxy-6-tridecylbenzoic acid	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0012508	-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0012567	13-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0012598	17-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0060101	12 Hydroxy arachidonic acid	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0006111	12-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0061118	12-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0061119	12(R)-HETE	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0038694	Crispane	C20H32O3	M+NH4	338.2690	-1.1
	HMDB0240344	2-({(9Z,12Z)-1-hydroxyoctadeca-9,12-dien-1-ylidene}amino}acetic acid	C20H35NO3	M+H	338.2690	-1.1
341.0081	HMDB0141539	[3-(4-oxo-4H-chromen-2-yl)phenyl]oxidanesulfonic acid	C15H10O6S	M+Na	341.0090	-2.7
341.2223	HMDB0061306	5-({[(2E)-6,6-dimethylhept-2-en-4-yn-1-yl](methyl)amino}methyl)naphthalene-1,2-diol	C21H25NO2	M+NH4	341.2224	-0.2
	HMDB0061305	4-({[(2E)-6,6-dimethylhept-2-en-4-yn-1-yl](methyl)amino}methyl)naphthalene-1,2-diol	C21H25NO2	M+NH4	341.2224	-0.2
	HMDB0030359	14,19-Dihydroaspidospermatine	C21H28N2O2	M+H	341.2224	-0.2
342.0689	HMDB0156309	286-43-3	C9H13N2O9P	M+NH4	342.0697	-2.3
	HMDB0060282	Uridine 3'-monophosphate	C9H13N2O9P	M+NH4	342.0697	-2.3
	HMDB0011641	Uridine 2'-phosphate	C9H13N2O9P	M+NH4	342.0697	-2.3
	HMDB0001271	Pseudouridine 5'-phosphate	C9H13N2O9P	M+NH4	342.0697	-2.3

	HMDB0000288	Uridine 5'-monophosphate	C9H13N2O9P	M+NH4	342.0697	-2.3
343.0518	HMDB0015034	Triazolam	C17H12Cl2N4	M+H	343.0512	1.8
344.2275	HMDB0061835	Heptaethylene glycol	C14H30O8	M+NH4	344.2279	-1.1
344.3517	HMDB0002337	Homophytanic acid	C21H42O2	M+NH4	344.3523	-1.8
	HMDB0035670	4-Hydroxy-6-heneicosanone	C21H42O2	M+NH4	344.3523	-1.8
	HMDB0035669	8-Hydroxy-6-heneicosanone	C21H42O2	M+NH4	344.3523	-1.8
	HMDB0035671	6-Hydroxy-4-heneicosanone	C21H42O2	M+NH4	344.3523	-1.8
	HMDB0035668	6-Hydroxy-8-heneicosanone	C21H42O2	M+NH4	344.3523	-1.8
	HMDB0031319	2,3,7,11,15-Pentamethylhexadecanoic acid	C21H42O2	M+NH4	344.3523	-1.8
	HMDB0002345	Heneicosanoic acid	C21H42O2	M+NH4	344.3523	-1.8
346.0309	HMDB0155253	ACMC-9hv8	C9H13N3O8S	M+Na	346.0316	-1.9
	HMDB0155255	[4-hydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)-2-(hydroxymethyl)oxolan-3-yl]oxidanesulfonic acid	C9H13N3O8S	M+Na	346.0316	-1.9
	HMDB0155254	[4-hydroxy-2-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)-5-(hydroxymethyl)oxolan-3-yl]oxidanesulfonic acid	C9H13N3O8S	M+Na	346.0316	-1.9
346.2734	HMDB0062579	6217-54-5	C22H32O2	M+NH4	346.2741	-1.9
	HMDB0167219	2-methoxy-4-[(8E,11E)-pentadeca-8,11,14-trien-1-yl]phenol	C22H32O2	M+NH4	346.2741	-1.9
	HMDB0167215	2-methoxy-3-[(8E,11E)-pentadeca-8,11,14-trien-1-yl]phenol	C22H32O2	M+NH4	346.2741	-1.9
	HMDB0030053	Neogrifolin	C22H32O2	M+NH4	346.2741	-1.9
	HMDB0038908	(Z,Z)-2-Methyl-5-(8,11,14-pentadecatrienyl)-1,3-benzenediol	C22H32O2	M+NH4	346.2741	-1.9
	HMDB0030446	Grifolin	C22H32O2	M+NH4	346.2741	-1.9
	HMDB0035185	Retinol acetate	C22H32O2	M+NH4	346.2741	-1.9
	HMDB0002183	Docosahexaenoic acid	C22H32O2	M+NH4	346.2741	-1.9
	HMDB0013649	Eicosapentaenoyl Ethanolamide	C22H35NO2	M+H	346.2741	-1.9
346.2942	HMDB0011534	MG(16:1(9Z))	C19H36O4	M+NH4	346.2952	-2.8
	HMDB0011565	MG(16:1(9Z))	C19H36O4	M+NH4	346.2952	-2.8
	HMDB0031044	Avocadoene 2-acetate	C19H36O4	M+NH4	346.2952	-2.8
	HMDB0031045	Avocadoene 4-acetate	C19H36O4	M+NH4	346.2952	-2.8
	HMDB0031043	Avocadoene 1-acetate	C19H36O4	M+NH4	346.2952	-2.8
346.3312	HMDB0032477	Polyoxyethylene monostearate	C20H40O3	M+NH4	346.3316	-1.1
	HMDB0158832	7-hydroxy-3,7,11,15-tetramethylhexadecanoic acid	C20H40O3	M+NH4	346.3316	-1.1
	HMDB0158831	3-hydroxy-3,7,11,15-tetramethylhexadecanoic acid	C20H40O3	M+NH4	346.3316	-1.1
	HMDB0158834	15-hydroxy-3,7,11,15-tetramethylhexadecanoic acid	C20H40O3	M+NH4	346.3316	-1.1
	HMDB0158833	11-hydroxy-3,7,11,15-tetramethylhexadecanoic acid	C20H40O3	M+NH4	346.3316	-1.1
	HMDB0158838	omega-hydroxyphytanic acid	C20H40O3	M+NH4	346.3316	-1.1
	HMDB0158835	3-(hydroxymethyl)-7,11,15-trimethylhexadecanoic acid	C20H40O3	M+NH4	346.3316	-1.1
	HMDB0158837	11-(hydroxymethyl)-3,7,15-trimethylhexadecanoic acid	C20H40O3	M+NH4	346.3316	-1.1
	HMDB0061659	2(R)-hydroxyicosanoic acid	C20H40O3	M+NH4	346.3316	-1.1
	HMDB0061664	12-hydroxyicosanoic acid	C20H40O3	M+NH4	346.3316	-1.1
	HMDB0061665	15-hydroxyicosanoic acid	C20H40O3	M+NH4	346.3316	-1.1
	HMDB0061666	2-hydroxyphytanic acid	C20H40O3	M+NH4	346.3316	-1.1
	HMDB0062566	3-hydroxyicosanoic Acid	C20H40O3	M+NH4	346.3316	-1.1
	HMDB0158836	7-(hydroxymethyl)-3,11,15-trimethylhexadecanoic acid	C20H40O3	M+NH4	346.3316	-1.1
	HMDB0179890	[({[(3Z)-4-hydroxy-1-methoxy-2-oxo-2,3-dihydro-1H-indol-3-ylidene]methyl} imino)(methylsulfanyl)methyl]dimethylsulfanium	C14H17N2O3 S2	M+Na	347.0495	0.7
	HMDB0179888	[({[(3Z)-7-hydroxy-1-methoxy-2-oxo-2,3-dihydro-1H-indol-3-ylidene]methyl} imino)(methylsulfanyl)methyl]dimethylsulfanium	C14H17N2O3 S2	M+Na	347.0495	0.7
	HMDB0179886	[({[(3Z)-5-hydroxy-1-methoxy-2-oxo-2,3-dihydro-1H-indol-3-ylidene]methyl} imino)(methylsulfanyl)methyl]dimethylsulfanium	C14H17N2O3 S2	M+Na	347.0495	0.7

347.0497	HMDB0179884	[({[(3Z)-6-hydroxy-1-methoxy-2-oxo-2,3-dihydro-1H-indol-3-ylidene]methyl} imino)(methylsulfanyl)methyl]dimethylsulfanium	C14H17N2O3S2	M+Na	347.0495	0.7
	HMDB0179840	[({[(3E)-7-hydroxy-1-methoxy-2-oxo-2,3-dihydro-1H-indol-3-ylidene]methyl} imino)(methylsulfanyl)methyl]dimethylsulfanium	C14H17N2O3S2	M+Na	347.0495	0.7
	HMDB0179842	[({[(3E)-4-hydroxy-1-methoxy-2-oxo-2,3-dihydro-1H-indol-3-ylidene]methyl} imino)(methylsulfanyl)methyl]dimethylsulfanium	C14H17N2O3S2	M+Na	347.0495	0.7
	HMDB0179838	[({[(3E)-5-hydroxy-1-methoxy-2-oxo-2,3-dihydro-1H-indol-3-ylidene]methyl} imino)(methylsulfanyl)methyl]dimethylsulfanium	C14H17N2O3S2	M+Na	347.0495	0.7
	HMDB0179836	[({[(3E)-6-hydroxy-1-methoxy-2-oxo-2,3-dihydro-1H-indol-3-ylidene]methyl} imino)(methylsulfanyl)methyl]dimethylsulfanium	C14H17N2O3S2	M+Na	347.0495	0.7
348.0695	HMDB0011680	Coproporphyrinogen I	C10H11N4O7P	M+NH4	348.0704	-2.5
	HMDB0001044	2'-Deoxyguanosine 5'-monophosphate	C10H14N5O7P	M+H	348.0704	-2.5
	HMDB0003540	3'-AMP	C10H14N5O7P	M+H	348.0704	-2.5
	HMDB0011617	Adenosine 2'-phosphate	C10H14N5O7P	M+H	348.0704	-2.5
	HMDB0059594	2-hydroxy-dAMP	C10H14N5O7P	M+H	348.0704	-2.5
	HMDB0155033	Adenosine monophosphate	C10H14N5O7P	M+H	348.0704	-2.5
	HMDB0000045	Adenosine monophosphate	C10H14N5O7P	M+H	348.0704	-2.5
	HMDB0155034	Adenosine-3-phosphoric acid	C10H14N5O7P	M+H	348.0704	-2.5
	HMDB0014910	Malathion	C10H19O6PS2	M+NH4	348.0699	-1.1
	HMDB0059997	Dihydroxy-1H-indole glucuronide I	C14H15NO8	M+Na	348.0690	1.5
348.2741	HMDB0178044	6-{4-[cyano(hydroxy)methyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H15NO8	M+Na	348.0690	1.5
	HMDB0004708	9,12,13-TriHOME	C18H34O5	M+NH4	348.2744	-1.0
	HMDB0172549	9,-dihydroxy-18-oxooctadecanoic acid	C18H34O5	M+NH4	348.2744	-1.0
	HMDB0030936	5,8,12-Trihydroxy-9-octadecenoic acid	C18H34O5	M+NH4	348.2744	-1.0
	HMDB0038555	(9S,E,12S,13S)-9,12,13-Trihydroxy--octadecenoic acid	C18H34O5	M+NH4	348.2744	-1.0
348.2889	HMDB0004710	9,,13-TriHOME	C18H34O5	M+NH4	348.2744	-1.0
	HMDB0032257	Ethyl abietate	C22H34O2	M+NH4	348.2897	-2.3
	HMDB0039530	Ethyl icosapentate	C22H34O2	M+NH4	348.2897	-2.3
	HMDB0039133	4,8,12,15,19-Docosapentaenoic acid	C22H34O2	M+NH4	348.2897	-2.3
	HMDB0038909	2-Methyl-5-(8,11-pentadecadienyl)-1,3-benzenediol	C22H34O2	M+NH4	348.2897	-2.3
	HMDB0035024	ent-16-Kauren-19-ol acetate	C22H34O2	M+NH4	348.2897	-2.3
	HMDB0035581	1-Phenyl-1,3-hexadecanedione	C22H34O2	M+NH4	348.2897	-2.3
	HMDB0006528	Docosapentaenoic acid (22n-3)	C22H34O2	M+NH4	348.2897	-2.3
	HMDB0001976	Docosapentaenoic acid (22n-6)	C22H34O2	M+NH4	348.2897	-2.3
	HMDB0060113	Docosapentaenoic acid (22n-6)	C22H34O2	M+NH4	348.2897	-2.3
	HMDB0004080	Anandamide	C22H37NO2	M+H	348.2897	-2.3
348.3101	HMDB0013655	O-Arachidonoyl Ethanolamine	C22H37NO2	M+H	348.2897	-2.3
	HMDB0011533	MG(16)	C19H38O4	M+NH4	348.3108	-2.1
	HMDB0011564	MG(16)	C19H38O4	M+NH4	348.3108	-2.1
	HMDB0031074	Glycerol-1-monopalmitate	C19H38O4	M+NH4	348.3108	-2.1
	HMDB0072844	MG(i-16)	C19H38O4	M+NH4	348.3108	-2.1
	HMDB0072873	MG(i-16)	C19H38O4	M+NH4	348.3108	-2.1
	HMDB0157904	3,4,5-trihydroxy-6-[(3,4,5-trihydroxypentanoyl)oxy]oxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4

349.0733	HMDB0160646	3,4,5-trihydroxy-6-[(1,3,5-trihydroxy-4-oxopentan-2-yl)oxy]oxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
	HMDB0160647	3,4,5-trihydroxy-6-[(1,2,5-trihydroxy-4-oxopentan-3-yl)oxy]oxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
	HMDB0160645	3,4,5-trihydroxy-6-[(2,3,5-trihydroxy-4-oxopentyl)oxy]oxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
	HMDB0039723	3-O-alpha-D-Glucopyranuronosyl-D-xylose	C11H18O11	M+Na	349.0741	-2.4
	HMDB0160648	3,4,5-trihydroxy-6-[(3,4,5-trihydroxy-2-oxopentyl)oxy]oxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
	HMDB0187612	6-{[2,4-dihydroxy-2-(hydroxymethyl)oxolan-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
	HMDB0187614	3,4,5-trihydroxy-6-[(2,3,4-trihydroxyoxolan-2-yl)methoxy]oxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
	HMDB0157902	6-[(4-carboxy-1,3-dihydroxybutan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
	HMDB0157901	6-[(1-carboxy-3,4-dihydroxybutan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
	HMDB0157903	6-(4-carboxy-2,3-dihydroxybutoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
	HMDB0155257	6-{[2,4-dihydroxy-5-(hydroxymethyl)oxolan-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
	HMDB0148465	3,4,5-trihydroxy-6-[(4,5,6-trihydroxyoxan-3-yl)oxy]oxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
	HMDB0127655	3,4,5-trihydroxy-6-{[3-hydroxy-2,2-bis(hydroxymethyl)propanoyl]oxy}oxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
	HMDB0127654	6-[2-carboxy-2,2-bis(hydroxymethyl)ethoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
	HMDB0148464	3,4,5-trihydroxy-6-[(2,3,5-trihydroxyoxan-4-yl)oxy]oxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
	HMDB0155258	3,4,5-trihydroxy-6-[(3,4,5-trihydroxyoxolan-2-yl)methoxy]oxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
	HMDB0040737	Aldobiouronic acid D3	C11H18O11	M+Na	349.0741	-2.4
	HMDB0187613	6-{[4,5-dihydroxy-5-(hydroxymethyl)oxolan-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C11H18O11	M+Na	349.0741	-2.4
349.0889	HMDB0033581	trans-beta-D-glucosyl-2-hydroxycinnamic acid	C15H18O8	M+Na	349.0894	-1.4
	HMDB0135298	3,4,5-trihydroxy-6-[3-(3-oxopropyl)phenoxy]oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
	HMDB0135294	3,4,5-trihydroxy-6-[(1-oxo-3-phenylpropan-2-yl)oxy]oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
	HMDB0135296	3,4,5-trihydroxy-6-(3-oxo-1-phenylpropoxy)oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
	HMDB0135256	3,4,5-trihydroxy-6-[2-hydroxy-4-(prop-2-en-1-yl)phenoxy]oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
	HMDB0135257	3,4,5-trihydroxy-6-[2-hydroxy-5-(prop-2-en-1-yl)phenoxy]oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
	HMDB0134047	3,4,5-trihydroxy-6-[2-(3-hydroxyprop-1-en-1-yl)phenoxy]oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
	HMDB0134046	3,4,5-trihydroxy-6-[2-(3-oxopropyl)phenoxy]oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
	HMDB0128020	6-(3-ethenyl-5-methoxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
	HMDB0127979	6-(4-ethenyl-2-methoxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
	HMDB0125172	3,4,5-trihydroxy-6-[(3-phenylpropanoyl)oxy]oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
	HMDB0135300	3,4,5-trihydroxy-6-[4-(3-oxopropyl)phenoxy]oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
	HMDB0135305	3,4,5-trihydroxy-6-{4-[(1E)-3-hydroxyprop-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
	HMDB0177515	3,4,5-trihydroxy-6-[4-(3-methyloxiran-2-yl)phenoxy]oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
	HMDB0176426	3,4,5-trihydroxy-6-{[6-(3-methyloxiran-2-yl)hexa-3,5-diyn-1-yl]oxy}oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4

HMDB0176423	3,4,5-trihydroxy-6-[[[(7E)-9-hydroxynon-7-en-3,5-diyn-1-yl]oxy]oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
HMDB0176422	3,4,5-trihydroxy-6-[[[(2E)-9-hydroxynon-2-en-4,6-diyn-1-yl]oxy]oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
HMDB0171001	3,4,5-trihydroxy-6-{2-hydroxy-5-[(1Z)-prop-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
HMDB0171000	3,4,5-trihydroxy-6-{2-hydroxy-4-[(1Z)-prop-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
HMDB0170766	3,4,5-trihydroxy-6-{4-[(oxiran-2-yl)methyl]phenoxy}oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
HMDB0145842	CHEMBL35582	C15H18O8	M+Na	349.0894	-1.4
HMDB0135655	3,4,5-trihydroxy-6-[4-(3-hydroxyprop-1-en-1-yl)phenoxy]oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
HMDB0135308	3,4,5-trihydroxy-6-[(3-phenyloxiran-2-yl)methoxy]oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
HMDB0135302	3,4,5-trihydroxy-6-{3-[(1E)-3-hydroxyprop-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
HMDB0141878	3,4,5-trihydroxy-6-[(2-phenylpropanoyl)oxy]oxane-2-carboxylic acid	C15H18O8	M+Na	349.0894	-1.4
HMDB0060077	cis-beta-D-Glucosyl-2-hydroxycinnamate	C15H18O8	M+Na	349.0894	-1.4
HMDB0036735	Bilobalide A	C15H18O8	M+Na	349.0894	-1.4
HMDB0036936	1-O-p-Coumaroyl-beta-D-glucose	C15H18O8	M+Na	349.0894	-1.4
HMDB0039169	6-O-p-Coumaroyl-D-glucose	C15H18O8	M+Na	349.0894	-1.4
HMDB0039167	2-O-p-Coumaroyl-D-glucose	C15H18O8	M+Na	349.0894	-1.4
HMDB0039509	trans-p-Coumaric acid 4-glucoside	C15H18O8	M+Na	349.0894	-1.4
HMDB0157390	(1S,R,11S,15S)-4,5-dimethoxy-15-methyltetracyclo[8.7.,,heptadeca-2,4,6-triene-12,14-diol	C20H28O4	M+NH4	350.2326	-1.9
HMDB0157388	(1S,R,11S,15S)-4,5-dimethoxy-15-methyltetracyclo[8.7.,,heptadeca-2,4,6-triene-14,14-diol	C20H28O4	M+NH4	350.2326	-1.9
HMDB0169109	1-[6-(3,7-dimethylocta-2,6-dien-1-yl)-4-hydroxy-2,3-dimethoxyphenyl]ethan-1-one	C20H28O4	M+NH4	350.2326	-1.9
HMDB0169112	1-{2-[(2E)-3,7-dimethylocta-2,6-dien-1-yl]-4-hydroxy-3,6-dimethoxyphenyl}ethan-1-one	C20H28O4	M+NH4	350.2326	-1.9
HMDB0169665	(3Z)-3-ethylidene-6-hydroxy-7-methylidene-2-oxo-4-(propan-2-yl)-octahydro-1H-inden-1-yl (2Z)-2-methylbut-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177626	(1Z)-1-(2-hydroxyethylidene)-4-methylidene-2-oxo-7-(propan-2-yl)-octahydro-1H-inden-5-yl 3-methylbut-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177625	(1Z)-1-ethylidene-4-methylidene-2-oxo-7-(propan-2-yl)-octahydro-1H-inden-5-yl 4-hydroxy-3-methylbut-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177627	(1Z)-1-ethylidene-7-hydroxy-4-methylidene-2-oxo-7-(propan-2-yl)-octahydro-1H-inden-5-yl 3-methylbut-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177631	(1Z)-1-ethylidene-7-(1-hydroxypropan-2-yl)-4-methylidene-2-oxo-octahydro-1H-inden-5-yl 3-methylbut-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0157389	(1S,R,11S,15S)-4,5-dimethoxy-15-methyltetracyclo[8.7.,,heptadeca-2,4,6-triene-13,14-diol	C20H28O4	M+NH4	350.2326	-1.9
HMDB0157387	(1S,R,11S,15S)-15-(hydroxymethyl)-4,5-dimethoxytetracyclo[8.7.,,heptadeca-2,4,6-trien-14-ol	C20H28O4	M+NH4	350.2326	-1.9
HMDB0157385	(1S,S,11S,15S)-4,5-dimethoxy-15-methyltetracyclo[8.7.,,heptadeca-2,4,6-triene-3,14-diol	C20H28O4	M+NH4	350.2326	-1.9
HMDB0062410	4-{3-[(1E,3E,5E,8Z,E,12R)-12-hydroxytetradeca-1,3,5,8,-pentaen-1-yl]oxiran-2-yl}butanoic acid	C20H28O4	M+NH4	350.2326	-1.9
HMDB0157379	(1S,R,11S,15S)-4,5-dimethoxy-15-methyltetracyclo[8.7.,,heptadeca-2,4,6-triene-9,14-diol	C20H28O4	M+NH4	350.2326	-1.9
HMDB0157380	(1S,S,11S,15S)-4,5-dimethoxy-15-methyltetracyclo[8.7.,,heptadeca-2,4,6-triene-14,17-diol	C20H28O4	M+NH4	350.2326	-1.9
HMDB0157382	(1R,11R,15S)-4,5-dimethoxy-15-methyltetracyclo[8.7.,,heptadeca-2,4,6-triene-,14-diol	C20H28O4	M+NH4	350.2326	-1.9
HMDB0157381	(1S,R,11S,15S)-4,5-dimethoxy-15-methyltetracyclo[8.7.,,heptadeca-2,4,6-triene-14,16-diol	C20H28O4	M+NH4	350.2326	-1.9

HMDB0157386	(1S,R,11S,15S)-4,5-dimethoxy-15-methyltetracyclo[8.7.,heptadeca-2,4,6-triene-8,14-diol	C20H28O4	M+NH4	350.2326	-1.9
HMDB0157383	(S,11S,15S)-4,5-dimethoxy-15-methyltetracyclo[8.7.,heptadeca-2,4,6-triene-1,14-diol	C20H28O4	M+NH4	350.2326	-1.9
HMDB0157384	(1S,R,15R)-4,5-dimethoxy-15-methyltetracyclo[8.7.,heptadeca-2,4,6-triene-11,14-diol	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177628	(1Z)-1-ethylidene-6-hydroxy-4-methylidene-2-oxo-7-(propan-2-yl)-octahydro-1H-inden-5-yl 3-methylbut-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177629	(1Z)-1-ethylidene-7a-hydroxy-4-methylidene-2-oxo-7-(propan-2-yl)-octahydro-1H-inden-5-yl 3-methylbut-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0178403	6-hydroxy-13-(hydroxymethyl)-5,5,9-trimethyltetracyclo[11.2.1,? 籍hexadec-14-ene-7,12-dione	C20H28O4	M+NH4	350.2326	-1.9
HMDB0178404	6,16-dihydroxy-5,5,9,13-tetramethyltetracyclo[11.2.1,? 籍hexadec-14-ene-7,12-dione	C20H28O4	M+NH4	350.2326	-1.9
HMDB0178402	6-hydroxy-5-(hydroxymethyl)-5,9,13-trimethyltetracyclo[11.2.1,? 籍hexadec-14-ene-7,12-dione	C20H28O4	M+NH4	350.2326	-1.9
HMDB0178405	6-hydroxy-5,5,9,13-tetramethyl-15-oxapentacyclo[11.3.1,??heptadecane-7,12-dione	C20H28O4	M+NH4	350.2326	-1.9
HMDB0178407	6,8-dihydroxy-5,5,9,13-tetramethyltetracyclo[11.2.1,? 籍hexadec-14-ene-7,12-dione	C20H28O4	M+NH4	350.2326	-1.9
HMDB0178406	6,11-dihydroxy-5,5,9,13-tetramethyltetracyclo[11.2.1,? 籍hexadec-14-ene-7,12-dione	C20H28O4	M+NH4	350.2326	-1.9
HMDB0178401	6-hydroxy-9-(hydroxymethyl)-5,5,13-trimethyltetracyclo[11.2.1,? 籍hexadec-14-ene-7,12-dione	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177675	(1Z)-1-ethylidene-3-hydroxy-4-methylidene-2-oxo-7-(propan-2-yl)-octahydro-1H-inden-5-yl (2Z)-2-methylbut-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177672	(1Z)-1-ethylidene-6-hydroxy-4-methylidene-2-oxo-7-(propan-2-yl)-octahydro-1H-inden-5-yl (2Z)-2-methylbut-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177630	(1Z)-1-ethylidene-4-methylidene-2-oxo-7-(propan-2-yl)-octahydro-1H-inden-5-yl 3,3-dimethyloxirane-2-carboxylate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177632	(1Z)-1-ethylidene-3-hydroxy-4-methylidene-2-oxo-7-(propan-2-yl)-octahydro-1H-inden-5-yl 3-methylbut-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177667	(1Z)-1-(2-hydroxyethylidene)-4-methylidene-2-oxo-7-(propan-2-yl)-octahydro-1H-inden-5-yl (2Z)-2-methylbut-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177670	(1Z)-1-ethylidene-7a-hydroxy-4-methylidene-2-oxo-7-(propan-2-yl)-octahydro-1H-inden-5-yl (2Z)-2-methylbut-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177671	(1Z)-1-ethylidene-7-hydroxy-4-methylidene-2-oxo-7-(propan-2-yl)-octahydro-1H-inden-5-yl (2Z)-2-methylbut-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177668	(1Z)-1-ethylidene-4-methylidene-2-oxo-7-(propan-2-yl)-octahydro-1H-inden-5-yl (2Z)-2-(hydroxymethyl)but-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177669	(1Z)-1-ethylidene-4-methylidene-2-oxo-7-(propan-2-yl)-octahydro-1H-inden-5-yl (2Z)-4-hydroxy-2-methylbut-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177673	(1Z)-1-ethylidene-4-methylidene-2-oxo-7-(propan-2-yl)-octahydro-1H-inden-5-yl 2,3-dimethyloxirane-2-carboxylate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0177674	(1Z)-1-ethylidene-7-(1-hydroxypropan-2-yl)-4-methylidene-2-oxo-octahydro-1H-inden-5-yl (2Z)-2-methylbut-2-enoate	C20H28O4	M+NH4	350.2326	-1.9
HMDB0002358	Carnosic acid	C20H28O4	M+NH4	350.2326	-1.9
HMDB0036700	ent-7alpha,12beta-Dihydroxy-16-kauren-19,6beta-olide	C20H28O4	M+NH4	350.2326	-1.9
HMDB0035637	Petasitin	C20H28O4	M+NH4	350.2326	-1.9

	HMDB0036623	4-Deoxycohumulone	C20H28O4	M+NH4	350.2326	-1.9
	HMDB0012851	7'-Carboxy-gamma-tocotrienol	C20H28O4	M+NH4	350.2326	-1.9
	HMDB0030103	Hulupone	C20H28O4	M+NH4	350.2326	-1.9
	HMDB0030136	Adhulupone	C20H28O4	M+NH4	350.2326	-1.9
	HMDB0031375	(1(E),4E,6a,9b)-9-(3-Methylbutanoyloxy)-1(0),4,11(13)-germacatrien-12,6-olide	C20H28O4	M+NH4	350.2326	-1.9
	HMDB0036726	ent-15-Kaurene-17,19-dioic acid	C20H28O4	M+NH4	350.2326	-1.9
	HMDB0036761	7,18-Dihydroxykaurenolide	C20H28O4	M+NH4	350.2326	-1.9
	HMDB0031374	(1(E),4E,6a,9b)-9-(2-Methylbutanoyloxy)-1(0),4,11(13)-germacatrien-12,6-olide	C20H28O4	M+NH4	350.2326	-1.9
	HMDB0038966	(9Z,11S,16S)-1-Acetoxy-9,17-octadecadiene-12,14-diyne-11,16-diol	C20H28O4	M+NH4	350.2326	-1.9
	HMDB0036146	6-Angeloylfuranofukinol	C20H28O4	M+NH4	350.2326	-1.9
350.2893	HMDB0030935	9,,13-Trihydroxystearic acid	C18H36O5	M+NH4	350.2901	-2.3
	HMDB0034295	Floionolic acid	C18H36O5	M+NH4	350.2901	-2.3
	HMDB0062725	ethyl (5Z,8Z,14Z)-icosa-5,8,11,14-tetraenoate	C22H36O2	M+NH4	350.3054	-2.1
	HMDB0002226	Adrenic acid	C22H36O2	M+NH4	350.3054	-2.1
	HMDB0062580	Adrenic acid	C22H36O2	M+NH4	350.3054	-2.1
350.3046	HMDB0035677	3-Hydroxy-1-phenyl-1-hexadecanone	C22H36O2	M+NH4	350.3054	-2.1
	HMDB0035676	1-Hydroxy-1-phenyl-3-hexadecanone	C22H36O2	M+NH4	350.3054	-2.1
	HMDB0038910	2-Methyl-5-(8-pentadecenyl)-1,3-benzenediol	C22H36O2	M+NH4	350.3054	-2.1
	HMDB0185130	(13Z,16Z,19Z)-docosa-13,16,19,21-tetraenoic acid	C22H36O2	M+NH4	350.3054	-2.1
	HMDB0013625	Dihomo-gamma-Linolenoyl ethanolamide	C22H39NO2	M+H	350.3054	-2.2
	HMDB0014686	Adinazolam	C19H18ClN5	M+H	352.1323	-0.7
352.1321	HMDB0015186	Penicillin G	C16H18N2O4S	M+NH4	352.1326	-1.3
	HMDB0014853	Paroxetine	C19H20FNO3	M+Na	352.1319	0.5
352.2693	HMDB0039848	3-Oxotetradecanoic acid glycerides	C17H33O6	M+NH4	352.2688	1.4
	HMDB0002823	Docosatrienoic acid	C22H38O2	M+NH4	352.3210	-1.7
352.3204	HMDB0167408	2-methoxy-4-pentadecylphenol	C22H38O2	M+NH4	352.3210	-1.7
	HMDB0031099	(all-Z)-7,,13-Docosatrienoic acid	C22H38O2	M+NH4	352.3210	-1.7
	HMDB0167412	2-methoxy-3-pentadecylphenol	C22H38O2	M+NH4	352.3210	-1.7
	HMDB0060776	5-Hydroxydantrolene	C14H10N4O6	M+Na	353.0493	-1.8
	HMDB0134104	6-(2,3-dihydroxybenzoyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0134103	6-(2-carboxy-6-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0134102	6-(3-carboxy-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0134109	6-(3-carboxy-4-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0134111	6-(2,5-dihydroxybenzoyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0134110	6-(2-carboxy-4-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0166599	3,4,5-trihydroxy-6-[(6-hydroxy-2H-1,3-benzodioxol-5-yl)oxy]oxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0171099	6-(2-carboxy-3-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0171100	6-(2,6-dihydroxybenzoyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0240405	(2S,3S,4S,5R,6S)-6-(5-carboxy-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
353.0486	HMDB0240406	(2S,3S,4S,5R,6S)-6-(4-carboxy-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0126656	6-(3,5-dihydroxybenzoyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0126655	6-(3-carboxy-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0124991	6-(5-carboxy-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9

	HMDB0124990	6-(4-carboxy-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0124992	6-(3,4-dihydroxybenzoyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0125146	6-(2-formyl-3,5-dihydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0125147	6-(4-formyl-3,5-dihydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0126444	6-(4-carboxy-3-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0126445	6-(2-carboxy-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0126446	6-(2,4-dihydroxybenzoyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
	HMDB0240410	(2S,3S,4S,5R,6S)-6-(3-carboxy-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H14O10	M+Na	353.0479	1.9
355.0669	HMDB0130552	3,4,5-trihydroxy-6-[(8-hydroxy-2-oxo-2H-chromen-7-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0136748	3,4,5-trihydroxy-6-[(5-hydroxy-2-oxo-2H-chromen-6-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0141204	3,4,5-trihydroxy-6-[(3-hydroxy-2-oxo-2H-chromen-6-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0141202	3,4,5-trihydroxy-6-[(3-hydroxy-2-oxo-2H-chromen-7-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0141203	3,4,5-trihydroxy-6-[(7-hydroxy-2-oxo-2H-chromen-3-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0141208	3,4,5-trihydroxy-6-[(3-hydroxy-2-oxo-2H-chromen-5-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0141207	3,4,5-trihydroxy-6-[(8-hydroxy-2-oxo-2H-chromen-3-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0141206	3,4,5-trihydroxy-6-[(3-hydroxy-2-oxo-2H-chromen-8-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0141205	3,4,5-trihydroxy-6-[(6-hydroxy-2-oxo-2H-chromen-3-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0141209	3,4,5-trihydroxy-6-[(5-hydroxy-2-oxo-2H-chromen-3-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0136746	3,4,5-trihydroxy-6-[(5-hydroxy-2-oxo-2H-chromen-7-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0136749	3,4,5-trihydroxy-6-[(6-hydroxy-2-oxo-2H-chromen-5-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0130551	3,4,5-trihydroxy-6-[(7-hydroxy-2-oxo-2H-chromen-8-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0132255	3,4,5-trihydroxy-6-[(7-hydroxy-2-oxo-2H-chromen-6-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0132256	3,4,5-trihydroxy-6-[(6-hydroxy-2-oxo-2H-chromen-7-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0040570	2-O-p-Coumaroylhydroxycitric acid	C15H14O10	M+H	355.0660	2.6
	HMDB0136662	3,4,5-trihydroxy-6-[(7-hydroxy-2-oxo-2H-chromen-4-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0136747	3,4,5-trihydroxy-6-[(7-hydroxy-2-oxo-2H-chromen-5-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
	HMDB0136663	3,4,5-trihydroxy-6-[(4-hydroxy-2-oxo-2H-chromen-7-yl)oxy]oxane-2-carboxylic acid	C15H14O10	M+H	355.0660	2.6
355.2379	HMDB0002835	Danazol	C22H27NO2	M+NH4	355.2380	-0.3
	HMDB0144293	3-[(dimethylamino)methyl]-1,2-diphenylbut-3-en-2-yl propanoate	C22H27NO2	M+NH4	355.2380	-0.3
	HMDB0144294	4-(dimethylamino)-3-methyl-1,2-diphenylbutan-2-yl prop-2-enoate	C22H27NO2	M+NH4	355.2380	-0.3
	HMDB0030361	(-)-Aspidospermine	C22H30N2O2	M+H	355.2380	-0.3
356.1908	HMDB0164643	6-[(3,7-dihydroxyoctyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H26O9	M+NH4	356.1915	-2.0
	HMDB0164645	6-[(6,8-dihydroxyoctan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H26O9	M+NH4	356.1915	-2.0

	HMDB0164644	6-[(1,7-dihydroxyoctan-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H26O9	M+NH4	356.1915	-2.0
356.2786	HMDB0184684	PGE1,11-DEOXY	C20H34O4	M+NH4	356.2795	-2.6
	HMDB0002265	14,15-DiHETrE	C20H34O4	M+NH4	356.2795	-2.6
	HMDB0060106	15-Hydroperoxyeicosa-8Z,11Z,13E-trienoate	C20H34O4	M+NH4	356.2795	-2.6
	HMDB0002311	8,9-DiHETrE	C20H34O4	M+NH4	356.2795	-2.6
	HMDB0002314	11,12-DiHETrE	C20H34O4	M+NH4	356.2795	-2.6
	HMDB0002343	5,6-DHET	C20H34O4	M+NH4	356.2795	-2.6
	HMDB0002995	12-Keto-tetrahydro-leukotriene B4	C20H34O4	M+NH4	356.2795	-2.6
	HMDB0035379	Sterebin E	C20H34O4	M+NH4	356.2795	-2.6
	HMDB0012504	11-dihydro-leukotriene B4	C20H34O4	M+NH4	356.2795	-2.6
	HMDB0012838	6,7-dihydro-12-epi-LTB4	C20H34O4	M+NH4	356.2795	-2.6
360.1492	HMDB0000048	Melibiose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0182195	931-68-4	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0133305	6-({[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}methyl)oxane-2,3,4,5-tetrol	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0165105	AC1NAD98	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0163565	3,4,5-trihydroxy-6-[(2,3,4-trihydroxy-5-methoxypentyl)oxy]oxane-2-carboxylic acid	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0163568	3,4,5-trihydroxy-6-[(3,4,5-trihydroxy-1-methoxypentan-2-yl)oxy]oxane-2-carboxylic acid	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0163567	3,4,5-trihydroxy-6-[(1,2,4-trihydroxy-5-methoxypentan-3-yl)oxy]oxane-2-carboxylic acid	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0163566	3,4,5-trihydroxy-6-[(1,3,4-trihydroxy-5-methoxypentan-2-yl)oxy]oxane-2-carboxylic acid	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0029880	Neotrehalose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0006792	Epimelibiose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0029902	Galabiose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0000740	Lactulose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0011742	Kojibiose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0039876	Fagopyritol A1	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0039237	Glucinol	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0029882	Sakebiose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0029919	Maltulose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0029933	Mannobiose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0038489	Allolactose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0011740	Turanose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0006603	3-b-Galactopyranosyl glucose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0000055	Cellobiose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0000163	D-Maltose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0000186	Alpha-Lactose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0000258	Sucrose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0125600	Sucrose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0000975	Trehalose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0039727	Trehalulose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0005826	Galactinol	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0062114	gentiobiose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0002923	Isomaltose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0060068	Glucose-1,3-mannose oligosaccharide	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0029898	Inulobiose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0033368	DEAE-cellulose	C12H22O11	M+NH4	360.1500	-2.3
	HMDB0041627	beta-Lactose	C12H22O11	M+NH4	360.1500	-2.3
362.3257	HMDB0031923	,-Dihydroxyeicosanoic acid	C20H40O4	M+NH4	362.3265	-2.2
	HMDB0072856	MG(17)	C20H40O4	M+NH4	362.3265	-2.2
	HMDB0072852	MG(i-17)	C20H40O4	M+NH4	362.3265	-2.2
	HMDB0072851	MG(a-17)[rac]	C20H40O4	M+NH4	362.3265	-2.2
	HMDB0072848	MG/a-17)[rac]	C20H40O4	M+NH4	362.3265	-2.2
	HMDB0072846	MG(i-17)	C20H40O4	M+NH4	362.3265	-2.2
	HMDB0240306	Mg(17)[rac]	C20H40O4	M+NH4	362.3265	-2.2
	HMDB0072875	MG/17)	C20H40O4	M+NH4	362.3265	-2.2
	HMDB0179733	3,4,5-trihydroxy-6-{4-[(1E)-3-methoxyprop-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
	HMDB0133767	3,4,5-trihydroxy-6-(2-oxo-4-phenylbutoxy)oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6

363.1041

HMDB0133742	3,4,5-trihydroxy-6-[1-(3-phenyloxiran-2-yl)ethoxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133736	3,4,5-trihydroxy-6-{3-[(1E)-3-hydroxybut-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133739	3,4,5-trihydroxy-6-{4-[(1E)-3-hydroxybut-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133732	3,4,5-trihydroxy-6-{[(3E)-2-hydroxy-4-phenylbut-3-en-1-yl]oxy}oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133733	3,4,5-trihydroxy-6-{[(3E)-1-hydroxy-4-phenylbut-3-en-2-yl]oxy}oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133675	3,4,5-trihydroxy-6-[(2-methyl-3-phenylpropanoyl)oxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133657	3,4,5-trihydroxy-6-{2-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133653	3,4,5-trihydroxy-6-[(2-methyl-3-phenyloxiran-2-yl)methoxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133650	3,4,5-trihydroxy-6-{4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133765	3,4,5-trihydroxy-6-[(3-oxo-1-phenylbutan-2-yl)oxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133769	3,4,5-trihydroxy-6-(3-oxo-1-phenylbutoxy)oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133771	3,4,5-trihydroxy-6-[3-(3-oxobutyl)phenoxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0179549	3,4,5-trihydroxy-6-[4-hydroxy-5-methyl-2-(prop-1-en-2-yl)phenoxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0179550	3,4,5-trihydroxy-6-[4-hydroxy-2-methyl-5-(prop-1-en-2-yl)phenoxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0170985	3,4,5-trihydroxy-6-{2-methoxy-4-[(1Z)-prop-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0160088	3,4,5-trihydroxy-6-[(4-phenylbutanoyl)oxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0157137	3,4,5-trihydroxy-6-[(2-phenylbutanoyl)oxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0151264	3,4,5-trihydroxy-6-[4-(3-hydroxy-2-methylprop-1-en-1-yl)phenoxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0141024	3,4,5-trihydroxy-6-[(3-phenylbutanoyl)oxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0135652	3,4,5-trihydroxy-6-{[3-(4-methoxyphenyl)prop-2-en-1-yl]oxy}oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0135244	3,4,5-trihydroxy-6-[2-methoxy-4-(prop-2-en-1-yl)phenoxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133773	3,4,5-trihydroxy-6-[4-(3-oxobutyl)phenoxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133647	3,4,5-trihydroxy-6-{3-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133645	3,4,5-trihydroxy-6-[(2E)-3-hydroxy-2-(phenylmethylidene)propoxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0060021	trans-isoeugenol-O-glucuronide	C16H20O8	M+Na	363.1050	-2.6
HMDB0035441	Oenanthoside A	C16H20O8	M+Na	363.1050	-2.6
HMDB0133643	3,4,5-trihydroxy-6-[4-(2-methyl-3-oxopropyl)phenoxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133641	3,4,5-trihydroxy-6-[3-(2-methyl-3-oxopropyl)phenoxy]oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133636	6-(2-benzyl-3-oxopropoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133639	3,4,5-trihydroxy-6-(2-methyl-3-oxo-1-phenylpropoxy)oxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0133635	6-[(2-benzyl-1-oxopropan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H20O8	M+Na	363.1050	-2.6
HMDB0030678	Linocinnamarin	C16H20O8	M+Na	363.1050	-2.6
HMDB0003033	Canrenone	C22H28O3	M+Na	363.1931	-2.7
HMDB0040635	Piperochromenoic acid	C22H28O3	M+Na	363.1931	-2.7
HMDB0149439	2,4-dihydroxy-5-methoxy-5-(methylamino)-3,4-diphenylpentanoic acid	C19H23NO5	M+NH4	363.1914	1.8

363.1921	HMDB0177100	4-hydroxy-4-[(7-hydroxy-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl]-2-methoxycyclohexa-2,5-dien-1-one	C19H23NO5	M+NH4	363.1914	1.8
	HMDB0149442	2-hydroxy-3-(3-hydroxyphenyl)-5-methoxy-5-(methylamino)-4-phenylpentanoic acid	C19H23NO5	M+NH4	363.1914	1.8
	HMDB0149441	2-hydroxy-4-(3-hydroxyphenyl)-5-methoxy-5-(methylamino)-3-phenylpentanoic acid	C19H23NO5	M+NH4	363.1914	1.8
	HMDB0149447	2-hydroxy-4-(2-hydroxyphenyl)-5-methoxy-5-(methylamino)-3-phenylpentanoic acid	C19H23NO5	M+NH4	363.1914	1.8
	HMDB0149448	2-hydroxy-3-(2-hydroxyphenyl)-5-methoxy-5-(methylamino)-4-phenylpentanoic acid	C19H23NO5	M+NH4	363.1914	1.8
	HMDB0149440	2,3-dihydroxy-5-methoxy-5-(methylamino)-3,4-diphenylpentanoic acid	C19H23NO5	M+NH4	363.1914	1.8
	HMDB0149444	2-hydroxy-3-(4-hydroxyphenyl)-5-methoxy-5-(methylamino)-4-phenylpentanoic acid	C19H23NO5	M+NH4	363.1914	1.8
	HMDB0149443	2-hydroxy-4-(4-hydroxyphenyl)-5-methoxy-5-(methylamino)-3-phenylpentanoic acid	C19H23NO5	M+NH4	363.1914	1.8
364.0645	HMDB0156245	3,4,5-trihydroxy-6-{{2-(phosphonooxy)propanoyl}oxy}oxane-2-carboxylic	C9H15O12P	M+NH4	364.0639	1.5
	HMDB0240438	2-Hydroxy-1,4-benzoxazin-3-one glucuronide	C14H15NO9	M+Na	364.0639	1.7
	HMDB0240378	HBOA glucuronide	C14H15NO9	M+Na	364.0639	1.7
	HMDB0154952	((3,4-dihydroxy-5-[6-(hydroxyamino)-9H-purin-9-yl]oxolan-2-yl)methoxy)phosphonic acid	C10H14N5O8P	M+H	364.0653	-2.1
	HMDB0240586	Guanosine 2'-monophosphate	C10H14N5O8P	M+H	364.0653	-2.1
	HMDB0001397	Guanosine monophosphate	C10H14N5O8P	M+H	364.0653	-2.1
	HMDB0011670	8-Oxo-dGMP	C10H14N5O8P	M+H	364.0653	-2.1
	HMDB0059639	Cyclic pyranopterin monophosphate	C10H14N5O8P	M+H	364.0653	-2.1
	HMDB0240587	Guanosine 3'-monophosphate	C10H14N5O8P	M+H	364.0653	-2.1
366.9605	HMDB0041856	Chlorpyrifos	C9H11Cl3NO3PS	M+NH4	366.9601	1.1
368.2062	HMDB0034915	Calonectrin	C19H26O6	M+NH4	368.2068	-1.5
	HMDB0036689	Millefin	C19H26O6	M+NH4	368.2068	-1.5
369.0795	HMDB0180029	3,4,5-trihydroxy-6-[2-hydroxy-4-(hydroxymethyl)-6-methoxyphenoxy]oxane-2-carboxylic acid	C14H18O10	M+Na	369.0792	0.8
	HMDB0156884	6-[4-(1,2-dihydroxyethyl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H18O10	M+Na	369.0792	0.8
	HMDB0156885	6-[5-(1,2-dihydroxyethyl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H18O10	M+Na	369.0792	0.8
	HMDB0171102	3,4,5-trihydroxy-6-(4-hydroxy-3,5-dimethoxyphenoxy)oxane-2-carboxylic acid	C14H18O10	M+Na	369.0792	0.8
	HMDB0171103	3,4,5-trihydroxy-6-(4-hydroxy-2,6-dimethoxyphenoxy)oxane-2-carboxylic acid	C14H18O10	M+Na	369.0792	0.8
	HMDB0039354	Methyl 6-O-galloyl-beta-D-glucopyranoside	C14H18O10	M+Na	369.0792	0.8
	HMDB0180028	3,4,5-trihydroxy-6-[2-hydroxy-5-(hydroxymethyl)-3-methoxyphenoxy]oxane-2-carboxylic acid	C14H18O10	M+Na	369.0792	0.8
370.0499	HMDB0180838	2-[2-chloro-4-fluoro-5-(4-hydroxy-1,3-dioxo-2,3,4,5,6,7-hexahydro-1H-isoindol-2-yl)phenoxy]acetic acid	C16H13ClFN O6	M+H	370.0488	2.9
	HMDB0180839	[2-Chloro-4-fluoro-5-[(1,3,4,5,6,7-hexahydro-5-hydroxy-1,3-dioxo-2H-isoindol)-2-yl]phenoxy]acetic acid	C16H13ClFN O6	M+H	370.0488	2.9
	HMDB0180840	2-[2-chloro-5-(1,3-dioxo-2,3,4,5,6,7-hexahydro-1H-isoindol-2-yl)-4-fluoro-3-hydroxyphenoxy]acetic acid	C16H13ClFN O6	M+H	370.0488	2.9
	HMDB0180841	2-[6-chloro-3-(1,3-dioxo-2,3,4,5,6,7-hexahydro-1H-isoindol-2-yl)-4-fluoro-2-hydroxyphenoxy]acetic acid	C16H13ClFN O6	M+H	370.0488	2.9
	HMDB0062299	(5S,6E,8E,Z,14R,15S)-5,14,15-trihydroxyicosa-6,8,,12-tetraenoic acid	C20H32O5	M+NH4	370.2588	1.6
	HMDB0164486	5-hydroxy-1-(4-hydroxy-3,5-dimethoxyphenyl)dodecan-3-one	C20H32O5	M+NH4	370.2588	1.6

370.2594	HMDB0062798	(6E,8Z,11Z)-5-hydroperoxy-15-hydroxyicos-6,8,11,13-tetraenoic acid	C20H32O5	M+NH4	370.2588	1.6
	HMDB0062291	13,14-dihydro-15-oxolipoxin A4	C20H32O5	M+NH4	370.2588	1.6
	HMDB0183411	(5Z)-7-[3-hydroxy-5-oxo-2-(3-oxooctyl)cyclopentyl]hept-5-enoic acid	C20H32O5	M+NH4	370.2588	1.6
	HMDB0186059	7-hydroxy-7-{2-[(1E)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopent-1-en-1-yl}heptanoic acid	C20H32O5	M+NH4	370.2588	1.6
	HMDB0062691	7-[3-hydroxy-5-oxo-2-(3-oxooct-1-en-1-yl)cyclopentyl]heptanoic acid	C20H32O5	M+NH4	370.2588	1.6
	HMDB0186065	7-{4-hydroxy-2-[(1E)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopent-1-en-1-yl}heptanoic acid	C20H32O5	M+NH4	370.2588	1.6
	HMDB0186066	2-hydroxy-7-{2-[(1E)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopent-1-en-1-yl}heptanoic acid	C20H32O5	M+NH4	370.2588	1.6
	HMDB0186064	7-{2-[(1E)-3,8-dihydroxyoct-1-en-1-yl]-5-oxocyclopent-1-en-1-yl}heptanoic acid	C20H32O5	M+NH4	370.2588	1.6
	HMDB0186062	7-{2-[3-(1-hydroxyhexyl)oxiran-2-yl]-5-oxocyclopent-1-en-1-yl}heptanoic acid	C20H32O5	M+NH4	370.2588	1.6
	HMDB0186063	7-{5-[(1E)-3-hydroxyoct-1-en-1-yl]-2-oxo-6-oxabicyclo[3.1]hexan-1-yl}heptanoic acid	C20H32O5	M+NH4	370.2588	1.6
	HMDB0186060	7-{3-hydroxy-2-[(1E)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopent-1-en-1-yl}heptanoic acid	C20H32O5	M+NH4	370.2588	1.6
	HMDB0186061	7-{2-[(1E)-3,7-dihydroxyoct-1-en-1-yl]-5-oxocyclopent-1-en-1-yl}heptanoic acid	C20H32O5	M+NH4	370.2588	1.6
	HMDB0035064	Cinnassiol D4	C20H32O5	M+NH4	370.2588	1.6
	HMDB0034676	Cinnassiol D1	C20H32O5	M+NH4	370.2588	1.6
	HMDB0035338	Sterebin B	C20H32O5	M+NH4	370.2588	1.6
	HMDB0035339	Sterebin C	C20H32O5	M+NH4	370.2588	1.6
	HMDB0036756	Acorusnol	C20H32O5	M+NH4	370.2588	1.6
	HMDB0002122	Prostaglandin F3a	C20H32O5	M+NH4	370.2588	1.6
	HMDB0001509	-Hydroxy-leukotriene B4	C20H32O5	M+NH4	370.2588	1.6
	HMDB0001452	Thromboxane A2	C20H32O5	M+NH4	370.2588	1.6
	HMDB0001381	Prostaglandin H2	C20H32O5	M+NH4	370.2588	1.6
	HMDB0001335	Prostaglandin I2	C20H32O5	M+NH4	370.2588	1.6
	HMDB0001320	(13E)-11a-Hydroxy-9,15-dioxoprost-13-enoic acid	C20H32O5	M+NH4	370.2588	1.6
	HMDB0001403	Prostaglandin D2	C20H32O5	M+NH4	370.2588	1.6
	HMDB0002132	8-iso-PGF3a	C20H32O5	M+NH4	370.2588	1.6
	HMDB0002363	Levuglandin E2	C20H32O5	M+NH4	370.2588	1.6
	HMDB0005844	8-isoprostaglandin E2	C20H32O5	M+NH4	370.2588	1.6
	HMDB0005082	Lipoxin B4	C20H32O5	M+NH4	370.2588	1.6
	HMDB0005077	8-iso-15-keto-PGF2a	C20H32O5	M+NH4	370.2588	1.6
	HMDB0004385	Lipoxin A4	C20H32O5	M+NH4	370.2588	1.6
	HMDB0004240	15-Keto-prostaglandin F2a	C20H32O5	M+NH4	370.2588	1.6
	HMDB0002776	13,14-Dihydro-15-keto-PGE2	C20H32O5	M+NH4	370.2588	1.6
	HMDB0002400	Levuglandin D2	C20H32O5	M+NH4	370.2588	1.6
	HMDB0001220	Prostaglandin E2	C20H32O5	M+NH4	370.2588	1.6
	HMDB0012481	(5Z)-(15S)-11alpha-Hydroxy-9,15-dioxoprostanoate	C20H32O5	M+NH4	370.2588	1.6
	HMDB0012587	15-Epi-lipoxin A4	C20H32O5	M+NH4	370.2588	1.6
	HMDB0060042	13,14-Dihydro-15-keto-PGD2	C20H32O5	M+NH4	370.2588	1.6
	HMDB0060041	11b-PGE2	C20H32O5	M+NH4	370.2588	1.6
	HMDB0012564	13,14-Dihydro-15-oxo-lipoxin A4	C20H32O5	M+NH4	370.2588	1.6
371.3147	HMDB0040270	Diethylhexyl adipate	C22H42O4	M+H	371.3156	-2.4
	HMDB0041619	Diethyl hexanedioate	C22H42O4	M+H	371.3156	-2.4
372.0993	HMDB0041837	16,17-dimethoxy-5,7-diox-13-azapentacyclo[11.8.,,]henicosa-1(13),2,4(8),9,14,16,18,-octaen-13-ylum chloride	C20H18ClNO4	M+H	372.0997	-1.1
	HMDB0014559	Ampicillin	C16H19N3O4S	M+Na	372.0988	1.2
	HMDB0015428	Cefradine	C16H19N3O4S	M+Na	372.0988	1.2
372.1855	HMDB0041513	Isopropyl apiosylglucoside	C14H26O10	M+NH4	372.1864	-2.5
	HMDB0160361	6-[(1-carboxy-1,2,4,5-tetrahydroxypentan-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O13	M+H	373.0977	-1.8
	HMDB0160359	6-[(1-carboxy-2,3,4,5-tetrahydroxypentyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O13	M+H	373.0977	-1.8

373.0970	HMDB0160360	6-[(1-carboxy-1,3,4,5-tetrahydroxypentan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O13	M+H	373.0977	-1.8
	HMDB0160362	6-[(5-carboxy-1,3,4,5-tetrahydroxypentan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O13	M+H	373.0977	-1.8
	HMDB0160364	3,4,5-trihydroxy-6-[(2,3,4,5,6-pentahydroxyhexanoyl)oxy]oxane-2-carboxylic acid	C12H20O13	M+H	373.0977	-1.8
	HMDB0160363	6-[(5-carboxy-2,3,4,5-tetrahydroxypentyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O13	M+H	373.0977	-1.8
	HMDB0144646	2-[4-(2-chloro-1,2-diphenylethenyl)phenoxy]ethan-1-ol	C22H19ClO2	M+Na	373.0966	1.1
374.3052	HMDB0002007	Tetracosahexaenoic acid	C24H36O2	M+NH4	374.3054	-0.4
	HMDB0013025	6,9,12,15,18,21-Tetracosahexaenoic acid	C24H36O2	M+NH4	374.3054	-0.4
	HMDB0060117	Tetracosahexaenoic acid, n-3	C24H36O2	M+NH4	374.3054	-0.4
374.3259	HMDB0062009	Glyceryl monooleate	C21H40O4	M+NH4	374.3265	-1.6
	HMDB0011536	MG/18:1(11Z))	C21H40O4	M+NH4	374.3265	-1.6
	HMDB0011537	MG/18:1(9Z))	C21H40O4	M+NH4	374.3265	-1.6
	HMDB0011566	MG(18:1(11Z))	C21H40O4	M+NH4	374.3265	-1.6
	HMDB0011567	MG(18:1(9Z))	C21H40O4	M+NH4	374.3265	-1.6
	HMDB0034031	3-(2-Heptenyloxy)-2-hydroxypropyl undecanoate	C21H40O4	M+NH4	374.3265	-1.6
	HMDB0033372	Stearoyllactic acid	C21H40O4	M+NH4	374.3265	-1.6
	HMDB0094684	Glyceryl 1-oleate	C21H40O4	M+NH4	374.3265	-1.6
	HMDB0062003	MG/18:1)	C21H40O4	M+NH4	374.3265	-1.6
374.3628	HMDB0061660	2(R)-hydroydocosanoic acid	C22H44O3	M+NH4	374.3629	-0.2
376.0650	HMDB0161280	3,4,5-trihydroxy-6-(5-hydroxy-1H-indole-2-carbonyloxy)oxane-2-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
	HMDB0161283	7-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1H-indole-2-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
	HMDB0161281	6-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1H-indole-2-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
	HMDB0161282	3,4,5-trihydroxy-6-(6-hydroxy-1H-indole-2-carbonyloxy)oxane-2-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
	HMDB0161284	3,4,5-trihydroxy-6-(7-hydroxy-1H-indole-2-carbonyloxy)oxane-2-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
	HMDB0161286	3,4,5-trihydroxy-6-(4-hydroxy-1H-indole-2-carbonyloxy)oxane-2-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
	HMDB0161279	5-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1H-indole-2-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
	HMDB0134950	3,4,5-trihydroxy-6-(4-hydroxy-1H-indole-3-carbonyloxy)oxane-2-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
	HMDB0134949	4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1H-indole-3-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
	HMDB0134946	7-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1H-indole-3-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
	HMDB0134947	3,4,5-trihydroxy-6-(7-hydroxy-1H-indole-3-carbonyloxy)oxane-2-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
	HMDB0134944	3,4,5-trihydroxy-6-(6-hydroxy-1H-indole-3-carbonyloxy)oxane-2-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
	HMDB0134941	3,4,5-trihydroxy-6-(5-hydroxy-1H-indole-3-carbonyloxy)oxane-2-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
	HMDB0134943	6-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1H-indole-3-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
	HMDB0134940	5-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1H-indole-3-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
	HMDB0161285	4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1H-indole-2-carboxylic acid	C15H15NO9	M+Na	376.0639	2.9
376.3415	HMDB0011131	MG(18)	C21H42O4	M+NH4	376.3421	-1.7
	HMDB0072842	MG(i-18)	C21H42O4	M+NH4	376.3421	-1.7
	HMDB0031075	Glycerol 1-monostearate	C21H42O4	M+NH4	376.3421	-1.7
	HMDB0011535	MG/18)	C21H42O4	M+NH4	376.3421	-1.7
	HMDB0072877	MG(i-18)	C21H42O4	M+NH4	376.3421	-1.7
	HMDB0133701	3,4,5-trihydroxy-6-[3-(2-methyl-3-oxobutyl)phenoxy]oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0133705	6-(2-benzyl-3-oxobutoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6

377.1197	HMDB0151244	3,4,5-trihydroxy-6-[[3-(4-methoxyphenyl)-2-methylprop-2-en-1-yl]oxy]oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0133707	3,4,5-trihydroxy-6-(3-methyl-2-oxo-4-phenylbutoxy)oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0163615	3,4,5-trihydroxy-6-[(3-methyl-2-phenylbutanoyl)oxy]oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0163616	3,4,5-trihydroxy-6-[(2-methyl-4-oxo-3-phenylbutan-2-yl)oxy]oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0163617	3,4,5-trihydroxy-6-(2-methyl-4-oxo-3-phenylbutoxy)oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0163620	3,4,5-trihydroxy-6-[3-(3-methyl-1-oxobutan-2-yl)phenoxy]oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0163619	3,4,5-trihydroxy-6-[(3-methyl-1-oxo-2-phenylbutan-2-yl)oxy]oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0163622	3,4,5-trihydroxy-6-[4-(3-methyl-1-oxobutan-2-yl)phenoxy]oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0133703	3,4,5-trihydroxy-6-[4-(2-methyl-3-oxobutyl)phenoxy]oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0133698	3,4,5-trihydroxy-6-[(2-methyl-3-oxo-1-phenylbutan-2-yl)oxy]oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0133699	3,4,5-trihydroxy-6-(2-methyl-3-oxo-1-phenylbutoxy)oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0040797	Methyl heliantheneate F glucoside	C17H22O8	M+Na	377.1207	-2.6
	HMDB0126175	3,4,5-trihydroxy-6-[3-hydroxy-2-(3-methylbut-2-en-1-yl)phenoxy]oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0133001	3,4,5-trihydroxy-6-[4-(3-oxopentyl)phenoxy]oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0133204	3,4,5-trihydroxy-6-[5-hydroxy-2-(3-methylbut-2-en-1-yl)phenoxy]oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0133205	3,4,5-trihydroxy-6-[3-hydroxy-4-(3-methylbut-2-en-1-yl)phenoxy]oxane-2-carboxylic acid	C17H22O8	M+Na	377.1207	-2.6
	HMDB0040898	Methyl (R)-8-Hydroxy-9-decene-4,6-diynoate glucoside	C17H22O8	M+Na	377.1207	-2.6
	HMDB0181292	3,4,5-trihydroxy-6-[(3-hydroxy-1,7-dioxo-3a,4,5,6,7,7a-hexahydro-1H-isoindol-6-yl)oxy]oxane-2-carboxylic acid	C14H17NO10	M+NH4	377.1191	1.7
	HMDB0154757	3,4,5-trihydroxy-6-[3-hydroxy-5-(hydroxymethyl)-2-methylpyridine-4-carbonyloxy]oxane-2-carboxylic acid	C14H17NO10	M+NH4	377.1191	1.7
	HMDB0154756	3-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-5-(hydroxymethyl)-2-methylpyridine-4-carboxylic acid	C14H17NO10	M+NH4	377.1191	1.7
	HMDB0181258	3,4,5-trihydroxy-6-(4-hydroxy-2-oxo-1aH,1bH,2H,4aH,5H,6H,6aH-oxireno[2,3-e]isoindol-6-yl)oxy]oxane-2-carboxylic acid	C14H17NO10	M+NH4	377.1191	1.7
	HMDB0030934	Triglochinin	C14H17NO10	M+NH4	377.1191	1.7
	HMDB0181268	3,4,5-trihydroxy-6-[(3-hydroxy-1,5-dioxo-3a,4,5,6,7,7a-hexahydro-1H-isoindol-6-yl)oxy]oxane-2-carboxylic acid	C14H17NO10	M+NH4	377.1191	1.7
	HMDB0181283	3,4,5-trihydroxy-6-(5-hydroxy-3-oxo-1aH,2H,2aH,3H,5aH,6H,6aH-oxireno[2,3-f]isoindol-2-yl)oxy]oxane-2-carboxylic acid	C14H17NO10	M+NH4	377.1191	1.7
377.2078	HMDB0014722	Enalapril	C20H28N2O5	M+H	377.2071	1.9
	HMDB0015036	Remifentanyl	C20H28N2O5	M+H	377.2071	1.9
	HMDB0177095	1-[(3,4-dimethoxyphenyl)methyl]-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinoline-7,8-diol	C20H25NO5	M+NH4	377.2071	1.9
	HMDB0177094	1-[(3,4-dimethoxyphenyl)methyl]-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinoline-4,7-diol	C20H25NO5	M+NH4	377.2071	1.9
	HMDB0177096	1-[(3,4-dimethoxyphenyl)methyl]-7-hydroxy-6-methoxy-2-methyl-1,2,3,4-tetrahydro-2H-isoquinolin-2-one	C20H25NO5	M+NH4	377.2071	1.9
	HMDB0177093	1-[(3,4-dimethoxyphenyl)(hydroxy)methyl]-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-ol	C20H25NO5	M+NH4	377.2071	1.9

	HMDB0177090	1-[(3,4-dimethoxyphenyl)methyl]-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinoline-3,7-diol	C20H25NO5	M+NH4	377.2071	1.9
	HMDB0177091	1-[(3,4-dimethoxyphenyl)methyl]-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinoline-1,7-diol	C20H25NO5	M+NH4	377.2071	1.9
	HMDB0135481	3-(3,4-dimethoxyphenyl)-N-[2-(4-hydroxy-3-methoxyphenyl)ethyl]propanimidic acid	C20H25NO5	M+NH4	377.2071	1.9
	HMDB0135482	3-(3,4-dimethoxyphenyl)-N-[2-(3-hydroxy-4-methoxyphenyl)ethyl]propanimidic acid	C20H25NO5	M+NH4	377.2071	1.9
	HMDB0135480	N-[2-(3,4-dimethoxyphenyl)ethyl]-3-(3-hydroxy-4-methoxyphenyl)propanimidic acid	C20H25NO5	M+NH4	377.2071	1.9
	HMDB0135483	N-[2-(3,4-dimethoxyphenyl)ethyl]-3-(4-hydroxy-3-methoxyphenyl)propanimidic acid	C20H25NO5	M+NH4	377.2071	1.9
380.2438	HMDB0154722	(2R,S,14R,15S)-14,17-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetraacyclo[8.7.,heptadec-6-en-5-one	C21H30O5	M+NH4	380.2431	1.7
	HMDB0154725	(2R,R,14R,15S)-8,14-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetraacyclo[8.7.,heptadec-6-en-5-one	C21H30O5	M+NH4	380.2431	1.7
	HMDB0154726	(2R,R,14S,15S)-13,14-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetraacyclo[8.7.,heptadec-6-en-5-one	C21H30O5	M+NH4	380.2431	1.7
	HMDB0154728	(2R,R,14R,15S)-14-hydroxy-14-(2-hydroxyacetyl)-15-(hydroxymethyl)-2-methyltetraacyclo[8.7.,heptadec-6-en-5-one	C21H30O5	M+NH4	380.2431	1.7
	HMDB0154727	(2S,R,14R,15S)-14-hydroxy-14-(2-hydroxyacetyl)-2-(hydroxymethyl)-15-methyltetraacyclo[8.7.,heptadec-6-en-5-one	C21H30O5	M+NH4	380.2431	1.7
	HMDB0154912	(2S,15R)-17-hydroxy-14-(2-hydroxyacetyl)-2-methyl-5-oxotetraacyclo[8.7.,heptadecane-15-carbaldehyde	C21H30O5	M+NH4	380.2431	1.7
	HMDB0158175	(2R,14S,15S)-14-acetyl-13,14,17-trihydroxy-2,15-dimethyltetraacyclo[8.7.,heptadec-6-en-5-one	C21H30O5	M+NH4	380.2431	1.7
	HMDB0158174	(2R,14R,15S)-14-acetyl-8,14,17-trihydroxy-2,15-dimethyltetraacyclo[8.7.,heptadec-6-en-5-one	C21H30O5	M+NH4	380.2431	1.7
	HMDB0158178	(2R,14R,15S)-14-acetyl-4,14,17-trihydroxy-2,15-dimethyltetraacyclo[8.7.,heptadec-6-en-5-one	C21H30O5	M+NH4	380.2431	1.7
	HMDB0158179	(2R,14R,15S)-14-acetyl-6,14,17-trihydroxy-2,15-dimethyltetraacyclo[8.7.,heptadec-6-en-5-one	C21H30O5	M+NH4	380.2431	1.7
	HMDB0158177	(2R,14R,15S)-14-acetyl-14,17-dihydroxy-15-(hydroxymethyl)-2-methyltetraacyclo[8.7.,heptadec-6-en-5-one	C21H30O5	M+NH4	380.2431	1.7
	HMDB0158176	(2S,14R,15S)-14-acetyl-14,17-dihydroxy-2-(hydroxymethyl)-15-methyltetraacyclo[8.7.,heptadec-6-en-5-one	C21H30O5	M+NH4	380.2431	1.7
	HMDB0170454	5,6-dihydroxy-4,6-bis(3-methylbut-2-en-1-yl)-2-(3-methylbutanoyl)cyclohex-4-ene-1,3-dione	C21H30O5	M+NH4	380.2431	1.7
	HMDB0170453	5,6-dihydroxy-4-(3-methylbutanoyl)-2,6-bis(3-methylbut-2-en-1-yl)cyclohex-4-ene-1,3-dione	C21H30O5	M+NH4	380.2431	1.7
	HMDB0154724	(2R,R,14R,15S)-6,14-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetraacyclo[8.7.,heptadec-6-en-5-one	C21H30O5	M+NH4	380.2431	1.7
	HMDB0154723	(2R,R,14R,15S)-4,14-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetraacyclo[8.7.,heptadec-6-en-5-one	C21H30O5	M+NH4	380.2431	1.7
	HMDB0014879	Cortisol	C21H30O5	M+NH4	380.2431	1.7
	HMDB0000063	Cortisol	C21H30O5	M+NH4	380.2431	1.7
	HMDB0000319	18-Hydroxycorticosterone	C21H30O5	M+NH4	380.2431	1.7
	HMDB0006758	17a,21-Dihydroxy-5b-pregnane-3,11,-trione	C21H30O5	M+NH4	380.2431	1.7
	HMDB0034090	(R)-Humulone	C21H30O5	M+NH4	380.2431	1.7
	HMDB0030026	Isohumulone A	C21H30O5	M+NH4	380.2431	1.7
	HMDB0030138	Adhumulone	C21H30O5	M+NH4	380.2431	1.7
	HMDB0032095	5-Hydroxy-4-methoxy-5-(1-oxo-9,12,15-hexadecatrienyl)-2(5H)-furanone	C21H30O5	M+NH4	380.2431	1.7
381.1655	HMDB0037847	N-(1-Deoxy-1-fructosyl)tryptophan	C18H24N2O7	M+H	381.1656	-0.3
	HMDB0168638	3,4,5-trihydroxy-6-(3-methyl-1-{1H-pyrrolo[2,3-b]pyridin-2-yl}butoxy)oxane-2-carboxylic acid	C18H24N2O7	M+H	381.1656	-0.3
	HMDB0168640	3,4,5-trihydroxy-6-(2-methyl-4-{1H-pyrrolo[2,3-b]pyridin-2-yl}butoxy)oxane-2-carboxylic acid	C18H24N2O7	M+H	381.1656	-0.3

	HMDB0168642	3,4,5-trihydroxy-6-[(2-methyl-4-{1H-pyrrolo[2,3-b]pyridin-2-yl}butan-2-yl)oxy]oxane-2-carboxylic acid	C18H24N2O7	M+H	381.1656	-0.3
381.1812	HMDB0033466	Di-4-coumaroylputrescine	C22H24N2O4	M+H	381.1809	0.8
	HMDB0041143	8-Methyldihydrochelerythrine	C22H21NO4	M+NH4	381.1809	0.8
383.3301	HMDB0001093	5a-Cholesta-8,24-dien-3-one	C27H42O	M+H	383.3308	-1.9
	HMDB0154864	(1S,2R,11R,15R)-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadeca-7,9-dien-5-one	C27H42O	M+H	383.3308	-1.9
	HMDB0002394	Cholesta-4,6-dien-3-one	C27H42O	M+H	383.3308	-1.9
	HMDB0003896	7-Dehydrodesmosterol	C27H42O	M+H	383.3308	-1.9
	HMDB0184839	(1S,2R,S,11S,15R)-2,15-dimethyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadec-7-en-5-one	C27H42O	M+H	383.3308	-1.9
384.2388	HMDB0187151	(5Z)-7-[(1R,4S,5R,6R)-6-[(1E,3S)-3-hydroperoxyocta-1,7-dien-1-yl]-2,3-dioxabicyclo[2.2.1]heptan-5-yl]hept-5-enoic acid	C20H30O6	M+NH4	384.2381	1.9
	HMDB0187379	(5Z)-7-{3-hydroxy-2-[(1E)-3-hydroxy-8-oxooct-1-en-1-yl]-5-oxocyclopentyl}hept-5-enoic acid	C20H30O6	M+NH4	384.2381	1.9
	HMDB0036863	Anhydrocinnzeylanol	C20H30O6	M+NH4	384.2381	1.9
	HMDB0012551	12-oxo--dihydroxy-leukotriene B4	C20H30O6	M+NH4	384.2381	1.9
	HMDB0012549	12-oxo-,11-dihydro--COOH-LTB4	C20H30O6	M+NH4	384.2381	1.9
	HMDB0037062	Sporotrichiol	C20H30O6	M+NH4	384.2381	1.9
	HMDB0006059	-Carboxy-leukotriene B4	C20H30O6	M+NH4	384.2381	1.9
385.3456	HMDB0006842	5alpha-cholesta-7,24-dien-3beta-ol	C27H44O	M+H	385.3465	-2.3
	HMDB0184863	(2S,15R)-2,15-dimethyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadecan-7-ylum-5-olate	C27H44O	M+H	385.3465	-2.3
	HMDB0184133	(1S,2S,S,11S,15R)-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-8-en-5-one	C27H44O	M+H	385.3465	-2.3
	HMDB0155071	(1S,2R,S,11S,15R)-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-one	C27H44O	M+H	385.3465	-2.3
	HMDB0154878	(2S,15R)-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-9-en-7-ylum-5-olate	C27H44O	M+H	385.3465	-2.3
	HMDB0062414	5alpha-cholest-8-en-3-one	C27H44O	M+H	385.3465	-2.3
	HMDB0012178	5Alpha-cholesta-8-en-3-one	C27H44O	M+H	385.3465	-2.3
	HMDB0006719	5,6-trans-Vitamin D3	C27H44O	M+H	385.3465	-2.3
	HMDB0006560	Tachysterol 3	C27H44O	M+H	385.3465	-2.3
	HMDB0006505	Lumisterol 3	C27H44O	M+H	385.3465	-2.3
	HMDB0006500	Previtamin D3	C27H44O	M+H	385.3465	-2.3
	HMDB0006271	Zymosterol intermediate 2	C27H44O	M+H	385.3465	-2.3
	HMDB0002719	Desmosterol	C27H44O	M+H	385.3465	-2.3
	HMDB0002027	8-Dehydrocholesterol	C27H44O	M+H	385.3465	-2.3
	HMDB0000921	Cholestenone	C27H44O	M+H	385.3465	-2.3
	HMDB0014315	Vitamin D3	C27H44O	M+H	385.3465	-2.3
	HMDB0000032	7-Dehydrocholesterol	C27H44O	M+H	385.3465	-2.3
	HMDB0034399	N2-gamma-L-Glutamyl-L-ornithine	C27H44O	M+H	385.3465	-2.3
	HMDB0059615	5-alpha-Cholesta-7,24-dien-3-beta-ol	C27H44O	M+H	385.3465	-2.3
	HMDB0000876	Vitamin D3	C27H44O	M+H	385.3465	-2.3
386.0254	HMDB0180648	2-[2,4-dichloro-5-(methanesulfonylazaniumyl)phenyl]-4-(fluoromethylidene)-5-methyl-3-oxo-2,3-dihydro-1H-1,2,4-triazol-1-ide	C11H11Cl2FN4O3S	M+NH4	386.0251	0.7
386.2011	HMDB0041255	(2S)-2-Butanol O-[b-D-Apiofuranosyl-(1->6)-b-D-glucopyranoside]	C15H28O10	M+NH4	386.2021	-2.5
387.1922	HMDB0061331	Heroin	C21H23NO5	M+NH4	387.1914	1.9
	HMDB0036765	Romucosine D	C21H23NO5	M+NH4	387.1914	1.9
	HMDB0033084	7-Hydroxydehydroglucine	C21H23NO5	M+NH4	387.1914	1.9
	HMDB0030730	3-(1,1-Dimethyl-2-propenyl)-8-(3-methyl-2-butenyl)xanthyletin	C24H28O3	M+Na	387.1931	-2.2
388.2533	HMDB0094680	Octaethylene glycol	C16H34O9	M+NH4	388.2541	-2.1
388.3412	HMDB0040270	Diethylhexyl adipate	C22H42O4	M+NH4	388.3421	-2.4
	HMDB0041619	Diocetyl hexanedioate	C22H42O4	M+NH4	388.3421	-2.4
	HMDB0029830	N-Caffeoyltryptophan	C20H18N2O5	M+Na	389.1108	0.3
	HMDB0139425	4-hydroxy-4-{5-hydroxy-2-oxa-6,11-diazatetracyclo[7.5.2?.hexadeca-1(15),5,9,12(16),13-pentaen-3-yl]-2-methoxycyclohexa-2,5-dien-1-one	C20H18N2O5	M+Na	389.1108	0.3

389.1109	HMDB0139424	3-(4-hydroxy-3-methoxyphenyl)-2-oxa-6,11-diazatetracyclo[7.5.2?,hexadeca-1(15),5,9,12(16),13-pentaene-4,5-diol	C20H18N2O5	M+Na	389.1108	0.3
	HMDB0139422	3-(4-hydroxy-3-methoxyphenyl)-2-oxa-6,11-diazatetracyclo[7.5.2?,hexadeca-1(15),5,9,12(16),13-pentaene-5,7-diol	C20H18N2O5	M+Na	389.1108	0.3
	HMDB0139423	3-(4-hydroxy-3-methoxyphenyl)-2-oxa-6,11-diazatetracyclo[7.5.2?,hexadeca-1(15),5,9,12(16),13-pentaene-5,8-diol	C20H18N2O5	M+Na	389.1108	0.3
	HMDB0139421	5-{5-hydroxy-2-oxa-6,11-diazatetracyclo[7.5.2?,hexadeca-1(15),5,9,12(16),13-pentaen-3-yl}-3-methoxybenzene-1,2-diol	C20H18N2O5	M+Na	389.1108	0.3
389.1260	HMDB0041837	16,17-dimethoxy-5,7-dioxo-13-azapentacyclo[11.8,,,]henicosa-1(13),2,4(8),9,14,16,18,-octaen-13-ylum chloride	C20H18ClNO ₄	M+NH ₄	389.1263	-0.7
	HMDB0181630	{2'-[(acetyloxy)methyl]-1',5'-dimethyl-8'-oxaspiro[oxirane-2,12'-tricyclo[7.2.1,dodecan]-5'-en-1'-yl]oxidanesulfonic acid	C17H24O8S	M+H	389.1265	-1.2
	HMDB0181633	{[1'-(acetyloxy)-1',5'-dimethyl-8'-oxaspiro[oxirane-2,12'-tricyclo[7.2.1,dodecan]-5'-en-2'-yl]methoxy} sulfonic acid	C17H24O8S	M+H	389.1265	-1.2
	HMDB0177954	[3-(acetyloxy)-7,7a-dimethyl-4'-methylidene-2'-oxo-octahydrospiro[indene-2,3'-oxolane]-4-yl]oxidanesulfonic acid	C17H24O8S	M+H	389.1265	-1.2
	HMDB0151383	6-(2-benzyl-3-methanesulfinylpropoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C17H24O8S	M+H	389.1265	-1.2
390.1231	HMDB0160361	6-[(1-carboxy-1,2,4,5-tetrahydroxypentan-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O13	M+NH ₄	390.1242	-2.9
	HMDB0160359	6-[(1-carboxy-2,3,4,5-tetrahydroxypentyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O13	M+NH ₄	390.1242	-2.9
	HMDB0160360	6-[(1-carboxy-1,3,4,5-tetrahydroxypentan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O13	M+NH ₄	390.1242	-2.9
	HMDB0160363	6-[(5-carboxy-2,3,4,5-tetrahydroxypentyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O13	M+NH ₄	390.1242	-2.9
	HMDB0160364	3,4,5-trihydroxy-6-[(2,3,4,5,6-pentahydroxyhexanoyl)oxy]oxane-2-carboxylic acid	C12H20O13	M+NH ₄	390.1242	-2.9
	HMDB0160362	6-[(5-carboxy-1,3,4,5-tetrahydroxypentan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C12H20O13	M+NH ₄	390.1242	-2.9
390.3576	HMDB0062105	Diethylene glycol monostearate	C22H44O4	M+NH ₄	390.3578	-0.5
	HMDB0072839	MG(19)	C22H44O4	M+NH ₄	390.3578	-0.5
	HMDB0072840	MG(19)	C22H44O4	M+NH ₄	390.3578	-0.5
	HMDB0072876	MG(i-19)	C22H44O4	M+NH ₄	390.3578	-0.5
	HMDB0072881	MG(i-19)	C22H44O4	M+NH ₄	390.3578	-0.5
391.1073	HMDB0149477	{[1-methyl-6-(methyloxidaniumylidene)-2-oxo-4,5-diphenylpiperidin-1-ium-3-yl]oxy}trioxo- β - γ -sulfanuide	C19H20NO6S	M+H	391.1079	-1.4
	HMDB0170522	6-[[{(4E,6E)-7-carboxy-7-(hydroxymethyl)-2-methylhepta-4,6-dienoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H22O11	M+H	391.1235	1.8
	HMDB0170518	(2E,4E)-7-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-2,7-dimethylocta-2,4-dienedioic acid	C16H22O11	M+H	391.1235	1.8
	HMDB0170532	6-[(3-{3-[(1E)-2-carboxy-2-methyleth-1-en-1-yl]oxiran-2-yl}-2-methylpropanoyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H22O11	M+H	391.1235	1.8
	HMDB0170519	6-[[{(4E,6E)-7-carboxy-2-hydroxy-2,7-dimethylhepta-4,6-dienoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H22O11	M+H	391.1235	1.8
	HMDB0170520	6-[[{(2E,4E)-7-carboxy-7-hydroxy-2,7-dimethylhepta-2,4-dienoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H22O11	M+H	391.1235	1.8
	HMDB0170521	(2E,4E)-2-[[{(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]methyl]-7-methylocta-2,4-dienedioic acid	C16H22O11	M+H	391.1235	1.8
	HMDB0170537	6-[[{(4E,6E)-7-carboxy-2-(hydroxymethyl)-7-methylhepta-4,6-dienoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H22O11	M+H	391.1235	1.8

391.1242	HMDB0170523	6-{[(2E,4E)-7-carboxy-2-(hydroxymethyl)-7-methylhepta-2,4-dienoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H22O11	M+H	391.1235	1.8
	HMDB0170536	(2E,4E)-7-{[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]methyl}-2-methylocta-2,4-dienedioic acid	C16H22O11	M+H	391.1235	1.8
	HMDB0170526	6-{[(4E,6E)-7-carboxy-3-hydroxy-2,7-dimethylhepta-4,6-dienoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H22O11	M+H	391.1235	1.8
	HMDB0170527	6-{[(2E,4E)-7-carboxy-6-hydroxy-2,7-dimethylhepta-2,4-dienoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H22O11	M+H	391.1235	1.8
	HMDB0170529	6-{[(4E)-5-(3-carboxy-3-methyloxiran-2-yl)-2-methylpent-4-enoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H22O11	M+H	391.1235	1.8
	HMDB0170530	6-{3-[(1E)-4-carboxy-4-methylbut-1-en-1-yl]-2-methyloxirane-2-carbonyloxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H22O11	M+H	391.1235	1.8
	HMDB0170533	6-{[(2E)-3-[3-(2-carboxy-2-methylethyl)oxiran-2-yl]-2-methylprop-2-enoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H22O11	M+H	391.1235	1.8
	HMDB0170525	(2E)-6-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-2,7-dimethylocta-2,4-dienedioic acid	C16H22O11	M+H	391.1235	1.8
	HMDB0034223	2,3,4,5,6-Penta-O-acetyl-D-glucose	C16H22O11	M+H	391.1235	1.8
	HMDB0035608	Monotropein	C16H22O11	M+H	391.1235	1.8
	HMDB0170538	6-{[(2E,4E)-7-carboxy-7-(hydroxymethyl)-2-methylhepta-2,4-dienoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H22O11	M+H	391.1235	1.8
	HMDB0062742	12alpha-hydroxy-3-oxo-5beta-cholan-24-oic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0156541	5-hydroxy-4-[(1S,2R,S,11S,15S)-5-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0156542	4-[(1S,2R,S,11S,15R)-5,17-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0156544	4-[(1S,2S,S,11S,15R)-5-hydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadec-7-en-14-yl]]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0156543	4-[(1S,2R,S,11S,15S)-5,13-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0156545	4-[(1S,2R,R,11S,15S)-5-hydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadec-7-en-14-yl]]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0156546	4-hydroxy-4-[(1S,2R,S,11S,15S)-5-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0156547	4-[(1S,2R,S,11S,15R)-5,6-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0156548	4-[(1S,2R,S,11S,15R)-5,9-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0157446	4-[(1S,2S,7S,R,11S,15R)-16-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0159760	4-[(1S,2S,7S,11S,14R,15R)-5-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0160999	4-[(1S,2R,S,11S,15R)-5-hydroxy-2,15-dimethyl-8-oxotetracyclo[8.7.,heptadecan-14-yl]]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0184494	4-[(2R,15R)-8-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0184497	4-[(2S,15S)-15-(hydroxymethyl)-2-methyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0184495	4-[(2S,15S)-13-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]]pentanoic acid	C24H38O4	M+H	391.2843	-2.0

391.2835	HMDB0184496	4-[(2S,15R)-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]-5-hydroxypentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0184498	4-[(2R,15R)-2-(hydroxymethyl)-15-methyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0184499	4-[(2S,15S)-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]-4-hydroxypentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0062796	7alpha-hydroxy-3-oxo-5beta-cholan-24-oic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0000503	7alpha-hydroxy-3-oxo-5beta-cholan-24-oic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0159759	4-[(1S,2S,7R,R,11S,15S)-5,9-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-yl]pent-4-enoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0159748	4-[(1S,2S,7R,11S,15R)-5-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0159167	4-[(1S,2S,R,11S,15R)-9-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0157455	4-[(1S,2S,7S,R,11S,15S)-5,16-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-yl]pent-4-enoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0157686	4-[(1S,2S,7S,R,11S,15S)-5,9-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-yl]pent-4-enoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0158251	4-[(2S,15S)-13-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0158250	4-[(2R,15R)-8-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0158255	4-[(2S,15S)-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]-4-hydroxypentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0158252	4-[(2S,15S)-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]-5-hydroxypentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0158254	4-[(2R,15R)-2-(hydroxymethyl)-15-methyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0158253	4-[(2S,15S)-15-(hydroxymethyl)-2-methyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0158256	4-[(2S,15R)-4-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0158257	4-[(2R,15R)-6-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0158273	4-[(2S,15S)-5,17-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-yl]pent-4-enoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0158772	4-[(1S,2S,7R,R,11S,15S)-5,16-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-yl]pent-4-enoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0000328	12-Ketodeoxycholic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0000460	7-Hydroxy-3-oxocholanoic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0000467	Nutriacholic acid	C24H38O4	M+H	391.2843	-2.0
	HMDB0041454	D8'-Merulinic acid A	C24H38O4	M+H	391.2843	-2.0
	HMDB0012866	9'-Carboxy-alpha-chromanol	C24H38O4	M+H	391.2843	-2.0
393.3248	HMDB0184483	[(1S,2S,7S,R,11S,14R,15R)-14-(4-carboxybutan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadecan-9-yl]oxidanyl	C24H39O3	M+NH4	393.3237	2.7
	HMDB0155061	(2R,14S,15S)-14-hydroxy-14-(2-hydroxyacetyl)-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadec-6-ene-5,17-dione	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0157239	2-[(2R,14S,15S)-14,17-dihydroxy-15-(hydroxymethyl)-2-methyl-5-oxotetracyclo[8.7.,heptadec-6-en-14-yl]-2-oxoacetaldehyde	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0185103	SCHEMBL11796127	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0185102	(1S,2R,S,11S,14R,15S)-6,14-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7.,heptadec-6-ene-5,17-dione	C21H28O6	M+NH4	394.2224	-2.8

394.2213	HMDB0185101	(1S,2R,S,11S,14R,15S)-4,14-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7,,heptadec-6-ene-5,17-dione	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0185104	6-hydroxycortisone	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0185106	18-Hydroxycortisone	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0185105	(1S,2S,S,11S,14R,15S)-14-hydroxy-14-(2-hydroxyacetyl)-2-(hydroxymethyl)-15-methyltetracyclo[8.7,,heptadec-6-ene-5,17-dione	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0155060	(2S,14S,15S)-14-hydroxy-14-(2-hydroxyacetyl)-2-(hydroxymethyl)-15-methyltetracyclo[8.7,,heptadec-6-ene-5,17-dione	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0155059	(2R,14S,15S)-8,14-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7,,heptadec-6-ene-5,17-dione	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0158867	18-Oxocortisol	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0154915	(2R,15R)-17-hydroxy-14-(2-hydroxyacetyl)-2-methyl-5-oxotetracyclo[8.7,,heptadec-6-ene-15-carboxylic acid	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0155056	(2R,14S,15S)-4,14-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7,,heptadec-6-ene-5,17-dione	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0155058	(2R,14R,15S)-13,14-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7,,heptadec-6-ene-5,17-dione	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0155057	(2R,14S,15S)-6,14-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7,,heptadec-6-ene-5,17-dione	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0000332	18-Oxocortisol	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0031932	11,12,14-Trihydroxy-7-methoxy-8,11,13-abietatrien-,6-olide	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0039557	12alpha-Hydroxy-13,18-dehydroparain	C21H28O6	M+NH4	394.2224	-2.8
	HMDB0061016	16α-hydroxyprednisolone	C21H28O6	M+NH4	394.2224	-2.8
396.2375	HMDB0157224	(1S,2S,S,11S,14S,15R)-14,17-dihydroxy-14-(2-hydroxyacetyl)-2-methyl-5-oxotetracyclo[8.7,,heptadecane-15-carbaldehyde	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0154916	(2S,15R)-8,17-dihydroxy-14-(2-hydroxyacetyl)-2-methyl-5-oxotetracyclo[8.7,,heptadecane-15-carbaldehyde	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0154917	(2S,15R)-13,17-dihydroxy-14-(2-hydroxyacetyl)-2-methyl-5-oxotetracyclo[8.7,,heptadecane-15-carbaldehyde	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0154918	(2R,15R)-17-hydroxy-14-(2-hydroxyacetyl)-2-(hydroxymethyl)-5-oxotetracyclo[8.7,,heptadecane-15-carbaldehyde	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0155050	(1S,2R,S,11S,14S,15S)-6,14,17-trihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7,,heptadec-6-en-5-one	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0155049	(1S,2R,S,11S,14S,15S)-4,14,17-trihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7,,heptadec-6-en-5-one	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0155051	(1S,2R,S,11S,14S,15S)-8,14,17-trihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7,,heptadec-6-en-5-one	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0155053	(1S,2S,S,11S,14S,15S)-14,17-dihydroxy-14-(2-hydroxyacetyl)-2-(hydroxymethyl)-15-methyltetracyclo[8.7,,heptadec-6-en-5-one	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0155052	(1S,2R,S,11S,14R,15S)-13,14,17-trihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7,,heptadec-6-en-5-one	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0154735	(2R,14R,15S)-14,17-dihydroxy-14-(2-hydroxyacetyl)-15-(hydroxymethyl)-2-methyltetracyclo[8.7,,heptadec-6-en-5-one	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0154734	(2S,14R,15S)-14,17-dihydroxy-14-(2-hydroxyacetyl)-2-(hydroxymethyl)-15-methyltetracyclo[8.7,,heptadec-6-en-5-one	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0155054	18-Hydroxycortisol	C21H30O6	M+NH4	396.2381	-1.4

	HMDB0154730	(2R,14R,15S)-4,14,17-trihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7,,heptadec-6-en-5-one	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0154731	(2R,14R,15S)-6,14,17-trihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7,,heptadec-6-en-5-one	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0154732	(2R,14R,15S)-8,14,17-trihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7,,heptadec-6-en-5-one	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0154733	(2R,14S,15S)-13,14,17-trihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7,,heptadec-6-en-5-one	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0061033	6-beta-hydrocortisol	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0030105	Humulinone	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0032770	Eremopetasitenin C1	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0040702	Sugetriol triacetate	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0036889	Arachisprenol 11	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0032773	Eremopetasitenin D1	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0030045	Quillaic acid 3-[galactosyl-(1->2)-[rhamnosyl-(1->3)]-glucuronide] 28-[6-acetyl-glucosyl-(1->3)-[xylosyl-(1->4)-rhamnosyl-(1->2)]-4-acetyl-fucosyl] ester	C21H30O6	M+NH4	396.2381	-1.4
	HMDB0000418	18-Hydroxycortisol	C21H30O6	M+NH4	396.2381	-1.4
398.2577	HMDB0171073	17-(sulfooxy)octadecanoic acid	C18H36O6S	M+NH4	398.2571	1.5
	HMDB0171076	SCHEMBL5993398	C18H36O6S	M+NH4	398.2571	1.5
	HMDB0171079	2-(sulfooxy)octadecanoic acid	C18H36O6S	M+NH4	398.2571	1.5
399.1435	HMDB0062709	Ademetionine	C15H22N6O5S	M+H	399.1445	-2.5
	HMDB0146123	3-(2,4-dihydroxyphenyl)-6-[(3,3-dimethyloxiran-2-yl)methyl]-5,7-dimethoxy-2H-chromen-2-one	C22H22O7	M+H	399.1438	-0.8
	HMDB0146120	5,7-dimethoxy-6-(3-methylbut-2-en-1-yl)-3-(2,3,4-trihydroxyphenyl)-2H-chromen-2-one	C22H22O7	M+H	399.1438	-0.8
	HMDB0146122	3-(2,4-dihydroxyphenyl)-6-(4-hydroxy-3-methylbut-2-en-1-yl)-5,7-dimethoxy-2H-chromen-2-one	C22H22O7	M+H	399.1438	-0.8
	HMDB0146119	5,7-dimethoxy-6-(3-methylbut-2-en-1-yl)-3-(2,4,5-trihydroxyphenyl)-2H-chromen-2-one	C22H22O7	M+H	399.1438	-0.8
	HMDB0137488	5-hydroxy-2-(4-hydroxy-2-methoxyphenyl)-8-(4-hydroxy-3-methylbut-2-en-1-yl)-7-methoxy-4H-chromen-4-one	C22H22O7	M+H	399.1438	-0.8
	HMDB0137486	2-(3,4-dihydroxy-2-methoxyphenyl)-5-hydroxy-7-methoxy-8-(3-methylbut-2-en-1-yl)-4H-chromen-4-one	C22H22O7	M+H	399.1438	-0.8
	HMDB0137487	8-[(3,3-dimethyloxiran-2-yl)methyl]-5-hydroxy-2-(4-hydroxy-2-methoxyphenyl)-7-methoxy-4H-chromen-4-one	C22H22O7	M+H	399.1438	-0.8
	HMDB0137485	2-(4,5-dihydroxy-2-methoxyphenyl)-5-hydroxy-7-methoxy-8-(3-methylbut-2-en-1-yl)-4H-chromen-4-one	C22H22O7	M+H	399.1438	-0.8
	HMDB0137484	5,6-dihydroxy-2-(4-hydroxy-2-methoxyphenyl)-7-methoxy-8-(3-methylbut-2-en-1-yl)-4H-chromen-4-one	C22H22O7	M+H	399.1438	-0.8
	HMDB0038921	5'-Methoxycurcumin	C22H22O7	M+H	399.1438	-0.8
	HMDB0034030	Dulxanthone E	C22H22O7	M+H	399.1438	-0.8
400.2168	HMDB0033237	1,2,-Trihydroxydihydro-trans-linalyl oxide 7-O-beta-D-glucopyranoside	C16H30O10	M+NH4	400.2177	-2.3
	HMDB0172274	2-(4,12-dimethyl-8-methylidenetridecyl)-2,7-dimethyl-3,4-dihydro-2H-1-benzopyran-6-ol	C27H44O2	M+H	401.3414	-1.8
	HMDB0174261	17-hydroxy-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7,,heptadec-9-en-5-one	C27H44O2	M+H	401.3414	-1.8
	HMDB0174260	14-(1-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7,,heptadec-9-en-5-one	C27H44O2	M+H	401.3414	-1.8
	HMDB0174265	2-(hydroxymethyl)-15-methyl-14-(6-methylheptan-2-yl)tetracyclo[8.7,,heptadec-9-en-5-one	C27H44O2	M+H	401.3414	-1.8
	HMDB0174262	8-hydroxy-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7,,heptadec-9-en-5-one	C27H44O2	M+H	401.3414	-1.8
	HMDB0174263	13-hydroxy-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7,,heptadec-9-en-5-one	C27H44O2	M+H	401.3414	-1.8
	HMDB0174264	15-(hydroxymethyl)-2-methyl-14-(6-methylheptan-2-yl)tetracyclo[8.7,,heptadec-9-en-5-one	C27H44O2	M+H	401.3414	-1.8

HMDB0174266	14-(2-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-9-en-5-one	C27H44O2	M+H	401.3414	-1.8
HMDB0174267	14-(6-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-9-en-5-one	C27H44O2	M+H	401.3414	-1.8
HMDB0172275	2,7-dimethyl-2-(4,8,12-trimethyltridec-12-en-1-yl)-3,4-dihydro-2H-1-benzopyran-6-ol	C27H44O2	M+H	401.3414	-1.8
HMDB0172273	2-(8,12-dimethyl-4-methylidenetridecyl)-2,7-dimethyl-3,4-dihydro-2H-1-benzopyran-6-ol	C27H44O2	M+H	401.3414	-1.8
HMDB0155085	SCHEMBL141218	C27H44O2	M+H	401.3414	-1.8
HMDB0154867	(1S,2R,11R,15R)-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadeca-7,9-diene-5,17-diol	C27H44O2	M+H	401.3414	-1.8
HMDB0154866	(1S,2R,11R,15R)-14-(1-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadeca-7,9-dien-5-ol	C27H44O2	M+H	401.3414	-1.8
HMDB0155080	(2R,15S)-13-hydroxy-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-one	C27H44O2	M+H	401.3414	-1.8
HMDB0155083	(2R,15S)-15-(hydroxymethyl)-2-methyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-one	C27H44O2	M+H	401.3414	-1.8
HMDB0155082	(2S,15R)-2-(hydroxymethyl)-15-methyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-one	C27H44O2	M+H	401.3414	-1.8
HMDB0155081	(2R,15S)-14-(1-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-one	C27H44O2	M+H	401.3414	-1.8
HMDB0155084	(2R,15R)-14-(6-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-one	C27H44O2	M+H	401.3414	-1.8
HMDB0155086	(2R,15R)-9-hydroxy-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-one	C27H44O2	M+H	401.3414	-1.8
HMDB0155087	(2R,15R)-14-(7-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-one	C27H44O2	M+H	401.3414	-1.8
HMDB0174268	14-(7-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-9-en-5-one	C27H44O2	M+H	401.3414	-1.8
HMDB0184144	(2S,15S)-14-(1-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+H	401.3414	-1.8
HMDB0184845	(1S,2R,R,11S,15S)-15-(hydroxymethyl)-2-methyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadec-7-en-5-ol	C27H44O2	M+H	401.3414	-1.8
HMDB0184846	(1S,2R,S,11S,15S)-14-(2-hydroxy-6-methylhept-5-en-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-ol	C27H44O2	M+H	401.3414	-1.8
HMDB0184848	(1S,2R,S,11S,15R)-14-(7-hydroxy-6-methylhept-5-en-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-ol	C27H44O2	M+H	401.3414	-1.8
HMDB0184847	(1S,2R,S,11S,15R)-2,15-dimethyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadec-7-ene-5,6-diol	C27H44O2	M+H	401.3414	-1.8
HMDB0184849	(1S,2R,S,11S,15R)-2,15-dimethyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadec-7-ene-5,9-diol	C27H44O2	M+H	401.3414	-1.8
HMDB0184851	(1S,2R,S,11S,15R)-14-[4-(3,3-dimethyloxiran-2-yl)butan-2-yl]-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-ol	C27H44O2	M+H	401.3414	-1.8
HMDB0184850	(1S,2R,S,11S,15R)-14-(4-hydroxy-6-methylhept-5-en-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-ol	C27H44O2	M+H	401.3414	-1.8
HMDB0185576	(2R)-2-(8,12-dimethyl-4-methylidenetridecyl)-2,8-dimethyl-3,4-dihydro-2H-1-benzopyran-6-ol	C27H44O2	M+H	401.3414	-1.8
HMDB0185577	(2R)-2-(4,12-dimethyl-8-methylidenetridecyl)-2,8-dimethyl-3,4-dihydro-2H-1-benzopyran-6-ol	C27H44O2	M+H	401.3414	-1.8
HMDB0184842	(1S,2R,S,11S,15R)-2,15-dimethyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadec-7-ene-5,17-diol	C27H44O2	M+H	401.3414	-1.8
HMDB0184843	(1S,2R,S,11S,15S)-2,15-dimethyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadec-7-ene-5,13-diol	C27H44O2	M+H	401.3414	-1.8
HMDB0184841	(1S,2R,S,11S,15S)-14-(1-hydroxy-6-methylhept-5-en-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-ol	C27H44O2	M+H	401.3414	-1.8
HMDB0184143	(2S,15S)-13-hydroxy-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+H	401.3414	-1.8
HMDB0184146	(2S,15S)-15-(hydroxymethyl)-2-methyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+H	401.3414	-1.8
HMDB0184145	(2R,15R)-2-(hydroxymethyl)-15-methyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+H	401.3414	-1.8
HMDB0184147	(2S,15R)-14-(6-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+H	401.3414	-1.8

	HMDB0184148	(2S,15S)-14-(2-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+H	401.3414	-1.8
	HMDB0184150	(2S,15R)-14-(7-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+H	401.3414	-1.8
	HMDB0184149	(R,14R)-,14-dimethyl-15-(6-methylheptan-2-yl)-3-oxapentacyclo[9.7.,??]octadecan-7-one	C27H44O2	M+H	401.3414	-1.8
	HMDB0184168	(2S,15R)-17-hydroxy-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+H	401.3414	-1.8
	HMDB0184844	(1S,2S,S,11S,15R)-2-(hydroxymethyl)-15-methyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadec-7-en-5-ol	C27H44O2	M+H	401.3414	-1.8
	HMDB0185578	(2R)-2,8-dimethyl-2-(4,8,12-trimethyltridec-12-en-1-yl)-3,4-dihydro-2H-1-benzopyran-6-ol	C27H44O2	M+H	401.3414	-1.8
	HMDB0003550	Calcidiol	C27H44O2	M+H	401.3414	-1.8
	HMDB0060132	27alpha-Hydroxy-8-dehydrocholesterol	C27H44O2	M+H	401.3414	-1.8
	HMDB0060131	3beta-Hydroxy-5-cholestenal	C27H44O2	M+H	401.3414	-1.8
	HMDB0015504	Alfacalcidol	C27H44O2	M+H	401.3414	-1.8
	HMDB0000501	7-Ketocholesterol	C27H44O2	M+H	401.3414	-1.8
	HMDB0001993	7a-Hydroxy-cholestene-3-one	C27H44O2	M+H	401.3414	-1.8
	HMDB0006722	25-Hydroxytachysterol3	C27H44O2	M+H	401.3414	-1.8
	HMDB0006721	5,6-trans-25-Hydroxyvitamin D3	C27H44O2	M+H	401.3414	-1.8
	HMDB0035585	1-Phenyl-1,3-heneicosanedione	C27H44O2	M+H	401.3414	-1.8
	HMDB0034328	(3beta,5alpha,6a)-Cholesta-8,14-diene-3,6-diol	C27H44O2	M+H	401.3414	-1.8
	HMDB0036012	5-Methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone	C27H44O2	M+H	401.3414	-1.8
	HMDB0039871	5-(12,15-Heneicosadienyl)-1,3-benzenediol	C27H44O2	M+H	401.3414	-1.8
402.1789	HMDB0062731	dodecamethylpentasiloxane	C12H36O4Si5	M+NH4	402.1798	-2.3
	HMDB0038642	Fumitremorgin C	C22H25N3O3	M+Na	402.1788	0.2
403.1782	HMDB0154859	[(2S,15S)-13,17-dihydroxy-2,15-dimethyl-14-oxotetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic	C19H30O7S	M+H	403.1785	-0.7
	HMDB0154858	[(2S,15S)-8,17-dihydroxy-2,15-dimethyl-14-oxotetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic	C19H30O7S	M+H	403.1785	-0.7
	HMDB0154860	[(2R,15S)-17-hydroxy-2-(hydroxymethyl)-15-methyl-14-oxotetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C19H30O7S	M+H	403.1785	-0.7
	HMDB0154861	[(2S,15S)-17-hydroxy-15-(hydroxymethyl)-2-methyl-14-oxotetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C19H30O7S	M+H	403.1785	-0.7
	HMDB0156622	[(2R,15R)-8,13-dihydroxy-2,15-dimethyl-3-oxotetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic	C19H30O7S	M+H	403.1785	-0.7
	HMDB0156623	[(2S,15R)-13-hydroxy-2-(hydroxymethyl)-15-methyl-3-oxotetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C19H30O7S	M+H	403.1785	-0.7
	HMDB0156624	[(2S,15S)-13-hydroxy-15-(hydroxymethyl)-2-methyl-3-oxotetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic	C19H30O7S	M+H	403.1785	-0.7
	HMDB0159868	[(2R,15S)-13,14,17-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-yl]oxidanesulfonic acid	C19H30O7S	M+H	403.1785	-0.7
	HMDB0164473	{[1-(4-hydroxy-3-methoxyphenyl)-3-oxododecan-5-yl]oxy}sulfonic acid	C19H30O7S	M+H	403.1785	-0.7
	HMDB0154857	[(2S,15S)-5-hydroxy-15-(hydroxymethyl)-2-methyl-14-oxotetracyclo[8.7.,heptadecan-9-yl]oxidanesulfonic	C19H30O7S	M+H	403.1785	-0.7
	HMDB0154853	[(2R,15S)-9-hydroxy-2-(hydroxymethyl)-15-methyl-14-oxotetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C19H30O7S	M+H	403.1785	-0.7
	HMDB0154854	[(2R,15S)-5-hydroxy-2-(hydroxymethyl)-15-methyl-14-oxotetracyclo[8.7.,heptadecan-9-yl]oxidanesulfonic acid	C19H30O7S	M+H	403.1785	-0.7
	HMDB0154856	[(2S,15S)-9-hydroxy-15-(hydroxymethyl)-2-methyl-14-oxotetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic	C19H30O7S	M+H	403.1785	-0.7
	HMDB0154851	[(2S,15S)-5,13-dihydroxy-2,15-dimethyl-14-oxotetracyclo[8.7.,heptadecan-9-yl]oxidanesulfonic	C19H30O7S	M+H	403.1785	-0.7

	HMDB0154850	[(2S,15S)-9,13-dihydroxy-2,15-dimethyl-14-oxotetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic	C19H30O7S	M+H	403.1785	-0.7
	HMDB0154848	[(2R,15S)-5,8-dihydroxy-2,15-dimethyl-14-oxotetracyclo[8.7.,heptadecan-9-yl]oxidanesulfonic	C19H30O7S	M+H	403.1785	-0.7
	HMDB0154847	[(2R,15S)-8,9-dihydroxy-2,15-dimethyl-14-oxotetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic	C19H30O7S	M+H	403.1785	-0.7
	HMDB0164472	[4-(5-hydroxy-3-oxododecyl)-2-methoxyphenyl]oxidanesulfonic acid	C19H30O7S	M+H	403.1785	-0.7
403.2319	HMDB0034159	Acetyl tributyl citrate	C20H34O8	M+H	403.2326	-1.8
	HMDB0159620	3,4,5-trihydroxy-6-[(5E)-tetradec-5-enoyloxy]oxane-2-carboxylic acid	C20H34O8	M+H	403.2326	-1.8
	HMDB0159809	3,4,5-trihydroxy-6-[(5Z)-tetradec-5-enoyloxy]oxane-2-carboxylic acid	C20H34O8	M+H	403.2326	-1.8
	HMDB0176329	6-(1,3-dioxotetradecan-2-yl)-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H34O8	M+H	403.2326	-1.8
404.3877	HMDB0154868	(1R,2S,11R,15R)-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-9-en-5-ol	C27H46O	M+NH4	404.3887	-2.4
	HMDB0000871	5alpha-Cholestanone	C27H46O	M+NH4	404.3887	-2.4
	HMDB0001170	Lathosterol	C27H46O	M+NH4	404.3887	-2.4
	HMDB0006841	5alpha-Cholest-8-en-3beta-ol	C27H46O	M+NH4	404.3887	-2.4
	HMDB0011182	5-L-Glutamyl-L-tyrosine	C27H46O	M+NH4	404.3887	-2.4
	HMDB0029815	Doristerol	C27H46O	M+NH4	404.3887	-2.4
	HMDB0000067	Cholesterol	C27H46O	M+NH4	404.3887	-2.4
	HMDB0062453	Cholesterol	C27H46O	M+NH4	404.3887	-2.4
	HMDB0185228	Cholesterol	C27H46O	M+NH4	404.3887	-2.4
	HMDB0059604	5-beta-Cholestan-3-one	C27H46O	M+NH4	404.3887	-2.4
	HMDB0160587	SCHEMBL13225924	C27H46O	M+NH4	404.3887	-2.4
405.1568	HMDB0180114	(4-[(9-hydroxy-8-methylnonanoyl)oxy]methyl)-2-methoxyphenyl]oxidanesulfonic acid	C18H28O8S	M+H	405.1578	-2.4
	HMDB0180124	(2-hydroxy-6-methoxy-4-[(8-methylnonanoyl)oxy]methyl)phenyl]oxidanesulfonic acid	C18H28O8S	M+H	405.1578	-2.4
	HMDB0180118	(1-[(4-hydroxy-3-methoxyphenyl)methoxy]-8-methyl-1-oxononan-2-yl)oxy)sulfonic acid	C18H28O8S	M+H	405.1578	-2.4
	HMDB0180115	(9-[(4-hydroxy-3-methoxyphenyl)methoxy]-2-methyl-9-oxononyl)oxy)sulfonic acid	C18H28O8S	M+H	405.1578	-2.4
	HMDB0180112	(4-[(8-hydroxy-8-methylnonanoyl)oxy]methyl)-2-methoxyphenyl]oxidanesulfonic acid	C18H28O8S	M+H	405.1578	-2.4
	HMDB0180117	(4-[(2-hydroxy-8-methylnonanoyl)oxy]methyl)-2-methoxyphenyl]oxidanesulfonic acid	C18H28O8S	M+H	405.1578	-2.4
405.3135	HMDB0001093	5a-Cholesta-8,24-dien-3-one	C27H42O	M+Na	405.3128	1.8
	HMDB0154864	(1S,2R,11R,15R)-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadeca-7,9-dien-5-one	C27H42O	M+Na	405.3128	1.8
	HMDB0002394	Cholesta-4,6-dien-3-one	C27H42O	M+Na	405.3128	1.8
	HMDB0003896	7-Dehydrodesmosterol	C27H42O	M+Na	405.3128	1.8
	HMDB0184839	(1S,2R,S,11S,15R)-2,15-dimethyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadec-7-en-5-one	C27H42O	M+Na	405.3128	1.8
406.1559	HMDB0166021	6-[(1,3,4,5,6,7-hexahydroxyheptan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H24O13	M+NH4	406.1555	1.0
	HMDB0166022	6-[(1,2,4,5,6,7-hexahydroxyheptan-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H24O13	M+NH4	406.1555	1.0
	HMDB0166020	6-[(2,3,4,5,6,7-hexahydroxyheptyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H24O13	M+NH4	406.1555	1.0
	HMDB0166023	6-[(1,2,3,5,6,7-hexahydroxyheptan-4-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H24O13	M+NH4	406.1555	1.0
	HMDB0005021	Quetiapine	C21H25N3O2S	M+Na	406.1560	-0.2
408.1339	HMDB0149477	{[1-methyl-6-(methyloxidaniumylidene)-2-oxo-4,5-diphenylpiperidin-1-ium-3-yl]oxy}trioxo-4,5-sulfanuide	C19H20NO6S	M+NH4	408.1344	-1.2
	HMDB0062742	12alpha-hydroxy-3-oxo-5beta-cholan-24-oic acid	C24H38O4	M+NH4	408.3108	-1.8
	HMDB0156541	5-hydroxy-4-[(1S,2R,S,11S,15S)-5-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8

408.3101

HMDB0156542	4-[(1S,2R,S,11S,15R)-5,17-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0156546	4-hydroxy-4-[(1S,2R,S,11S,15S)-5-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0156545	4-[(1S,2R,R,11S,15S)-5-hydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0156544	4-[(1S,2S,S,11S,15R)-5-hydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0156543	4-[(1S,2R,S,11S,15S)-5,13-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0156548	4-[(1S,2R,S,11S,15R)-5,9-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0156547	4-[(1S,2R,S,11S,15R)-5,6-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0159759	4-[(1S,2S,7R,R,11S,15S)-5,9-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-yl]pent-4-enoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0159760	4-[(1S,2S,7S,11S,14R,15R)-5-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0160999	4-[(1S,2R,S,11S,15R)-5-hydroxy-2,15-dimethyl-8-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0184494	4-[(2R,15R)-8-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0184495	4-[(2S,15S)-13-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0184497	4-[(2S,15S)-15-(hydroxymethyl)-2-methyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0184496	4-[(2S,15R)-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]-5-hydroxypentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0184498	4-[(2R,15R)-2-(hydroxymethyl)-15-methyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0184499	4-[(2S,15S)-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]-4-hydroxypentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0062796	7alpha-hydroxy-3-oxo-5beta-cholan-24-oic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0000503	7alpha-hydroxy-3-oxo-5beta-cholan-24-oic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0159748	4-[(1S,2S,7R,11S,15R)-5-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0159167	4-[(1S,2S,R,11S,15R)-9-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0157446	4-[(1S,2S,7S,R,11S,15R)-16-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0157455	4-[(1S,2S,7S,R,11S,15S)-5,16-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-yl]pent-4-enoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0157686	4-[(1S,2S,7S,R,11S,15S)-5,9-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-yl]pent-4-enoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0158251	4-[(2S,15S)-13-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0158250	4-[(2R,15R)-8-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0158255	4-[(2S,15S)-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]-4-hydroxypentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
HMDB0158253	4-[(2S,15S)-15-(hydroxymethyl)-2-methyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8

	HMDB0158254	4-[(2R,15R)-2-(hydroxymethyl)-15-methyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
	HMDB0158252	4-[(2S,15S)-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]-5-hydroxypentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
	HMDB0158257	4-[(2R,15R)-6-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
	HMDB0158256	4-[(2S,15R)-4-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+NH4	408.3108	-1.8
	HMDB0158273	4-[(2S,15S)-5,17-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-yl]pent-4-enoic acid	C24H38O4	M+NH4	408.3108	-1.8
	HMDB0158772	4-[(1S,2S,7R,R,11S,15S)-5,16-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-yl]pent-4-enoic acid	C24H38O4	M+NH4	408.3108	-1.8
	HMDB0000328	12-Ketodeoxycholic acid	C24H38O4	M+NH4	408.3108	-1.8
	HMDB0000460	7-Hydroxy-3-oxocholanoic acid	C24H38O4	M+NH4	408.3108	-1.8
	HMDB0000467	Nutriacholic acid	C24H38O4	M+NH4	408.3108	-1.8
	HMDB0041454	D8'-Merulinic acid A	C24H38O4	M+NH4	408.3108	-1.8
	HMDB0012866	9'-Carboxy-alpha-chromanol	C24H38O4	M+NH4	408.3108	-1.8
409.0561	HMDB0179773	6-{1-carboxy-2-[5-(prop-1-yn-1-yl)thiophen-2-yl]ethoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H18O9S	M+Na	409.0564	-0.7
	HMDB0179772	3,4,5-trihydroxy-6-({3-[1-oxo-5-(prop-1-yn-1-yl)-1-yl]thiophen-2-yl}propanoyl)oxy)oxane-2-carboxylic acid	C16H18O9S	M+Na	409.0564	-0.7
	HMDB0179774	3,4,5-trihydroxy-6-({2-hydroxy-3-[5-(prop-1-yn-1-yl)thiophen-2-yl]propanoyl}oxy)oxane-2-carboxylic acid	C16H18O9S	M+Na	409.0564	-0.7
	HMDB0179770	3,4,5-trihydroxy-6-({3-hydroxy-3-[5-(prop-1-yn-1-yl)thiophen-2-yl]propanoyl}oxy)oxane-2-carboxylic acid	C16H18O9S	M+Na	409.0564	-0.7
	HMDB0179769	6-{2-carboxy-1-[5-(prop-1-yn-1-yl)thiophen-2-yl]ethoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H18O9S	M+Na	409.0564	-0.7
	HMDB0166967	3,4,5-trihydroxy-6-({[(5E)-5-[(5-methylthiophen-2-yl)methylidene]-2-oxooxolan-3-yl]oxy}oxane-2-carboxylic acid	C16H18O9S	M+Na	409.0564	-0.7
	HMDB0166965	3,4,5-trihydroxy-6-[(5-{[(2E)-5-oxooxolan-2-ylidene]methyl}thiophen-2-yl)methoxy]oxane-2-carboxylic acid	C16H18O9S	M+Na	409.0564	-0.7
	HMDB0127836	{[1-(3-hydroxy-4-methoxyphenyl)-3-(2,4,6-trihydroxyphenyl)propan-2-yl]oxy}sulfonic acid	C16H18O9S	M+Na	409.0564	-0.7
	HMDB0127835	{5-[2-hydroxy-3-(2,4,6-trihydroxyphenyl)propyl]-2-methoxyphenyl}oxidanesulfonic acid	C16H18O9S	M+Na	409.0564	-0.7
	HMDB0127773	{4-[2-hydroxy-3-(2,4,6-trihydroxyphenyl)propyl]-2-methoxyphenyl}oxidanesulfonic acid	C16H18O9S	M+Na	409.0564	-0.7
	HMDB0127774	{[1-(4-hydroxy-3-methoxyphenyl)-3-(2,4,6-trihydroxyphenyl)propan-2-yl]oxy}sulfonic acid	C16H18O9S	M+Na	409.0564	-0.7
410.0542	HMDB0036354	1-Pentenyl glucosinolate	C12H21NO9S ₂	M+Na	410.0550	-1.9
	HMDB0038417	4-Pentenylglucosinolate	C12H21NO9S ₂	M+Na	410.0550	-1.9
	HMDB0137712	5-hydroxy-2-({1-hydroxy-3-[3-(sulfooxy)phenyl]prop-2-en-1-ylidene}amino)-4-methoxybenzoic acid	C17H15NO9S	M+H	410.0540	0.4
	HMDB0170914	{4-[1,3-dihydroxy-4-(4-hydroxyphenyl)-2,5-dioxocyclopent-3-en-1-yl]phenyl}oxidanesulfonic acid	C17H12O9S	M+NH4	410.0540	0.4
	HMDB0170936	{4-[3-hydroxy-3-(4-hydroxyphenyl)-2,4,5-trioxocyclopentyl]phenyl}oxidanesulfonic acid	C17H12O9S	M+NH4	410.0540	0.4
	HMDB0170937	{4-[1-hydroxy-3-(4-hydroxyphenyl)-2,4,5-trioxocyclopentyl]phenyl}oxidanesulfonic acid	C17H12O9S	M+NH4	410.0540	0.4
	HMDB0170904	{2-hydroxy-5-[2-hydroxy-4-(4-hydroxyphenyl)-3,5-dioxocyclopent-1-en-1-yl]phenyl}oxidanesulfonic acid	C17H12O9S	M+NH4	410.0540	0.4
	HMDB0170909	{2-hydroxy-5-[3-hydroxy-4-(4-hydroxyphenyl)-2,5-dioxocyclopent-3-en-1-yl]phenyl}oxidanesulfonic acid	C17H12O9S	M+NH4	410.0540	0.4
	HMDB0170932	{2-hydroxy-5-[3-(4-hydroxyphenyl)-2,4,5-trioxocyclopentyl]phenyl}oxidanesulfonic acid	C17H12O9S	M+NH4	410.0540	0.4

	HMDB0170913	{4-[2,4-dihydroxy-4-(4-hydroxyphenyl)-3,5-dioxocyclopent-1-en-1-yl]phenyl}oxidanesulfonic acid	C17H12O9S	M+NH4	410.0540	0.4
	HMDB0170918	{4-[3-(2,4-dihydroxyphenyl)-4-hydroxy-2,5-dioxocyclopent-3-en-1-yl]phenyl}oxidanesulfonic acid	C17H12O9S	M+NH4	410.0540	0.4
410.2530	HMDB0062274	(4Z,7Z,S,11E)--hydroperoxy-12-[(1R,4S,5S,6R)-6-[(2Z)-pent-2-en-1-yl]-2,3-dioxabicyclo[2.2.1]heptan-5-yl]dodeca-4,7,11-trienoic acid	C22H32O6	M+NH4	410.2537	-1.7
	HMDB0062282	3-[(1R,4S,5S,6R)-6-[(1E,3S,5Z,8Z,11Z)-3-hydroperoxytetradeca-1,5,8,11-tetraen-1-yl]-2,3-dioxabicyclo[2.2.1]heptan-5-yl]propanoic acid	C22H32O6	M+NH4	410.2537	-1.7
	HMDB0062292	14-Hydroperoxy-H4-neuroprostane	C22H32O6	M+NH4	410.2537	-1.7
	HMDB0034662	Dihydrofukinolide	C22H32O6	M+NH4	410.2537	-1.7
412.2573	HMDB0159726	[(1S,2S,7R,R,11S,15R)-14-(4-carboxybutan-2-yl)-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-9-yl]oxidanyl	C24H37O4	M+Na	412.2584	-2.7
412.2850	HMDB0015648	Fesoterodine	C26H37NO3	M+H	412.2846	0.9
413.2655	HMDB0062742	12alpha-hydroxy-3-oxo-5beta-cholan-24-oic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0156541	5-hydroxy-4-[(1S,2R,S,11S,15S)-5-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0156542	4-[(1S,2R,S,11S,15R)-5,17-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0156545	4-[(1S,2R,R,11S,15S)-5-hydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0156546	4-hydroxy-4-[(1S,2R,S,11S,15S)-5-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0156544	4-[(1S,2S,S,11S,15R)-5-hydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0156543	4-[(1S,2R,S,11S,15S)-5,13-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0156548	4-[(1S,2R,S,11S,15R)-5,9-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0156547	4-[(1S,2R,S,11S,15R)-5,6-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0159759	4-[(1S,2S,7R,R,11S,15S)-5,9-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-yl]pent-4-enoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0159760	4-[(1S,2S,7S,11S,14R,15R)-5-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0160999	4-[(1S,2R,S,11S,15R)-5-hydroxy-2,15-dimethyl-8-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0184494	4-[(2R,15R)-8-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0184495	4-[(2S,15S)-13-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0184497	4-[(2S,15S)-15-(hydroxymethyl)-2-methyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0184496	4-[(2S,15R)-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]-5-hydroxypentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0184498	4-[(2R,15R)-2-(hydroxymethyl)-15-methyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0184499	4-[(2S,15S)-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]-4-hydroxypentanoic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0062796	7alpha-hydroxy-3-oxo-5beta-cholan-24-oic acid	C24H38O4	M+Na	413.2662	-1.8
	HMDB0000503	7alpha-hydroxy-3-oxo-5beta-cholan-24-oic acid	C24H38O4	M+Na	413.2662	-1.8

HMDB0159748	4-[(1S,2S,7R,11S,15R)-5-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0159167	4-[(1S,2S,R,11S,15R)-9-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0157446	4-[(1S,2S,7S,R,11S,15R)-16-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0157455	4-[(1S,2S,7S,R,11S,15S)-5,16-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-yl]pent-4-enoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0157686	4-[(1S,2S,7S,R,11S,15S)-5,9-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-yl]pent-4-enoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0158251	4-[(2S,15S)-13-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0158250	4-[(2R,15R)-8-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0158253	4-[(2S,15S)-15-(hydroxymethyl)-2-methyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0158255	4-[(2S,15S)-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]-4-hydroxypentanoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0158252	4-[(2S,15S)-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]-5-hydroxypentanoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0158254	4-[(2R,15R)-2-(hydroxymethyl)-15-methyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0158257	4-[(2R,15R)-6-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0158256	4-[(2S,15R)-4-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0158273	4-[(2S,15S)-5,17-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-yl]pent-4-enoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0158772	4-[(1S,2S,7R,R,11S,15S)-5,16-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-yl]pent-4-enoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0000328	12-Ketodeoxycholic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0000460	7-Hydroxy-3-oxocholanoic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0000467	Nutriacholic acid	C24H38O4	M+Na	413.2662	-1.8
HMDB0041454	D8'-Merulinic acid A	C24H38O4	M+Na	413.2662	-1.8
HMDB0012866	9'-Carboxy-alpha-chromanol	C24H38O4	M+Na	413.2662	-1.8
HMDB0031689	1-Hexanol arabinosylglucoside	C17H32O10	M+NH4	414.2334	-1.9
HMDB0148762	5-hydroxy-4-(4-hydroxypentyl)-8,8-dimethyl-6-(3-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+H	415.2115	-2.7
HMDB0147026	5-hydroxy-4-(5-hydroxypentyl)-8,8-dimethyl-6-(2-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+H	415.2115	-2.7
HMDB0147023	8-hydroxy-12,12-dimethyl-9-(2-methylbutanoyl)-6-pentyl-3,11,14-trioxatetracyclo[8.5.,pentadeca-1,5,7,9-tetraen-4-one	C24H30O6	M+H	415.2115	-2.7
HMDB0148759	5-hydroxy-8-(hydroxymethyl)-8-methyl-6-(3-methylbutanoyl)-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+H	415.2115	-2.7
HMDB0147024	5-hydroxy-6-(4-hydroxy-2-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+H	415.2115	-2.7
HMDB0147025	5-hydroxy-6-[2-(hydroxymethyl)butanoyl]-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+H	415.2115	-2.7
HMDB0147021	5-hydroxy-6-(3-hydroxy-2-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+H	415.2115	-2.7
HMDB0147022	5-hydroxy-4-(4-hydroxypentyl)-8,8-dimethyl-6-(2-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+H	415.2115	-2.7
HMDB0147020	5-hydroxy-6-(2-hydroxy-2-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+H	415.2115	-2.7
HMDB0147019	5-hydroxy-4-(1-hydroxypentyl)-8,8-dimethyl-6-(2-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+H	415.2115	-2.7

415.2104	HMDB0147018	5-hydroxy-8-(hydroxymethyl)-8-methyl-6-(2-methylbutanoyl)-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0148760	5-hydroxy-4-(1-hydroxypentyl)-8,8-dimethyl-6-(3-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0148761	5-hydroxy-6-(3-hydroxy-3-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0148763	8-hydroxy-12,12-dimethyl-9-(3-methylbutanoyl)-6-pentyl-3,11,14-trioxatetracyclo[8.5.,pentadeca-1,5,7,9-tetraen-4-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0168750	7-{[(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-5-hydroxy-2H-chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0168748	7-{[(2E,6Z)-9-(3,3-dimethyloxiran-2-yl)-5,8-dihydroxy-3,7-dimethylnona-2,6-dien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0168747	7-{[(2E)-5-hydroxy-5-[3-(1-hydroxy-4-methylpent-3-en-1-yl)-3-methyloxiran-2-yl]-3-methylpent-2-en-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0168749	7-{[(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-8-hydroxy-2H-chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0168746	7-({3-[(3Z)-2,5-dihydroxy-4,8-dimethylnona-3,7-dien-1-yl]-3-methyloxiran-2-yl}methoxy)-2H-chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0168744	7-{[(2E,6Z,E)-5,8,12-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0168745	7-{[(2E,6Z)-5,8,9-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0168743	7-{[(2E,6Z)-5,8,12-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0168742	7-{[(2E,6Z)-5,8-dihydroxy-7-(hydroxymethyl)-3,11-dimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0168740	7-{[(2E,6Z)-4,5,8-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0168739	7-{[(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-6-hydroxy-2H-chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0168741	7-{[(2Z,6Z)-5,8-dihydroxy-3-(hydroxymethyl)-7,11-dimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0148765	5-hydroxy-4-(5-hydroxypentyl)-8,8-dimethyl-6-(3-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0148764	5-hydroxy-6-(4-hydroxy-3-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+H	415.2115	-2.7
	HMDB0037039	4-O-Methylmelleolide	C24H30O6	M+H	415.2115	-2.7
	HMDB0030404	Armillaripin	C24H30O6	M+H	415.2115	-2.7
416.2470	HMDB0039380	Armillarin	C24H30O6	M+H	415.2115	-2.7
	HMDB0041407	Clausarinol	C24H30O6	M+H	415.2115	-2.7
	HMDB0014838	Eplerenone	C24H30O6	M+H	415.2115	-2.7
416.2470	HMDB0173670	{14-acetyl-2,15-dimethyltetracyclo[8.7.,]heptadecan-5-yl}oxidanesulfonic acid	C21H34O5S	M+NH4	416.2465	1.2
	HMDB0240590	SCHEMBL782131	C21H34O5S	M+NH4	416.2465	1.2
	HMDB0240591	SCHEMBL4191973	C21H34O5S	M+NH4	416.2465	1.2
	HMDB0172273	2-(8,12-dimethyl-4-methylidenetridecyl)-2,7-dimethyl-3,4-dihydro-2H-1-benzopyran-6-ol	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0174260	14-(1-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-9-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0174261	17-hydroxy-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-9-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0174262	8-hydroxy-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-9-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0174265	2-(hydroxymethyl)-15-methyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-9-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0174264	15-(hydroxymethyl)-2-methyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-9-en-5-one	C27H44O2	M+NH4	418.3680	-2.5

HMDB0174263	13-hydroxy-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-9-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
HMDB0174267	14-(6-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-9-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
HMDB0174266	14-(2-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-9-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
HMDB0172275	2,7-dimethyl-2-(4,8,12-trimethyltridec-12-en-1-yl)-3,4-dihydro-2H-1-benzopyran-6-ol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0172274	2-(4,12-dimethyl-8-methylidenetridecyl)-2,7-dimethyl-3,4-dihydro-2H-1-benzopyran-6-ol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0155087	(2R,15R)-14-(7-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
HMDB0154867	(1S,2R,11R,15R)-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadeca-7,9-diene-5,17-diol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0154866	(1S,2R,11R,15R)-14-(1-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadeca-7,9-dien-5-ol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0155080	(2R,15S)-13-hydroxy-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
HMDB0155082	(2S,15R)-2-(hydroxymethyl)-15-methyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
HMDB0155081	(2R,15S)-14-(1-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
HMDB0155083	(2R,15S)-15-(hydroxymethyl)-2-methyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
HMDB0155084	(2R,15R)-14-(6-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
HMDB0155085	SCHEMBL141218	C27H44O2	M+NH4	418.3680	-2.5
HMDB0155086	(2R,15R)-9-hydroxy-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
HMDB0174268	14-(7-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-9-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
HMDB0184144	(2S,15S)-14-(1-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
HMDB0184848	(1S,2R,S,11S,15R)-14-(7-hydroxy-6-methylhept-5-en-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-ol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0184845	(1S,2R,R,11S,15S)-15-(hydroxymethyl)-2-methyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadec-7-en-5-ol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0184846	(1S,2R,S,11S,15S)-14-(2-hydroxy-6-methylhept-5-en-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-ol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0184847	(1S,2R,S,11S,15R)-2,15-dimethyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadec-7-ene-5,6-diol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0184850	(1S,2R,S,11S,15R)-14-(4-hydroxy-6-methylhept-5-en-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-ol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0184851	(1S,2R,S,11S,15R)-14-[4-(3,3-dimethylloxiran-2-yl)butan-2-yl]-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-ol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0184849	(1S,2R,S,11S,15R)-2,15-dimethyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadec-7-ene-5,9-diol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0185578	(2R)-2,8-dimethyl-2-(4,8,12-trimethyltridec-12-en-1-yl)-3,4-dihydro-2H-1-benzopyran-6-ol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0185577	(2R)-2-(4,12-dimethyl-8-methylidenetridecyl)-2,8-dimethyl-3,4-dihydro-2H-1-benzopyran-6-ol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0184841	(1S,2R,S,11S,15S)-14-(1-hydroxy-6-methylhept-5-en-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-ol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0184844	(1S,2S,S,11S,15R)-2-(hydroxymethyl)-15-methyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadec-7-en-5-ol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0184842	(1S,2R,S,11S,15R)-2,15-dimethyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadec-7-ene-5,17-diol	C27H44O2	M+NH4	418.3680	-2.5
HMDB0184143	(2S,15S)-13-hydroxy-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
HMDB0184147	(2S,15R)-14-(6-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+NH4	418.3680	-2.5

	HMDB0184145	(2R,15R)-2-(hydroxymethyl)-15-methyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0184146	(2S,15S)-15-(hydroxymethyl)-2-methyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0184148	(2S,15S)-14-(2-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0184149	(R,14R)-,14-dimethyl-15-(6-methylheptan-2-yl)-3-oxapentacyclo[9.7.??]octadecan-7-one	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0184150	(2S,15R)-14-(7-hydroxy-6-methylheptan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0184168	(2S,15R)-17-hydroxy-2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-8-en-5-one	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0184843	(1S,2R,S,11S,15S)-2,15-dimethyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadec-7-ene-5,13-diol	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0185576	(2R)-2-(8,12-dimethyl-4-methylidenetriacyl)-2,8-dimethyl-3,4-dihydro-2H-1-benzopyran-6-ol	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0003550	Calcidiol	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0060132	27alpha-Hydroxy-8-dehydrocholesterol	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0060131	3beta-Hydroxy-5-cholestenal	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0015504	Alfacalcidol	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0000501	7-Ketocholesterol	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0001993	7a-Hydroxy-cholestene-3-one	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0006722	25-Hydroxytachysterol3	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0006721	5,6-trans-25-Hydroxyvitamin D3	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0035585	1-Phenyl-1,3-heneicosanedione	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0034328	(3beta,5alpha,6a)-Cholesta-8,14-diene-3,6-diol	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0036012	5-Methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone	C27H44O2	M+NH4	418.3680	-2.5
	HMDB0039871	5-(12,15-Heneicosadienyl)-1,3-benzenediol	C27H44O2	M+NH4	418.3680	-2.5
419.3147	HMDB0187189	[(1S,2S,R,11S,14S,15R,17R,23S)-,14,16,-tetramethyl-22-azaheptacyclo[12.,??]tetracos-4-en-7-yl]oxidanyl	C27H42NO	M+Na	419.3159	-2.8
	HMDB0039317	Hexadecyl ferulate	C26H42O4	M+H	419.3156	-2.1
	HMDB0012515	11'-Carboxy-alpha-chromanol	C26H42O4	M+H	419.3156	-2.1
422.0348	HMDB0000295	Uridine 5'-diphosphate	C9H14N2O12P2	M+NH4	422.0360	-2.9
	HMDB0156308	UDP - Na	C9H14N2O12P2	M+NH4	422.0360	-2.9
	HMDB0185420	3-[(2-aminophenyl)sulfanyl]-3-(4-methoxyphenyl)-2-(sulfooxy)propanoic acid	C16H17NO7S2	M+Na	422.0339	2.2
428.0360	HMDB0001341	ADP	C10H15N5O10P2	M+H	428.0367	-1.6
	HMDB0160059	ADP	C10H15N5O10P2	M+H	428.0367	-1.6
	HMDB0000061	Adenosine 3',5'-diphosphate	C10H15N5O10P2	M+H	428.0367	-1.6
	HMDB0000960	dGDP	C10H15N5O10P2	M+H	428.0367	-1.6
429.2392	HMDB0015119	Nandrolone phenpropionate	C27H34O3	M+Na	429.2400	-1.9
	HMDB0015163	Irbesartan	C25H28N6O	M+H	429.2397	-1.2
	HMDB0177927	3,4,5-trihydroxy-6-({4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3-methyl-2,4,5,6,7,7a-hexahydro-1H-inden-7-yl}methoxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
	HMDB0179237	3,4,5-trihydroxy-6-([2-(hydroxymethyl)-1,1,5-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-yl]oxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
	HMDB0179236	3,4,5-trihydroxy-6-([2-hydroxy-1,1,5-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-yl]methoxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
	HMDB0179240	3,4,5-trihydroxy-6-([5-(hydroxymethyl)-1,1,2-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-yl]oxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2

HMDB0179239	3,4,5-trihydroxy-6-({2-hydroxy-1,1,2-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-5-yl}methoxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0179243	3,4,5-trihydroxy-6-({4-hydroxy-1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-yl}oxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0179242	3,4,5-trihydroxy-6-({2-hydroxy-1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-4-yl}oxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0179245	3,4,5-trihydroxy-6-({2-hydroxy-1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-6-yl}oxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0179248	3,4,5-trihydroxy-6-({2-hydroxy-1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-3-yl}oxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0179249	3,4,5-trihydroxy-6-({3-hydroxy-1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-yl}oxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0179234	3,4,5-trihydroxy-6-{{1-(hydroxymethyl)-1,2,5-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-yl}oxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0179233	3,4,5-trihydroxy-6-({2-hydroxy-1,2,5-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-1-yl}methoxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0177931	3,4,5-trihydroxy-6-({4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-7-yl}oxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0177932	3,4,5-trihydroxy-6-{{[(2E)-3-(7-hydroxy-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl)-2-methylprop-2-en-1-yl]oxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0177935	6-[(2E)-2-[(3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl)methylidene]-3-hydroxypropoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0177934	6-[(2Z)-2-[(3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl)methylidene]-3-hydroxypropoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0177939	3,4,5-trihydroxy-6-{{[(2E)-3-(2-hydroxy-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl)-2-methylprop-2-en-1-yl]oxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0177938	3,4,5-trihydroxy-6-({4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-2-yl}oxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0177943	3,4,5-trihydroxy-6-{{[(2E)-3-(1-hydroxy-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl)-2-methylprop-2-en-1-yl]oxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0177942	3,4,5-trihydroxy-6-({4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-1-yl}oxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0177946	6-{{[3-(3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl)-2-methyloxiran-2-yl]methoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0179246	3,4,5-trihydroxy-6-({6-hydroxy-1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-yl}oxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0179252	6-({7a-hydroxy-1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0179251	3,4,5-trihydroxy-6-({2-hydroxy-1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-7a-yl}oxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2

430.2426

HMDB0182106	6-[[{(3Z)-1-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]}-5-hydroxy-4-methylpent-3-en-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0182110	3,4,5-trihydroxy-6-({7-[(3Z)-5-hydroxy-4-methylpent-3-en-1-yl]-1,7-dimethyltricyclo[2.2.1,heptan-3-yl]oxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0182107	6-[[{(2Z)-5-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]}-4-hydroxy-2-methylpent-2-en-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0182111	3,4,5-trihydroxy-6-{{(2Z)-5-{5-hydroxy-2,3-dimethyltricyclo[2.2.1,heptan-3-yl]}-2-methylpent-2-en-1-yl]oxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0182114	6-{{3-(2-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]ethyl}-2-methyloxiran-2-yl)methoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0182118	3,4,5-trihydroxy-6-({3-[(3Z)-5-hydroxy-4-methylpent-3-en-1-yl]-2,3-dimethyltricyclo[2.2.1,heptan-1-yl]oxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0182119	3,4,5-trihydroxy-6-{{(2Z)-5-{1-hydroxy-2,3-dimethyltricyclo[2.2.1,heptan-3-yl]}-2-methylpent-2-en-1-yl]oxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0182324	3,4,5-trihydroxy-6-{{-methyl-8-oxo-2-(prop-1-en-2-yl)spiro[4.5]decan-6-yl}methoxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0183508	6-{{(8aR)-4-hydroxy-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0182103	6-[(2Z)-2-(3-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]propylidene)-3-hydroxypropoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0182099	6-[[{(2Z)-5-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]}-5-hydroxy-2-methylpent-2-en-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0179253	3,4,5-trihydroxy-6-({7-hydroxy-1,1,4,7-tetramethyl-1H,1aH,2H,3H,5H,6H,7H,7aH,7bH-cyclopropa[e]azulen-7b-yl]oxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0179254	6-({7b-hydroxy-1,1,4,7-tetramethyl-1H,1aH,2H,3H,5H,6H,7H,7aH,7bH-cyclopropa[e]azulen-7-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0179283	3,4,5-trihydroxy-6-{{1-methyl-4-(6-methyl-4-oxohept-5-en-2-yl)cyclohex-2-en-1-yl]oxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0182090	3,4,5-trihydroxy-6-({7-[(3Z)-5-hydroxy-4-methylpent-3-en-1-yl]-7-methyltricyclo[2.2.1,heptan-1-yl]methoxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0182094	3,4,5-trihydroxy-6-({3-[(3Z)-5-hydroxy-4-methylpent-3-en-1-yl]-2-methyltricyclo[2.2.1,heptan-3-yl]methoxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0182091	3,4,5-trihydroxy-6-{{(2Z)-5-[2-(hydroxymethyl)-3-methyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-en-1-yl]oxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0182095	3,4,5-trihydroxy-6-{{(2Z)-5-[3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-en-1-yl]oxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0182098	6-[[{(3Z)-1-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]}-5-hydroxy-4-methylpent-3-en-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0182102	6-[(2E)-2-(3-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]propylidene)-3-hydroxypropoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0183507	6-{{(4aR)-3-hydroxy-4,4a-dimethyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalen-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2

HMDB0177928	3,4,5-trihydroxy-6-{{(2E)-3-[7-(hydroxymethyl)-3-methyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl]-2-methylprop-2-en-1-yl]oxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0030082	5-(2,3-Dihydroxy-3-methylbutyl)-4-(3,4-epoxy-4-methylpentanoyl)-3,4-dihydroxy-2-isopentanoyl-2-cyclopenten-1-one	C21H32O8	M+NH4	430.2435	-2.2
HMDB0039636	Abscisic alcohol 11-glucoside	C21H32O8	M+NH4	430.2435	-2.2
HMDB0137926	6-[(5-formyl-1,1,4a-trimethyl-6-methylidene-decahydronaphthalen-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0150712	6-[(2,5,5,8a-tetramethyl-6-oxo-1,4,4a,5,6,7,8,8a-octahydronaphthalen-1-yl)methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0163089	3,4,5-trihydroxy-6-({2,2,4-trimethyl-3-[(3Z)-3-methyl-5-oxopent-3-en-1-yl]cyclohex-3-en-1-yl}oxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0166726	6-[2,6-di-tert-butyl-4-(hydroxymethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0166729	6-(2,4-di-tert-butyl-3-hydroxy-6-methylphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0166730	6-(2,6-di-tert-butyl-3-hydroxy-4-methylphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0166731	6-[2-tert-butyl-6-(1-hydroxy-2-methylpropan-2-yl)-4-methylphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0166734	6-[(3,5-di-tert-butyl-1-methyl-4-oxocyclohexa-2,5-dien-1-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0177924	3,4,5-trihydroxy-6-{{(2E)-3-[3-(hydroxymethyl)-7-methyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl]-2-methylprop-2-en-1-yl]oxy}oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0177923	3,4,5-trihydroxy-6-({4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-7-methyl-2,4,5,6,7,7a-hexahydro-1H-inden-3-yl}methoxy)oxane-2-carboxylic acid	C21H32O8	M+NH4	430.2435	-2.2
HMDB0036836	Cascarillin	C22H32O7	M+Na	431.2040	2.7
HMDB0036864	Anhydrocinnzeylanine	C22H32O7	M+Na	431.2040	2.7
HMDB0031673	Armillarilin	C24H30O7	M+H	431.2064	-2.9
HMDB0030815	Mammea E/BA	C24H30O7	M+H	431.2064	-2.9
HMDB0038788	Melleolide H	C24H30O7	M+H	431.2064	-2.9
HMDB0030814	Mammea E/BB	C24H30O7	M+H	431.2064	-2.9
HMDB0168750	7-[[{(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-5-hydroxy-2H-chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
HMDB0148759	5-hydroxy-8-(hydroxymethyl)-8-methyl-6-(3-methylbutanoyl)-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
HMDB0147025	5-hydroxy-6-[2-(hydroxymethyl)butanoyl]-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
HMDB0147026	5-hydroxy-4-(5-hydroxypentyl)-8,8-dimethyl-6-(2-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
HMDB0147023	8-hydroxy-12,12-dimethyl-9-(2-methylbutanoyl)-6-pentyl-3,11,14-trioxatetracyclo[8.5.,pentadeca-1,5,7,9-tetraen-4-one	C24H30O6	M+NH4	432.2381	-2.5
HMDB0147024	5-hydroxy-6-(4-hydroxy-2-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
HMDB0147022	5-hydroxy-4-(4-hydroxypentyl)-8,8-dimethyl-6-(2-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
HMDB0147021	5-hydroxy-6-(3-hydroxy-2-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
HMDB0147020	5-hydroxy-6-(2-hydroxy-2-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
HMDB0147019	5-hydroxy-4-(1-hydroxypentyl)-8,8-dimethyl-6-(2-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
HMDB0147018	5-hydroxy-8-(hydroxymethyl)-8-methyl-6-(2-methylbutanoyl)-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5

432.2370	HMDB0148763	8-hydroxy-12,12-dimethyl-9-(3-methylbutanoyl)-6-pentyl-3,11,14-trioxatetracyclo[8.5.,pentadeca-1,5,7,9-tetraen-4-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0148762	5-hydroxy-4-(4-hydroxypentyl)-8,8-dimethyl-6-(3-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0168747	7-[(2E)-5-hydroxy-5-[3-(1-hydroxy-4-methylpent-3-en-1-yl)-3-methyloxiran-2-yl]-3-methylpent-2-en-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0168748	7-[(2E,6Z)-9-(3,3-dimethyloxiran-2-yl)-5,8-dihydroxy-3,7-dimethylnona-2,6-dien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0168749	7-[(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-8-hydroxy-2H-chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0168746	7-[(3Z)-2,5-dihydroxy-4,8-dimethylnona-3,7-dien-1-yl]-3-methyloxiran-2-yl]methoxy}-2H-chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0168743	7-[(2E,6Z)-5,8,12-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0168745	7-[(2E,6Z)-5,8,9-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0168742	7-[(2E,6Z)-5,8-dihydroxy-7-(hydroxymethyl)-3,11-dimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0168744	7-[(2E,6Z,E)-5,8,12-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0168740	7-[(2E,6Z)-4,5,8-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0168739	7-[(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-6-hydroxy-2H-chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0168741	7-[(2Z,6Z)-5,8-dihydroxy-3-(hydroxymethyl)-7,11-dimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0148765	5-hydroxy-4-(5-hydroxypentyl)-8,8-dimethyl-6-(3-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0148764	5-hydroxy-6-(4-hydroxy-3-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0148761	5-hydroxy-6-(3-hydroxy-3-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0148760	5-hydroxy-4-(1-hydroxypentyl)-8,8-dimethyl-6-(3-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0037039	4-O-Methylmellecolide	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0030404	Armillaripin	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0039380	Armillarin	C24H30O6	M+NH4	432.2381	-2.5
433.2404	HMDB0041407	Clausarinol	C24H30O6	M+NH4	432.2381	-2.5
	HMDB0014838	Eplerenone	C24H30O6	M+NH4	432.2381	-2.5
433.2404	HMDB0014498	Buclizine	C28H33ClN2	M+H	433.2405	-0.2
	HMDB0144921	(12aS)-4,7-bis(dimethylamino)-3,4,,12,12a-pentahydroxy-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11-dione	C22H30N2O7	M+H	435.2126	1.7
	HMDB0145030	(12aS)-4,7-bis(dimethylamino)-3,,11a,12,12a-pentahydroxy-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11-dione	C22H30N2O7	M+H	435.2126	1.7
	HMDB0145026	(12aS)-4,7-bis(dimethylamino)-2,3,,12,12a-pentahydroxy-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11-dione	C22H30N2O7	M+H	435.2126	1.7
	HMDB0145021	N-[(4aS)--(dimethylamino)-2,4a,5,7-tetrahydroxy-4,6-dioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1-yl]-N-methylmethanamine oxide	C22H30N2O7	M+H	435.2126	1.7
	HMDB0145011	(12aS)-4,7-bis(dimethylamino)-3,5a,,12,12a-pentahydroxy-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11-dione	C22H30N2O7	M+H	435.2126	1.7

435.2133	HMDB0144941	(12aS)-4,7-bis(dimethylamino)-3,8,,12,12a-pentahydroxy-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11-dione	C22H30N2O7	M+H	435.2126	1.7
	HMDB0145001	(12aR)-4,7-bis(dimethylamino)-3,4a,,12,12a-pentahydroxy-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11-dione	C22H30N2O7	M+H	435.2126	1.7
	HMDB0144991	(12aS)-4,7-bis(dimethylamino)-3,5,,12,12a-pentahydroxy-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11-dione	C22H30N2O7	M+H	435.2126	1.7
	HMDB0144981	(12aS)-4,7-bis(dimethylamino)-3,6,,12,12a-pentahydroxy-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11-dione	C22H30N2O7	M+H	435.2126	1.7
	HMDB0144951	(12aS)-4,7-bis(dimethylamino)-3,9,,12,12a-pentahydroxy-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11-dione	C22H30N2O7	M+H	435.2126	1.7
	HMDB0154188	5-[2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)ethyl]-4,6-bis(3-methylbut-2-en-1-yl)benzene-1,3-diol	C25H32O5	M+Na	435.2142	-2.0
	HMDB0154182	5-[1-hydroxy-2-(4-hydroxy-3-methoxyphenyl)ethyl]-4,6-bis(3-methylbut-2-en-1-yl)benzene-1,3-diol	C25H32O5	M+Na	435.2142	-2.0
	HMDB0154176	5-[2-(4-hydroxy-3-methoxyphenyl)ethyl]-4-[(2E)-4-hydroxy-3-methylbut-2-en-1-yl]-6-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C25H32O5	M+Na	435.2142	-2.0
	HMDB0154195	4-[(3,3-dimethyloxiran-2-yl)methyl]-5-[2-(4-hydroxy-3-methoxyphenyl)ethyl]-6-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C25H32O5	M+Na	435.2142	-2.0
	HMDB0154200	5-[2-(2,5-dihydroxy-4-methoxyphenyl)ethyl]-4,6-bis(3-methylbut-2-en-1-yl)benzene-1,3-diol	C25H32O5	M+Na	435.2142	-2.0
	HMDB0154206	5-[2-(4-hydroxy-3-methoxyphenyl)ethyl]-4,6-bis(3-methylbut-2-en-1-yl)benzene-1,2,3-triol	C25H32O5	M+Na	435.2142	-2.0
	HMDB0154170	5-[2-(4-hydroxy-3-methoxyphenyl)ethyl]-4-(4-hydroxy-3-methylbut-2-en-1-yl)-6-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C25H32O5	M+Na	435.2142	-2.0
436.2166	HMDB0030157	Austalide K	C25H32O5	M+Na	435.2142	-2.0
	HMDB0040353	2-[4-(3-Hydroxypropyl)-2-methoxyphenoxy]-1,3-propanediol 1-glucoside	C19H30O10	M+NH4	436.2177	-2.6
	HMDB0161154	{4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-2-(hexanoyloxy)-4-oxobutyl} trimethylazanium	C19H34NO10	M+H	436.2177	-2.6
	HMDB0148763	8-hydroxy-12,12-dimethyl-9-(3-methylbutanoyl)-6-pentyl-3,11,14-trioxatetracyclo[8.5,,pentadeca-1,5,7,9-tetraen-4-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0148759	5-hydroxy-8-(hydroxymethyl)-8-methyl-6-(3-methylbutanoyl)-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0147026	5-hydroxy-4-(5-hydroxypentyl)-8,8-dimethyl-6-(2-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0147025	5-hydroxy-6-[2-(hydroxymethyl)butanoyl]-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0147023	8-hydroxy-12,12-dimethyl-9-(2-methylbutanoyl)-6-pentyl-3,11,14-trioxatetracyclo[8.5,,pentadeca-1,5,7,9-tetraen-4-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0147024	5-hydroxy-6-(4-hydroxy-2-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0147022	5-hydroxy-4-(4-hydroxypentyl)-8,8-dimethyl-6-(2-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0147020	5-hydroxy-6-(2-hydroxy-2-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0147021	5-hydroxy-6-(3-hydroxy-2-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0147019	5-hydroxy-4-(1-hydroxypentyl)-8,8-dimethyl-6-(2-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0147018	5-hydroxy-8-(hydroxymethyl)-8-methyl-6-(2-methylbutanoyl)-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0148762	5-hydroxy-4-(4-hydroxypentyl)-8,8-dimethyl-6-(3-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+Na	437.1935	-0.4

437.1933	HMDB0148760	5-hydroxy-4-(1-hydroxypentyl)-8,8-dimethyl-6-(3-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0148761	5-hydroxy-6-(3-hydroxy-3-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0168750	7-{[(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-5-hydroxy-2H-chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0168747	7-{[(2E)-5-hydroxy-5-[3-(1-hydroxy-4-methylpent-3-en-1-yl)-3-methyloxiran-2-yl]-3-methylpent-2-en-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0168748	7-{[(2E,6Z)-9-(3,3-dimethyloxiran-2-yl)-5,8-dihydroxy-3,7-dimethylnona-2,6-dien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0168746	7-({3-[(3Z)-2,5-dihydroxy-4,8-dimethylnona-3,7-dien-1-yl]-3-methyloxiran-2-yl}methoxy)-2H-chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0168749	7-{[(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-8-hydroxy-2H-chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0168743	7-{[(2E,6Z)-5,8,12-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0168745	7-{[(2E,6Z)-5,8,9-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0168742	7-{[(2E,6Z)-5,8-dihydroxy-7-(hydroxymethyl)-3,11-dimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0168744	7-{[(2E,6Z,E)-5,8,12-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0168740	7-{[(2E,6Z)-4,5,8-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0168739	7-{[(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-6-hydroxy-2H-chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0168741	7-{[(2Z,6Z)-5,8-dihydroxy-3-(hydroxymethyl)-7,11-dimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0148765	5-hydroxy-4-(5-hydroxypentyl)-8,8-dimethyl-6-(3-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0148764	5-hydroxy-6-(4-hydroxy-3-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M+Na	437.1935	-0.4
	HMDB0037039	4-O-Methylmelleolide	C24H30O6	M+Na	437.1935	-0.4
	HMDB0030404	Armillaripin	C24H30O6	M+Na	437.1935	-0.4
	HMDB0039380	Armillarin	C24H30O6	M+Na	437.1935	-0.4
	HMDB0041407	Clausarinol	C24H30O6	M+Na	437.1935	-0.4
	HMDB0014838	Eplerenone	C24H30O6	M+Na	437.1935	-0.4
438.0803	HMDB0144732	(12aS)-5,,12,12a-tetrahydroxy-6-methylidene-1,3,4,11-tetraoxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximide acid	C20H17NO9	M+Na	438.0795	1.7
	HMDB0144448	(6S,12aS)-6,,12a-trihydroxy-6-methyl-1,3,4,11,12-pentaoxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximide acid	C20H17NO9	M+Na	438.0795	1.7
	HMDB0144419	(6S,12aS)-3,6,,12a-tetrahydroxy-6-methyl-1,4,11,12-tetraoxo-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximide acid	C20H17NO9	M+Na	438.0795	1.7
	HMDB0144409	(6S,12aS)-6,,12,12a-tetrahydroxy-6-methyl-1,3,4,11-tetraoxo-1,2,3,4,4a,5,5a,6,11,11a,12a-decahydrotetracene-2-carboximide acid	C20H17NO9	M+Na	438.0795	1.7
	HMDB0144380	(4aR,5aS,6S,12aS)-3,6,,12,12a-pentahydroxy-6-methyl-1,4,11-trioxo-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboximide acid	C20H17NO9	M+Na	438.0795	1.7
	HMDB0142771	(12aS)-5,,12a-trihydroxy-6-methyl-1,3,4,11,12-pentaoxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximide acid	C20H17NO9	M+Na	438.0795	1.7
	HMDB0142695	(12aS)-3,5,,12a-tetrahydroxy-6-methyl-1,4,11,12-tetraoxo-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximide acid	C20H17NO9	M+Na	438.0795	1.7

	HMDB0142683	(12aS)-5,,12,12a-tetrahydroxy-6-methyl-1,3,4,11-tetraoxo-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C20H17NO9	M+Na	438.0795	1.7
	HMDB0142648	(4aR,5aR,12aS)-3,5,,12,12a-pentahydroxy-6-methyl-1,4,11-trioxo-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboximidic acid	C20H17NO9	M+Na	438.0795	1.7
	HMDB0152280	2-({hydroxy[2-hydroxy-4-(7-hydroxy-3,5-dimethoxy-4-oxo-4H-chromen-2-yl)phenyl]methylidene}amino)acetic acid	C20H17NO9	M+Na	438.0795	1.7
438.2974	HMDB0007004	CPA(18)	C21H41O6P	M+NH4	438.2979	-1.1
	HMDB0011152	LysoPE(P-16)	C21H44NO6P	M+H	438.2979	-1.1
444.0228	HMDB0154967	{4-hydroxy-2-[6-(hydroxyamino)-9H-purin-9-yl]-5-[(phosphonooxy)methyl]oxolan-3-yl} oxidanesulfonic acid	C10H14N5O11PS	M+H	444.0221	1.6
	HMDB0154968	{4-hydroxy-5-[6-(hydroxyamino)-9H-purin-9-yl]-2-[(phosphonooxy)methyl]oxolan-3-yl} oxidanesulfonic acid	C10H14N5O11PS	M+H	444.0221	1.6
	HMDB0036591	cycloartenol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156156	(6Z,E,14E,18E)-2,6,,15,19,23-hexamethyltetracos-2,6,,14,18,22-hexaen-4-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156155	(6Z,E,14E,18E)-2,6,,15,19,23-hexamethyltetracos-2,6,,14,18,22-hexaen-8-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156154	(6Z,E,14E,18E)-2,6,,15,19,23-hexamethyltetracos-2,6,,14,18,22-hexaen-12-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156151	(6E,E,14E,18Z)-2,6,,15,19,23-hexamethyltetracos-2,6,,14,18,22-hexaen-4-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156152	(6E,E,14E,18Z)-2,6,,15,19,23-hexamethyltetracos-2,6,,14,18,22-hexaen-8-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156150	squalene alcohol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156153	(6E,E,14E,18Z)-2,6,,15,19,23-hexamethyltetracos-2,6,,14,18,22-hexaen-12-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156149	(6Z,E,18E)-2,6,,15,19,23-hexamethyltetracos-2,6,,14,18,22-hexaen-1-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156147	(6Z,E,14E,18E)-2,6,,15,19,23-hexamethyltetracos-2,6,,14,18,22-hexaen-5-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156148	(2E,6E,E,14E)-6,11,15,19-tetramethyl-2-(4-methylpent-3-en-1-yl)icosa-2,6,,14,18-pentaen-1-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156146	(2Z,6E,E)-2-[(3Z)-4,8-dimethylnona-3,7-dien-1-yl]-7,11,15-trimethylhexadeca-2,6,,14-tetraen-1-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156143	(2Z,6E,Z)-2-[(3E)-4,8-dimethylnona-3,7-dien-1-yl]-7,11,15-trimethylhexadeca-2,6,,14-tetraen-1-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156145	(6Z,E,14E,18E)-2,6,,15,19,23-hexamethyltetracos-2,6,,14,18,22-hexaen-9-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156142	(6E,E,14E,18Z)-2,6,,15,19,23-hexamethyltetracos-2,6,,14,18,22-hexaen-5-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156144	(6E,E,14E,18Z)-2,6,,15,19,23-hexamethyltetracos-2,6,,14,18,22-hexaen-9-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156140	(6E,E,14E,18Z)-2,6,,15,19,23-hexamethyltetracos-2,6,,14,18,22-hexaen-1-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156157	2,2-dimethyl-3-[(3E,7E,11E,15Z)-3,7,12,16,-pentamethylhenicosa-3,7,11,15,19-pentaen-1-yl]oxirane	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156159	2-[(3E)-4,8-dimethylnona-3,7-dien-1-yl]-2-methyl-3-[(3E,7Z)-4,8,12-trimethyltrideca-3,7,11-trien-1-yl]oxirane	C30H50O	M+NH4	444.4200	-2.0
	HMDB0166796	14-(5-ethyl-6-methylheptan-2-yl)-2,6,15-trimethyltetracyclo[8.7,,heptadec-9-en-5-one	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156162	2,2-dimethyl-3-[(3Z,7E,11E,15E)-3,7,12,16,-pentamethylhenicosa-3,7,11,15,19-pentaen-1-yl]oxirane	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156158	2-methyl-2-(4-methylpent-3-en-1-yl)-3-[(3E,7E,11Z)-3,8,12,16-tetramethylheptadeca-3,7,11,15-tetraen-1-yl]oxirane	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156161	CHEMBL249	C30H50O	M+NH4	444.4200	-2.0

444.4191	HMDB0156160	2-[(3Z)-4,8-dimethylnona-3,7-dien-1-yl]-2-methyl-3-[(3E,7E)-4,8,12-trimethyltrideca-3,7,11-trien-1-yl]oxirane	C30H50O	M+NH4	444.4200	-2.0
	HMDB0156141	(2Z,6E,E,14Z)-6,11,15,19-tetramethyl-2-(4-methylpent-3-en-1-yl)icosa-2,6,,14,18-pentaen-1-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0033495	(Z)-24-ethylidenelophenol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0001242	Obtusifoliol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0175747	Germanicol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0035611	6-Hydroxy-8-heptacosanone	C30H50O	M+NH4	444.4200	-2.0
	HMDB0033684	25-Methylgramisterol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0038695	3beta-Cucurbita-5,24-dien-3-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0033195	Camelliol C	C30H50O	M+NH4	444.4200	-2.0
	HMDB0035920	Taraxasterol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0034066	29-Methylisofucosterol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0035128	(E)-2,6-Dimethyl-2,5-heptadienoic acid	C30H50O	M+NH4	444.4200	-2.0
	HMDB0036904	Cymbopogonol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0037032	Tirucallol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0034920	Taraxerol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0031438	Euphol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0001188	(S)-2,3-Epoxysqualene	C30H50O	M+NH4	444.4200	-2.0
	HMDB0036017	Mangiferursanone	C30H50O	M+NH4	444.4200	-2.0
	HMDB0035809	gamma-Taraxasterol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0036657	Epi-alpha-amyrin	C30H50O	M+NH4	444.4200	-2.0
	HMDB0036676	12beta--Ursen-12-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0033595	(3beta,4alpha,5alpha,9beta)-4,14-Dimethyl-9,19-cycloergost-24-en-3-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0032144	24-Methyl-28-norcycloart-25-en-3-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0040777	3beta-12,21-Baccharadien-3-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0030079	4,14-Dimethylergosta-8,25-dien-3-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0039445	Rheinanthrone	C30H50O	M+NH4	444.4200	-2.0
	HMDB0036758	Isomultiflorenol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0037799	4-Hydroxy-6-tetracosanone	C30H50O	M+NH4	444.4200	-2.0
	HMDB0037053	Cymbopogone	C30H50O	M+NH4	444.4200	-2.0
	HMDB0034348	(3beta,4alpha,5alpha,24Z)-4-Methylstigmasta-8(14),24(28)-dien-3-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0029420	L-trans-5-Hydroxy-2-piperidinecarboxylic acid	C30H50O	M+NH4	444.4200	-2.0
	HMDB0035123	3-Epimoretenol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0030674	(3beta,4alpha,5alpha,23E)-4,14-Dimethyl-9,19-cycloergost-23-en-3-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0030485	(3beta,4alpha,5alpha,23E)-4,14-Dimethylergosta-8,23-dien-3-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0001251	Lanosterin	C30H50O	M+NH4	444.4200	-2.0
	HMDB0059621	(3S)-2,3-epoxy-2,3-dihydrosqualene	C30H50O	M+NH4	444.4200	-2.0
	HMDB0039440	(3beta,4alpha,5alpha,24Z)-4-Methylstigmasta-8,24(28)-dien-3-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0033181	Camelliol A	C30H50O	M+NH4	444.4200	-2.0
	HMDB0033596	(3xi,4alpha,5alpha,14alpha)-4,14-Dimethylergosta-8,24-dien-3-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0030506	Cycloeucalanone	C30H50O	M+NH4	444.4200	-2.0
	HMDB0030912	(3beta,5alpha)-4,4-Dimethylergosta-8,24(28)-dien-3-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0034986	Chrysoeriol 7-[feruloyl-(->2)-glucuronyl-(1->2)-glucuronide]	C30H50O	M+NH4	444.4200	-2.0
	HMDB0034929	3beta-Tirucalla-7,24-dien-3-ol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0031957	3-Epiecloeucalenol	C30H50O	M+NH4	444.4200	-2.0
	HMDB0155737	3,4,5-trihydroxy-6-{{[4-hydroxy-5-(6-hydroxy-9H-purin-9-yl)-2-(hydroxymethyl)oxolan-3-yl]oxy}oxane-2-carboxylic acid	C16H20N4O11	M+H	445.1201	-2.8
	HMDB0155736	3,4,5-trihydroxy-6-{{[4-hydroxy-2-(6-hydroxy-9H-purin-9-yl)-5-(hydroxymethyl)oxolan-3-yl]oxy}oxane-2-carboxylic acid	C16H20N4O11	M+H	445.1201	-2.8
	HMDB0155735	6-{{[3,4-dihydroxy-5-(6-hydroxy-9H-purin-9-yl)oxolan-2-yl]methoxy}-3,4,5-trihydroxyoxane-2-carboxylic	C16H20N4O11	M+H	445.1201	-2.8

445.1189	HMDB0159384	3,4,5-trihydroxy-6-[(4-hydroxy-5-{4-hydroxy-1H-pyrazolo[3,4-d]pyrimidin-1-yl}-2-(hydroxymethyl)oxolan-3-yl)oxy]oxane-2-carboxylic acid	C16H20N4O11	M+H	445.1201	-2.8
	HMDB0159385	3,4,5-trihydroxy-6-[(4-hydroxy-2-{4-hydroxy-1H-pyrazolo[3,4-d]pyrimidin-1-yl}-5-(hydroxymethyl)oxolan-3-yl)oxy]oxane-2-carboxylic acid	C16H20N4O11	M+H	445.1201	-2.8
	HMDB0159386	6-[(3,4-dihydroxy-5-{4-hydroxy-1H-pyrazolo[3,4-d]pyrimidin-1-yl}oxolan-2-yl)methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H20N4O11	M+H	445.1201	-2.8
	HMDB0158893	6-[(1-carboxy-4,5,6,7,8-pentahydroxy-1-oxooctan-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O15	M+H	445.1188	0.2
	HMDB0158895	6-[(8-carboxy-1,2,3,5,6-pentahydroxy-8-oxooctan-4-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O15	M+H	445.1188	0.2
	HMDB0158898	6-[(8-carboxy-2,3,4,5,6-pentahydroxy-8-oxooctyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O15	M+H	445.1188	0.2
	HMDB0158896	6-[(8-carboxy-1,2,4,5,6-pentahydroxy-8-oxooctan-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O15	M+H	445.1188	0.2
	HMDB0158897	6-[(8-carboxy-1,3,4,5,6-pentahydroxy-8-oxooctan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O15	M+H	445.1188	0.2
	HMDB0158894	6-[(1-carboxy-3,5,6,7,8-pentahydroxy-1-oxooctan-4-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O15	M+H	445.1188	0.2
	HMDB0158899	6-[(4,5,6,7,8,9-hexahydroxy-2-oxononanoyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O15	M+H	445.1188	0.2
446.2741	HMDB0159351	6-[(7Z,Z)-hexadeca-7,-dienoyloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H36O8	M+NH4	446.2748	-1.7
	HMDB0166491	6-[(3Z)-hexadeca-3,15-dienoyloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H36O8	M+NH4	446.2748	-1.7
447.0663	HMDB0143134	{4-[2-chloro-1,2-bis(4-methoxyphenyl)ethenyl]phenyl}oxidanesulfonic acid	C22H19ClO6S	M+H	447.0664	-0.1
	HMDB0143136	{4-[1-chloro-2,2-bis(4-methoxyphenyl)ethenyl]phenyl}oxidanesulfonic acid	C22H19ClO6S	M+H	447.0664	-0.1
	HMDB0177730	6-[4-(3-chloro-1,2-dihydroxypropyl)-2-hydroxy-6-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H21ClO11	M+Na	447.0665	-0.4
	HMDB0177729	6-[5-(3-chloro-1,2-dihydroxypropyl)-2-hydroxy-3-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H21ClO11	M+Na	447.0665	-0.4
447.3460	HMDB0173067	14-(3,4-dihydroxy-6-methyl-5-methylideneheptan-2-yl)-4-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-one	C28H46O4	M+H	447.3469	-2.0
	HMDB0173066	14-(3,4-dihydroxy-6-methyl-5-methylideneheptan-2-yl)-5-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-4-one	C28H46O4	M+H	447.3469	-2.0
	HMDB0012557	13'-Carboxy-gamma-tocopherol	C28H46O4	M+H	447.3469	-2.0
	HMDB0032875	3,5,9-Trihydroxyergost-7-en-6-one	C28H46O4	M+H	447.3469	-2.0
	HMDB0032123	Quillaic acid 3-[galactosyl-(1->2)-[xylosyl-(1->3)]-glucuronide] 28-[apiosyl-(1->3)-xylosyl-(1->4)-rhamnosyl-(1->2)-[rhamnosyl-(1->3)]-4-acetyl-fucosyl] ester	C28H46O4	M+H	447.3469	-2.0
	HMDB0032107	(3beta,5alpha,6beta,7alpha,22E,24R)-Ergosta-8,22-diene-3,5,6,7-tetrol	C28H46O4	M+H	447.3469	-2.0
	HMDB0040999	Secasterone	C28H46O4	M+H	447.3469	-2.0
	HMDB0041527	3-Dehydroteasterone	C28H46O4	M+H	447.3469	-2.0
448.2320	HMDB0031673	Armillarilin	C24H30O7	M+NH4	448.2330	-2.2
	HMDB0030815	Mammea E/BA	C24H30O7	M+NH4	448.2330	-2.2
	HMDB0038788	Melleolide H	C24H30O7	M+NH4	448.2330	-2.2
	HMDB0030814	Mammea E/BB	C24H30O7	M+NH4	448.2330	-2.2
	HMDB0162707	3,4,5-trihydroxy-6-{[(4Z)-1-oxo-1-(1,2,3,4-tetrahydropyridin-1-yl)undec-4-en-8,-diyn-3-yl]oxy}oxane-2-carboxylic acid	C22H27NO8	M+NH4	451.2075	1.6
	HMDB0162709	3,4,5-trihydroxy-6-{[11-oxo-11-(1,2,3,4-tetrahydropyridin-1-yl)undec-7-en-1,3-diyn-6-yl]oxy}oxane-2-carboxylic acid	C22H27NO8	M+NH4	451.2075	1.6

451.2082	HMDB0162771	3,4,5-trihydroxy-6-{{(4Z,6E,8Z)-9-(2-methyl-2H-azepin-7-yl)-3-oxonona-4,6,8-trien-1-yl}oxy}oxane-2-carboxylic acid	C22H27NO8	M+NH4	451.2075	1.6
	HMDB0162757	3,4,5-trihydroxy-6-{{7-[(1Z,5Z)-7-oxonona-1,3,5-trien-1-yl]-2H-azepin-2-yl}methoxy}oxane-2-carboxylic acid	C22H27NO8	M+NH4	451.2075	1.6
	HMDB0162759	3,4,5-trihydroxy-6-{{(4Z,8Z)-9-(2-methyl-2H-azepin-7-yl)-3-oxonona-4,6,8-trien-2-yl}oxy}oxane-2-carboxylic acid	C22H27NO8	M+NH4	451.2075	1.6
	HMDB0162713	3,4,5-trihydroxy-6-{{(4Z)-1-oxo-1-(1,2,3,4-tetrahydropyridin-1-yl)undec-4-en-8,-diyn-2-yl}oxy}oxane-2-carboxylic acid	C22H27NO8	M+NH4	451.2075	1.6
	HMDB0030158	Natsudaïdain	C25H32O6	M+Na	451.2091	-2.0
452.1634	HMDB0172623	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(pent-4-en-1-yl)thio(carbonimidyl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C16H26N4O6S2	M+NH4	452.1632	0.4
453.1662	HMDB0179387	3-{{2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl}-2-hydroxyhex-4-enoic acid	C16H25N3O9S	M+NH4	453.1650	2.7
	HMDB0179389	(2Z)-4-{{2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl}-5-hydroxyhex-2-enoic acid	C16H25N3O9S	M+NH4	453.1650	2.7
	HMDB0179386	2-{{2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl}-3-hydroxyhex-4-enoic acid	C16H25N3O9S	M+NH4	453.1650	2.7
	HMDB0179390	(2Z)-5-{{2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl}-4-hydroxyhex-2-enoic acid	C16H25N3O9S	M+NH4	453.1650	2.7
	HMDB0035068	Melleolide M	C23H29ClO7	M+H	453.1675	-2.8
454.1693	HMDB0164397	3,4,5-trihydroxy-6-{{4-({4-[(2E)-4-methyl-5-oxooxolan-2-ylidene]butyl}amino)butanoyl}oxy}oxane-2-carboxylic	C19H29NO10	M+Na	454.1684	2.1
	HMDB0142502	{3-[(1E)-1-{4-[2-(methylamino)ethoxy]phenyl}-2-phenylbut-1-en-1-yl]phenyl}oxidanesulfonic acid	C25H27NO5S	M+H	454.1683	2.3
	HMDB0142467	{{[(3E)-4-{4-[2-(methylamino)ethoxy]phenyl}-3,4-diphenylbut-3-en-1-yl}oxy}sulfonic acid	C25H27NO5S	M+H	454.1683	2.3
	HMDB0142461	{4-[(1E)-1-{4-[2-(methylamino)ethoxy]phenyl}-1-phenylbut-1-en-2-yl]phenyl}oxidanesulfonic acid	C25H27NO5S	M+H	454.1683	2.3
	HMDB0142463	{4-[(1Z)-1-{4-[2-(methylamino)ethoxy]phenyl}-2-phenylbut-1-en-1-yl]phenyl}oxidanesulfonic acid	C25H27NO5S	M+H	454.1683	2.3
	HMDB0142457	{3-[(1E)-1-{4-[2-(methylamino)ethoxy]phenyl}-1-phenylbut-1-en-2-yl]phenyl}oxidanesulfonic acid	C25H27NO5S	M+H	454.1683	2.3
	HMDB0142459	{3-[(1Z)-1-{4-[2-(methylamino)ethoxy]phenyl}-2-phenylbut-1-en-1-yl]phenyl}oxidanesulfonic acid	C25H27NO5S	M+H	454.1683	2.3
	HMDB0142455	{{[(3Z)-4-{4-[2-(methylamino)ethoxy]phenyl}-3,4-diphenylbut-3-en-2-yl}oxy}sulfonic acid	C25H27NO5S	M+H	454.1683	2.3
	HMDB0061140	Endoxifen sulfate	C25H27NO5S	M+H	454.1683	2.3
	HMDB0142670	(12aS)-3,5,,12,12a-pentahydroxy-6-methyl-4-(methylamino)-1,11-dioxo-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximidic acid	C21H24N2O8	M+Na	455.1425	2.7
	HMDB0142763	(12aS)-5,,12,12a-tetrahydroxy-6-methyl-4-(methylamino)-1,3,11-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C21H24N2O8	M+Na	455.1425	2.7
	HMDB0142658	(12aS)-3,5,,12,12a-pentahydroxy-6-methyl-4-(methylamino)-1,11-dioxo-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C21H24N2O8	M+Na	455.1425	2.7

455.1437	HMDB0144388	(6S,12aS)-3,6,,12,12a-pentahydroxy-6-methyl-4-(methylamino)-1,11-dioxo-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C21H24N2O8	M+Na	455.1425	2.7
	HMDB0144398	(6S,12aS)-3,6,,12,12a-pentahydroxy-6-methyl-4-(methylamino)-1,11-dioxo-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximidic acid	C21H24N2O8	M+Na	455.1425	2.7
	HMDB0144445	(6S,12aS)-6,,12,12a-tetrahydroxy-6-methyl-4-(methylamino)-1,3,11-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C21H24N2O8	M+Na	455.1425	2.7
	HMDB0144446	(6S,12aR)-3,6,,12a-tetrahydroxy-6-methyl-4-(methylamino)-1,11,12-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C21H24N2O8	M+Na	455.1425	2.7
	HMDB0144967	(12aS)-7-(dimethylamino)-3,,12,12a-tetrahydroxy-1,4,11-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C21H24N2O8	M+Na	455.1425	2.7
	HMDB0142764	(12aR)-3,5,,12a-tetrahydroxy-6-methyl-4-(methylamino)-1,11,12-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C21H24N2O8	M+Na	455.1425	2.7
	HMDB0166567	2-amino-4-({2-[(1-carboxy-3-methoxy-3-oxopropyl)sulfanyl]-1-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C15H23N3O10S	M+NH4	455.1442	-1.2
455.1635	HMDB0181091	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1-hydroxy-2-methylidenepentan-3-yl)disulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C16H27N3O7S2	M+NH4	455.1629	1.4
	HMDB0181095	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(5-hydroxy-4-methylpent-1-en-3-yl)disulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C16H27N3O7S2	M+NH4	455.1629	1.4
456.1677	HMDB0146970	(1-{5-hydroxy-8,8-dimethyl-2-oxo-4-propyl-2H,8H-pyrano[2,3-f]chromen-6-yl}-2-methylpropoxy)sulfonic acid	C21H26O8S	M+NH4	456.1687	-2.1
	HMDB0147016	(1-{5-hydroxy-8,8-dimethyl-2-oxo-4-propyl-2H,8H-pyrano[2,3-f]chromen-6-yl}butoxy)sulfonic acid	C21H26O8S	M+NH4	456.1687	-2.1
	HMDB0150346	{3,15-dihydroxy-16,17-dimethoxytricyclo[12.3.1.1,nonadeca-1(17),2,4,6(19),14(18),15-hexaen-9-yl]oxidanesulfonic acid	C21H26O8S	M+NH4	456.1687	-2.1
	HMDB0175783	4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydopicene-3,14-diol	C30H50O2	M+NH4	460.4149	-2.2
	HMDB0173187	14-[(5Z)-1-hydroxy-5-(propan-2-yl)hept-5-en-2-yl]-2,6,15-trimethyltetraacyclo[8.7,,heptadec--en-5-ol	C30H50O2	M+NH4	460.4149	-2.2
	HMDB0173188	2,6,15-trimethyl-14-[(5Z)-5-(propan-2-yl)hept-5-en-2-yl]tetraacyclo[8.7,,heptadec--ene-5,17-diol	C30H50O2	M+NH4	460.4149	-2.2
	HMDB0169725	14-[(5Z)-8-hydroxy-5-(propan-2-yl)oct-5-en-2-yl]-2,15-dimethyltetraacyclo[8.7,,heptadec-7-en-5-ol	C30H50O2	M+NH4	460.4149	-2.2
	HMDB0169724	14-[(5Z)-7-hydroxy-6-methyl-5-propylideneheptan-2-yl]-2,15-dimethyltetraacyclo[8.7,,heptadec-7-en-5-ol	C30H50O2	M+NH4	460.4149	-2.2
	HMDB0169723	14-{4-[3-ethyl-2-(propan-2-yl)oxiran-2-yl]butan-2-yl}-2,15-dimethyltetraacyclo[8.7,,heptadec-7-en-5-ol	C30H50O2	M+NH4	460.4149	-2.2
	HMDB0169722	2,15-dimethyl-14-[(5Z)-5-(propan-2-yl)oct-5-en-2-yl]tetraacyclo[8.7,,heptadec-7-ene-5,9-diol	C30H50O2	M+NH4	460.4149	-2.2
	HMDB0169721	14-[(5Z)-7-hydroxy-5-(propan-2-yl)oct-5-en-2-yl]-2,15-dimethyltetraacyclo[8.7,,heptadec-7-en-5-ol	C30H50O2	M+NH4	460.4149	-2.2
	HMDB0169719	2,15-dimethyl-14-[(5Z)-5-(propan-2-yl)oct-5-en-2-yl]tetraacyclo[8.7,,heptadec-7-ene-5,6-diol	C30H50O2	M+NH4	460.4149	-2.2
	HMDB0169718	14-[(5Z)-2-hydroxy-5-(propan-2-yl)oct-5-en-2-yl]-2,15-dimethyltetraacyclo[8.7,,heptadec-7-en-5-ol	C30H50O2	M+NH4	460.4149	-2.2

HMDB0169720	14-[(5E)-4-hydroxy-5-(propan-2-yl)oct-5-en-2-yl]-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0169717	14-[(5Z)-6-hydroxy-6-methyl-5-propylideneheptan-2-yl]-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0169713	2,15-dimethyl-14-[(5Z)-5-(propan-2-yl)oct-5-en-2-yl]tetracyclo[8.7.,heptadec-7-ene-5,17-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0169714	2,15-dimethyl-14-[(5Z)-5-(propan-2-yl)oct-5-en-2-yl]tetracyclo[8.7.,heptadec-7-ene-5,13-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0169716	2-(hydroxymethyl)-15-methyl-14-[(5Z)-5-(propan-2-yl)oct-5-en-2-yl]tetracyclo[8.7.,heptadec-7-en-5-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0169715	15-(hydroxymethyl)-2-methyl-14-[(5Z)-5-(propan-2-yl)oct-5-en-2-yl]tetracyclo[8.7.,heptadec-7-en-5-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175771	6a-(hydroxymethyl)-4,4,6b,8a,11,11,14b-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricen-3-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175772	4-(hydroxymethyl)-4,6a,6b,8a,11,11,14b-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricen-3-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175777	4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricene-3,6-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0182811	2,5,,14,18,18-hexamethyl-6-(propan-2-yl)pentacyclo[11.8,??]henicos-12-ene-3,17-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0182810	6-(1-hydroxypropan-2-yl)-2,5,,14,18,18-hexamethylpentacyclo[11.8,??]henicos-12-en-17-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0181821	2,6,6,11,15-pentamethyl-14-(6-methylhept-5-en-2-yl)tetracyclo[8.7.,heptadec-9-ene-5,17-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175788	4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricene-3,9-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175789	4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricene-3,-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175786	4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricene-3,7-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175785	4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricene-3,12b-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175782	4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricene-3,14a-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175784	4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricene-3,13-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175779	4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricene-3,4a-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175778	4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricene-3,5-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175774	6b-(hydroxymethyl)-4,4,6a,8a,11,11,14b-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricen-3-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175773	14b-(hydroxymethyl)-4,4,6a,6b,8a,11,11-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricen-3-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0169712	14-[(5Z)-1-hydroxy-5-(propan-2-yl)oct-5-en-2-yl]-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0166809	14-(5-ethyl-7-hydroxy-6-methylheptan-2-yl)-2,6,15-trimethyltetracyclo[8.7.,heptadec-9-en-5-one	C30H50O2	M+NH4	460.4149	-2.2
HMDB0166811	14-(5-ethyl-5-hydroxy-6-methylheptan-2-yl)-2,6,15-trimethyltetracyclo[8.7.,heptadec-9-en-5-one	C30H50O2	M+NH4	460.4149	-2.2
HMDB0062379	3beta-hydroxylanost-8-en-32-al	C30H50O2	M+NH4	460.4149	-2.2

HMDB0164080	15-(1-hydroxy-5,6-dimethylhept-5-en-2-yl)-7,12,16-trimethylpentacyclo[9.7,,,octadecan-6-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0164081	15-(5,6-dimethylhept-5-en-2-yl)-7,12,16-trimethylpentacyclo[9.7,,,octadecan-6,18-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0164105	14-(1-hydroxy-5,6-dimethylhept-5-en-2-yl)-2,6,11,15-tetramethyltetraacyclo[8.7,,heptadec-1()-en-5-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0166810	14-[7-hydroxy-5-(propan-2-yl)heptan-2-yl]-2,6,15-trimethyltetraacyclo[8.7,,heptadec-9-en-5-one	C30H50O2	M+NH4	460.4149	-2.2
HMDB0166812	14-(5-ethyl-6-methylheptan-2-yl)-17-hydroxy-2,6,15-trimethyltetraacyclo[8.7,,heptadec-9-en-5-one	C30H50O2	M+NH4	460.4149	-2.2
HMDB0166808	14-[6-hydroxy-5-(propan-2-yl)heptan-2-yl]-2,6,15-trimethyltetraacyclo[8.7,,heptadec-9-en-5-one	C30H50O2	M+NH4	460.4149	-2.2
HMDB0166806	14-(5-ethyl-6-methylheptan-2-yl)-6-hydroxy-2,6,15-trimethyltetraacyclo[8.7,,heptadec-9-en-5-one	C30H50O2	M+NH4	460.4149	-2.2
HMDB0166807	14-(5-ethyl-2-hydroxy-6-methylheptan-2-yl)-2,6,15-trimethyltetraacyclo[8.7,,heptadec-9-en-5-one	C30H50O2	M+NH4	460.4149	-2.2
HMDB0166805	14-(5-ethyl-6-hydroxy-6-methylheptan-2-yl)-2,6,15-trimethyltetraacyclo[8.7,,heptadec-9-en-5-one	C30H50O2	M+NH4	460.4149	-2.2
HMDB0166804	14-(5-ethyl-6-methylheptan-2-yl)-6-(hydroxymethyl)-2,15-dimethyltetraacyclo[8.7,,heptadec-9-en-5-one	C30H50O2	M+NH4	460.4149	-2.2
HMDB0166801	14-(5-ethyl-1-hydroxy-6-methylheptan-2-yl)-2,6,15-trimethyltetraacyclo[8.7,,heptadec-9-en-5-one	C30H50O2	M+NH4	460.4149	-2.2
HMDB0166802	14-(5-ethyl-6-methylheptan-2-yl)-15-(hydroxymethyl)-2,6-dimethyltetraacyclo[8.7,,heptadec-9-en-5-one	C30H50O2	M+NH4	460.4149	-2.2
HMDB0166803	14-(5-ethyl-6-methylheptan-2-yl)-2-(hydroxymethyl)-6,15-dimethyltetraacyclo[8.7,,heptadec-9-en-5-one	C30H50O2	M+NH4	460.4149	-2.2
HMDB0166800	14-(5-ethyl-6-methylheptan-2-yl)-13-hydroxy-2,6,15-trimethyltetraacyclo[8.7,,heptadec-9-en-5-one	C30H50O2	M+NH4	460.4149	-2.2
HMDB0166799	14-(5-ethyl-6-methylheptan-2-yl)-8-hydroxy-2,6,15-trimethyltetraacyclo[8.7,,heptadec-9-en-5-one	C30H50O2	M+NH4	460.4149	-2.2
HMDB0165320	14-(1-hydroxy-6,6-dimethyl-5-methylideneheptan-2-yl)-2,6,15-trimethyltetraacyclo[8.7,,heptadec-9-en-5-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0165321	14-(6,6-dimethyl-5-methylideneheptan-2-yl)-2,6,15-trimethyltetraacyclo[8.7,,heptadec-9-ene-5,17-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0164106	14-(5,6-dimethylhept-5-en-2-yl)-2,6,11,15-tetramethyltetraacyclo[8.7,,heptadec-1()-ene-5,17-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175781	4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydopicene-1,3-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175775	8a-(hydroxymethyl)-4,4,6a,6b,11,11,14b-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydopicen-3-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175776	11-(hydroxymethyl)-4,4,6a,6b,8a,11,14b-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydopicen-3-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0034685	Myricadiol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0033232	(3beta,16alpha)-7-Baurene-3,16-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0039753	Atroviridin	C30H50O2	M+NH4	460.4149	-2.2
HMDB0034550	Maniladiol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0035033	Dehydrocyanaropicrin	C30H50O2	M+NH4	460.4149	-2.2
HMDB0034664	Coflodiol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0041145	3alpha-12-Ursene-3,24-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0035111	(3beta,21alphaH)-22()-Hopene-3,29-diol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0036056	(2xi,beta)-2,-Dihydroxy-3-oxo-12-ursen-28-oic acid	C30H50O2	M+NH4	460.4149	-2.2
HMDB0035769	Brein	C30H50O2	M+NH4	460.4149	-2.2
HMDB0012159	4,4-Dimethyl-14alpha-formyl-5alpha-cholesta-8-en-3beta-ol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0002391	Uvaol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0002360	Erythrodiol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0175696	Erythrodiol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0035826	Faradiol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0035960	Masticadienediol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0036838	betulin	C30H50O2	M+NH4	460.4149	-2.2
HMDB0033727	gamma-Taraxastanonol	C30H50O2	M+NH4	460.4149	-2.2
HMDB0035401	Arnidenediol	C30H50O2	M+NH4	460.4149	-2.2

	HMDB0181820	14-(1-hydroxy-6-methylhept-5-en-2-yl)-2,6,6,11,15-pentamethyltetracyclo[8.7.,,]heptadec-9-en-5-ol	C30H50O2	M+NH4	460.4149	-2.2
	HMDB0175780	4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricene-2,3-diol	C30H50O2	M+NH4	460.4149	-2.2
	HMDB0175787	4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricene-3,8-diol	C30H50O2	M+NH4	460.4149	-2.2
462.1454	HMDB0015194	Azlocillin	C20H23N5O6S	M+H	462.1442	2.6
	HMDB0155737	3,4,5-trihydroxy-6- {[4-hydroxy-5-(6-hydroxy-9H-purin-9-yl)-2-(hydroxymethyl)oxolan-3-yl]oxy} oxane-2-carboxylic acid	C16H20N4O11	M+NH4	462.1467	-2.8
	HMDB0155735	6- {[3,4-dihydroxy-5-(6-hydroxy-9H-purin-9-yl)oxolan-2-yl]methoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H20N4O11	M+NH4	462.1467	-2.8
	HMDB0155736	3,4,5-trihydroxy-6- {[4-hydroxy-2-(6-hydroxy-9H-purin-9-yl)-5-(hydroxymethyl)oxolan-3-yl]oxy} oxane-2-carboxylic acid	C16H20N4O11	M+NH4	462.1467	-2.8
	HMDB0159385	3,4,5-trihydroxy-6- [(4-hydroxy-2- {4-hydroxy-1H-pyrazolo[3,4-d]pyrimidin-1-yl}-5-(hydroxymethyl)oxolan-3-yl)oxy] oxane-2-carboxylic acid	C16H20N4O11	M+NH4	462.1467	-2.8
	HMDB0159384	3,4,5-trihydroxy-6- [(4-hydroxy-5- {4-hydroxy-1H-pyrazolo[3,4-d]pyrimidin-1-yl}-2-(hydroxymethyl)oxolan-3-yl)oxy] oxane-2-carboxylic acid	C16H20N4O11	M+NH4	462.1467	-2.8
	HMDB0159386	6- [(3,4-dihydroxy-5- {4-hydroxy-1H-pyrazolo[3,4-d]pyrimidin-1-yl} oxolan-2-yl) methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H20N4O11	M+NH4	462.1467	-2.8
	HMDB0158894	6- [(1-carboxy-3,5,6,7,8-pentahydroxy-1-oxooctan-4-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O15	M+NH4	462.1453	0.1
	HMDB0158899	6- [(4,5,6,7,8,9-hexahydroxy-2-oxononanoyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O15	M+NH4	462.1453	0.1
	HMDB0158896	6- [(8-carboxy-1,2,4,5,6-pentahydroxy-8-oxooctan-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O15	M+NH4	462.1453	0.1
	HMDB0158897	6- [(8-carboxy-1,3,4,5,6-pentahydroxy-8-oxooctan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O15	M+NH4	462.1453	0.1
	HMDB0158895	6- [(8-carboxy-1,2,3,5,6-pentahydroxy-8-oxooctan-4-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O15	M+NH4	462.1453	0.1
	HMDB0158893	6- [(1-carboxy-4,5,6,7,8-pentahydroxy-1-oxooctan-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O15	M+NH4	462.1453	0.1
	HMDB0158898	6- [(8-carboxy-2,3,4,5,6-pentahydroxy-8-oxooctyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O15	M+NH4	462.1453	0.1
462.3573	HMDB0011560	MG/24:6(6Z,9Z,12Z,15Z,18Z,21Z))	C28H44O4	M+NH4	462.3578	-1.0
	HMDB0033647	Torachryson 8-(6-oxalylglucoside)	C28H44O4	M+NH4	462.3578	-1.0
	HMDB0038977	(3beta,5alpha,6beta,9alpha,22E,24R)-5,9-Epidioxergosta-7,22-diene-3,6-diol	C28H44O4	M+NH4	462.3578	-1.0
	HMDB0032691	(3beta,5alpha,6alpha,7beta,14alpha,22E,24R)-5,6-Epoxyergosta-8,22-diene-3,7,14-triol	C28H44O4	M+NH4	462.3578	-1.0
	HMDB0032667	5,9-Epidioxy-3-hydroxyergost-7-en-6-one	C28H44O4	M+NH4	462.3578	-1.0
	HMDB0006227	1-a,24R,25-Trihydroxyvitamin D2	C28H44O4	M+NH4	462.3578	-1.0
463.1452	HMDB0001833	Aminopterin	C19H20N8O5	M+Na	463.1449	0.7
	HMDB0169075	3,4,5-trihydroxy-6- [2- ([3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy) methyl]phenoxy]oxane-2-carboxylic acid	C19H26O13	M+H	463.1446	1.3
464.1415	HMDB0182890	(7,7a-dimethyl-4'-methylidene-4- {[(2E)-3-(methylsulfanyl)prop-2-enoyl]oxy}-2'-oxooctahydrospiro[indene-2,3'-oxolane]-3-yl)oxidanesulfonic acid	C19H26O8S2	M+NH4	464.1407	1.7
464.3125	HMDB0240599	(2-aminoethoxy)[(2R)-2-hydroxy-3-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid	C23H46NO6P	M+H	464.3136	-2.3
	HMDB0160516	2-methyl-6- [(2S,15S)-9,13,16-trihydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,,heptadecan-14-yl]heptanoic acid	C27H44O6	M+H	465.3211	1.8

465.3219	HMDB0160517	6-[(2S,15R)-9,16-dihydroxy-2,15-dimethyl-5-oxotetracyclo[8.7,,heptadecan-14-yl]-7-hydroxy-2-methylheptanoic acid	C27H44O6	M+H	465.3211	1.8
	HMDB0160518	6-[(2R,15R)-9,16-dihydroxy-2-(hydroxymethyl)-15-methyl-5-oxotetracyclo[8.7,,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O6	M+H	465.3211	1.8
	HMDB0160515	2-methyl-6-[(2R,15R)-8,9,16-trihydroxy-2,15-dimethyl-5-oxotetracyclo[8.7,,heptadecan-14-yl]heptanoic acid	C27H44O6	M+H	465.3211	1.8
	HMDB0160519	6-[(2S,15R)-9,16-dihydroxy-15-(hydroxymethyl)-2-methyl-5-oxotetracyclo[8.7,,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O6	M+H	465.3211	1.8
	HMDB0160522	6-[(2S,15R)-9,16-dihydroxy-2,15-dimethyl-5-oxotetracyclo[8.7,,heptadecan-14-yl]-2-(hydroxymethyl)heptanoic acid	C27H44O6	M+H	465.3211	1.8
	HMDB0160521	6-[(2S,15S)-9,16-dihydroxy-2,15-dimethyl-5-oxotetracyclo[8.7,,heptadecan-14-yl]-6-hydroxy-2-methylheptanoic acid	C27H44O6	M+H	465.3211	1.8
	HMDB0160520	6-[(2S,15R)-9,16-dihydroxy-2,15-dimethyl-5-oxotetracyclo[8.7,,heptadecan-14-yl]-2-hydroxy-2-methylheptanoic acid	C27H44O6	M+H	465.3211	1.8
	HMDB0160523	2-methyl-6-[(2R,15R)-5,8,16-trihydroxy-2,15-dimethyl-9-oxotetracyclo[8.7,,heptadecan-14-yl]heptanoic acid	C27H44O6	M+H	465.3211	1.8
	HMDB0160526	6-[(2R,15R)-5,16-dihydroxy-2-(hydroxymethyl)-15-methyl-9-oxotetracyclo[8.7,,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O6	M+H	465.3211	1.8
	HMDB0160524	2-methyl-6-[(2S,15S)-5,13,16-trihydroxy-2,15-dimethyl-9-oxotetracyclo[8.7,,heptadecan-14-yl]heptanoic acid	C27H44O6	M+H	465.3211	1.8
	HMDB0160525	6-[(2S,15R)-5,16-dihydroxy-2,15-dimethyl-9-oxotetracyclo[8.7,,heptadecan-14-yl]-7-hydroxy-2-methylheptanoic acid	C27H44O6	M+H	465.3211	1.8
	HMDB0160528	6-[(2S,15R)-5,16-dihydroxy-2,15-dimethyl-9-oxotetracyclo[8.7,,heptadecan-14-yl]-2-hydroxy-2-methylheptanoic acid	C27H44O6	M+H	465.3211	1.8
	HMDB0160529	6-[(2S,15S)-5,16-dihydroxy-2,15-dimethyl-9-oxotetracyclo[8.7,,heptadecan-14-yl]-6-hydroxy-2-methylheptanoic acid	C27H44O6	M+H	465.3211	1.8
	HMDB0160527	6-[(2S,15R)-5,16-dihydroxy-15-(hydroxymethyl)-2-methyl-9-oxotetracyclo[8.7,,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O6	M+H	465.3211	1.8
	HMDB0160530	6-[(2S,15R)-5,16-dihydroxy-2,15-dimethyl-9-oxotetracyclo[8.7,,heptadecan-14-yl]-2-(hydroxymethyl)heptanoic acid	C27H44O6	M+H	465.3211	1.8
	HMDB0170464	138-56-5	C27H44O6	M+H	465.3211	1.8
	HMDB0172528	5,7',9',13'-tetramethyl-5'-oxaspiro[oxane-2,6'-pentacyclo[.8,2,,icosane]-5,11',16',19'-tetrol	C27H44O6	M+H	465.3211	1.8
466.0034	HMDB0154967	{4-hydroxy-2-[6-(hydroxyamino)-9H-purin-9-yl]-5-[(phosphonoxy)methyl]oxolan-3-yl} oxidanesulfonic acid	C10H14N5O11PS	M+Na	466.0040	-1.4
	HMDB0154968	{4-hydroxy-5-[6-(hydroxyamino)-9H-purin-9-yl]-2-[(phosphonoxy)methyl]oxolan-3-yl} oxidanesulfonic acid	C10H14N5O11PS	M+Na	466.0040	-1.4
	HMDB0240598	1-[(1Z)-octadec-1-enyl]-sn-glycero-3-phosphoethanolamine	C23H48NO6P	M+H	466.3292	-2.6
	HMDB0160537	[(2S,15S)-14-(6-carboxy-2-hydroxy-6-methylhexan-2-yl)-5,16-dihydroxy-2,15-dimethyltetracyclo[8.7,,heptadecan-9-yl]oxidanyl	C27H45O6	M+H	466.3289	-1.9
	HMDB0160536	[(2S,15R)-14-(6-carboxy-6-hydroxy-6-methylhexan-2-yl)-5,16-dihydroxy-2,15-dimethyltetracyclo[8.7,,heptadecan-9-yl]oxidanyl	C27H45O6	M+H	466.3289	-1.9
	HMDB0160535	[(2S,15R)-14-(6-carboxy-6-methylhexan-2-yl)-5,16-dihydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7,,heptadecan-9-yl]oxidanyl	C27H45O6	M+H	466.3289	-1.9

466.3280	HMDB0160538	[(2S,15R)-14-[6-carboxy-6-(hydroxymethyl)hexan-2-yl]-5,16-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-9-yl]oxidanyl	C27H45O6	M+H	466.3289	-1.9
	HMDB0160533	[(2S,15R)-14-(6-carboxy-1-hydroxy-6-methylhexan-2-yl)-5,16-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-9-yl]oxidanyl	C27H45O6	M+H	466.3289	-1.9
	HMDB0160532	[(2S,15S)-14-(6-carboxy-6-methylhexan-2-yl)-5,13,16-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-9-yl]oxidanyl	C27H45O6	M+H	466.3289	-1.9
	HMDB0160534	[(2R,15R)-14-(6-carboxy-6-methylhexan-2-yl)-5,16-dihydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-9-yl]oxidanyl	C27H45O6	M+H	466.3289	-1.9
	HMDB0160531	[(2R,15R)-14-(6-carboxy-6-methylhexan-2-yl)-5,8,16-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-9-yl]oxidanyl	C27H45O6	M+H	466.3289	-1.9
466.3516	HMDB0013154	12-Hydroxy-12-octadecanoylcarnitine	C25H49NO5	M+Na	466.3503	2.8
	HMDB0157631	6-[(2R,15R)-8,9-dihydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0157634	6-[(2S,15S)-9-hydroxy-15-(hydroxymethyl)-2-methyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0157632	6-[(2S,15S)-9,13-dihydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0157633	7-hydroxy-6-[(2S,15R)-9-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0157635	6-[(2R,15R)-9-hydroxy-2-(hydroxymethyl)-15-methyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0164013	19'-(hydroxymethyl)-5,7',9',13'-tetramethyl-5'-oxaspiro[oxane-2,6'-pentacyclo[.7,?,nonadecane]-16',18'-diol	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0160505	6-[(1S,2S,7S,11S,15R)-5,16-dihydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0160504	6-[(1S,2S,7R,R,11S,15R)-9,16-dihydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0157644	2-hydroxy-6-[(2S,15R)-5-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0157643	6-[(2R,15R)-5-hydroxy-2-(hydroxymethyl)-15-methyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0157646	6-[(2S,15R)-5-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]-2-(hydroxymethyl)heptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0157645	6-hydroxy-6-[(2S,15S)-5-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0157640	6-[(2S,15S)-5,13-dihydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0157641	7-hydroxy-6-[(2S,15R)-5-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0157642	6-[(2S,15S)-5-hydroxy-15-(hydroxymethyl)-2-methyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0157639	6-[(2R,15R)-5,8-dihydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4

	HMDB0157637	6-hydroxy-6-[(2S,15S)-9-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0157638	6-[(2S,15R)-9-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]-2-(hydroxymethyl)heptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0157636	2-hydroxy-6-[(2S,15R)-9-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]-2-methylheptanoic acid	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0032783	Porrigenin A	C27H44O5	M+NH4	466.3527	-2.4
	HMDB0034293	Asperagenin	C27H44O5	M+NH4	466.3527	-2.4
467.2030	HMDB0179776	(3E,5Z)-6-{4,4-dimethyl-3-[(3-methylbut-2-en-1-yl)oxy]-3,4-dihydro-2H-1,5-benzodioxepin-7-yl}-3-(hydroxymethyl)-2-(methoxymethylidene)hexa-3,5-dienoic acid	C25H32O7	M+Na	467.2040	-2.2
	HMDB0030156	Austalide J	C25H32O7	M+Na	467.2040	-2.2
	HMDB0062337	N-oleoyl tyrosine	C27H43NO4	M+Na	468.3084	-1.6
	HMDB0179451	6',11-dihydroxy-5',7',9,13-tetramethyl-5-oxaspiro[pentacyclo[.8.?,icosane-6,2'-piperidine]-16-one	C27H43NO4	M+Na	468.3084	-1.6
468.3077	HMDB0161447	2-oxo-3-(phosphonatoxy)propyl nonadecanoate	C22H41O7P	M+NH4	468.3085	-1.6
	HMDB0010379	LysoPC(14)	C22H46NO7P	M+H	468.3085	-1.6
	HMDB0061691	1-Heptadecanoylglycerophosphoethanolamine	C22H46NO7P	M+H	468.3085	-1.6
469.3123	HMDB0165682	3,4,5-trihydroxy-6-(octadecyloxy)oxane-2-carboxylic acid	C24H46O7	M+Na	469.3136	-2.7
	HMDB0165680	3,4,5-trihydroxy-6-(octadecan-2-yloxy)oxane-2-carboxylic acid	C24H46O7	M+Na	469.3136	-2.7
472.2744	HMDB0033370	Ethyl cellulose	C20H38O11	M+NH4	472.2752	-1.8
	HMDB0029925	Methyl cellulose	C20H38O11	M+NH4	472.2752	-1.8
476.1974	HMDB0041222	a-L-Fucopyranosyl-(1->2)-b-D-galactopyranosyl-(1->2)-D-xylose	C17H30O14	M+NH4	476.1974	0.0
477.1976	HMDB0035635	Adouetine X	C21H32O12	M+H	477.1967	2.0
479.1767	HMDB0038714	Kelampayoside A	C20H30O13	M+H	479.1759	1.6
	HMDB0032134	Gentiobiosyl 2-methyl-6-oxo-2E,4E-heptadienoate	C20H30O13	M+H	479.1759	1.6
479.3838	HMDB0030272	AC1L2U2M	C28H50N2O4	M+H	479.3843	-1.1
	HMDB0159392	1-(5-{[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]methyl}-3,4-dihydroxyoxolan-2-yl)-5-methanimidamido-1H-pyrazole-4-carboxylic acid	C16H22N4O12	M+NH4	480.1572	-2.6
	HMDB0159393	6-{1-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-5-methanimidamido-1H-pyrazole-4-carbonyloxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H22N4O12	M+NH4	480.1572	-2.6
	HMDB0159390	1-{4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-3-hydroxy-5-(hydroxymethyl)oxolan-2-yl}-5-methanimidamido-1H-pyrazole-4-carboxylic acid	C16H22N4O12	M+NH4	480.1572	-2.6
480.1560	HMDB0155765	1-(5-{[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]methyl}-3,4-dihydroxyoxolan-2-yl)-5-methanimidamido-1H-imidazole-4-carboxylic acid	C16H22N4O12	M+NH4	480.1572	-2.6
	HMDB0155764	1-{3-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl}-5-methanimidamido-1H-imidazole-4-carboxylic acid	C16H22N4O12	M+NH4	480.1572	-2.6
	HMDB0155766	6-{1-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-5-methanimidamido-1H-imidazole-4-carbonyloxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H22N4O12	M+NH4	480.1572	-2.6
	HMDB0155763	1-{4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-3-hydroxy-5-(hydroxymethyl)oxolan-2-yl}-5-methanimidamido-1H-imidazole-4-carboxylic acid	C16H22N4O12	M+NH4	480.1572	-2.6
	HMDB0159391	1-{3-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl}-5-methanimidamido-1H-pyrazole-4-carboxylic acid	C16H22N4O12	M+NH4	480.1572	-2.6
	HMDB0172575	2-oxo-3-(phosphonatoxy)propyl (1E)-icos-11-enoate	C23H41O7P	M+NH4	480.3085	-1.0
	HMDB0114758	LysoPA(:2(11Z,14Z))	C23H43O7P	M+NH4	480.3085	-1.0

480.3080	HMDB0062303	[(2R)-2-hydroxy-3-[(11Z)-icosa-11,14-dienoyloxy]propoxy]phosphonic acid	C23H43O7P	M+NH4	480.3085	-1.0
	HMDB0011476	LysoPE/18:1(9Z))	C23H46NO7P	M+H	480.3085	-1.0
	HMDB0011506	LysoPE(18:1(9Z))	C23H46NO7P	M+H	480.3085	-1.0
	HMDB0011505	LysoPE(18:1(11Z))	C23H46NO7P	M+H	480.3085	-1.0
	HMDB0011475	LysoPE/18:1(11Z))	C23H46NO7P	M+H	480.3085	-1.0
480.4039	HMDB0039713	(3beta,22R,23R,24S)-3,22,23-Trihydroxystigmastan-6-one	C29H50O4	M+NH4	480.4047	-1.7
	HMDB0034430	6-Deoxohomodolichosterone	C29H50O4	M+NH4	480.4047	-1.7
482.0384	HMDB0149975	3-carboxy-6,11-dihydroxy-7-[3-hydroxy-5-methoxy-4-(sulfooxy)phenyl]-2,4,6,9,11-hexaen-2-ylidene-1(13),2,4,6,9,11-hexaen-2-ylum	C19H13O12S	M+NH4	482.0388	-0.8
482.3235	HMDB0172583	2-hydroxy-3-(phosphonatooxy)propyl (11E)-icos-11-enoate	C23H43O7P	M+NH4	482.3241	-1.3
	HMDB0062305	Pa:(1(11z))	C23H45O7P	M+NH4	482.3241	-1.3
	HMDB0172584	SCHEMBL63612	C23H45O7P	M+NH4	482.3241	-1.3
	HMDB0010381	LysoPC(15)	C23H48NO7P	M+H	482.3241	-1.3
	HMDB0011130	LysoPE(18)	C23H48NO7P	M+H	482.3241	-1.3
	HMDB0011129	Pe(18)	C23H48NO7P	M+H	482.3241	-1.3
485.0726	HMDB0041969	Oxazepam glucuronide	C21H19CIN2O8	M+Na	485.0722	0.8
487.1036	HMDB0041380	Garciduel A	C27H18O9	M+H	487.1024	2.5
	HMDB0030279	Garciduel C	C27H18O9	M+H	487.1024	2.5
487.3306	HMDB0060159	Ebastine	C32H39NO2	M+NH4	487.3319	-2.7
488.2691	HMDB0157476	4-[(2S,15R)-2,15-dimethyl-5-oxo-16-(sulfooxy)tetracyclo[8.7,,heptadecan-14-yl]pentanoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0157501	4-[(2S,15S)-5-hydroxy-2,15-dimethyl-16-(sulfooxy)tetracyclo[8.7,,heptadecan-14-yl]pent-4-enoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0157500	4-[(2S,15S)-16-hydroxy-2,15-dimethyl-5-(sulfooxy)tetracyclo[8.7,,heptadecan-14-yl]pent-4-enoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0159181	4-[(1S,2S,7S,R,11S,15R)-2,15-dimethyl-5-oxo-9-(sulfooxy)tetracyclo[8.7,,heptadecan-14-yl]pentanoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0159184	4-[(2S,15R)-2,15-dimethyl-5-oxo-9-(sulfooxy)tetracyclo[8.7,,heptadecan-14-yl]pentanoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0159241	4-[(1S,2S,7S,R,11S,15R)-2,15-dimethyl-9-oxo-5-(sulfooxy)tetracyclo[8.7,,heptadecan-14-yl]pentanoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0159729	4-[(1S,2S,7R,R,11S,15R)-2,15-dimethyl-5-oxo-9-(sulfooxy)tetracyclo[8.7,,heptadecan-14-yl]pentanoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0157090	4-[(1S,2S,7R,R,11S,14R,15R)-2,15-dimethyl-16-oxo-5-(sulfooxy)tetracyclo[8.7,,heptadecan-14-yl]pentanoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0156579	4-[(2R,15R)-5-hydroxy-2,15-dimethyl-9-(sulfooxy)tetracyclo[8.7,,heptadec-7-en-14-yl]pentanoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0156578	4-[(2R,15R)-9-hydroxy-2,15-dimethyl-5-(sulfooxy)tetracyclo[8.7,,heptadec-7-en-14-yl]pentanoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0156575	4-[(2R,15R)-6-hydroxy-2,15-dimethyl-5-(sulfooxy)tetracyclo[8.7,,heptadec-7-en-14-yl]pentanoic acid	C24H38O7S	M+NH4	488.2676	3.0

	HMDB0156573	4-[(2R,15S)-2,15-dimethyl-5-(sulfooxy)tetracyclo[8.7,,heptadec-7-en-14-yl]-4-hydroxypentanoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0156571	4-[(2R,15S)-15-(hydroxymethyl)-2-methyl-5-(sulfooxy)tetracyclo[8.7,,heptadec-7-en-14-yl]pentanoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0156569	4-[(2S,15R)-2-(hydroxymethyl)-15-methyl-5-(sulfooxy)tetracyclo[8.7,,heptadec-7-en-14-yl]pentanoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0156567	4-[(2R,15S)-13-hydroxy-2,15-dimethyl-5-(sulfooxy)tetracyclo[8.7,,heptadec-7-en-14-yl]pentanoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0156563	4-[(2R,15S)-2,15-dimethyl-5-(sulfooxy)tetracyclo[8.7,,heptadec-7-en-14-yl]-5-hydroxypentanoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0156565	4-[(2R,15R)-17-hydroxy-2,15-dimethyl-5-(sulfooxy)tetracyclo[8.7,,heptadec-7-en-14-yl]pentanoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0184302	4-[(2S,15S)-9-hydroxy-2,15-dimethyl-5-(sulfooxy)tetracyclo[8.7,,heptadecan-14-yl]pent-4-enoic acid	C24H38O7S	M+NH4	488.2676	3.0
	HMDB0032799	(R)-1-O-[b-D-Glucopyranosyl-(1->6)-b-D-glucopyranoside]-1,3-octanediol	C20H38O12	M+NH4	488.2702	-2.2
488.9780	HMDB0142303	2-[3,5-dihydroxy-4-(sulfooxy)phenyl]-8-hydroxy-3-(sulfooxy)-3,4-dihydro-2H-1-benzopyran-6-olate	C15H13O13S2	M+Na	488.9768	2.5
489.3476	HMDB0014486	Terfenadine	C32H41NO2	M+NH4	489.3476	0.1
491.1560	HMDB0130657	3,4,5-trihydroxy-6-{[2-(3-hydroxyphenyl)-5-methoxy-6,8-dimethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-7-yl]oxy}oxane-2-carboxylic acid	C24H26O11	M+H	491.1548	2.5
	HMDB0130656	3,4,5-trihydroxy-6-[3-(7-hydroxy-5-methoxy-6,8-dimethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)phenoxy]oxane-2-carboxylic acid	C24H26O11	M+H	491.1548	2.5
	HMDB0130650	3,4,5-trihydroxy-6-{[2-(2-hydroxyphenyl)-5-methoxy-6,8-dimethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-7-yl]oxy}oxane-2-carboxylic acid	C24H26O11	M+H	491.1548	2.5
	HMDB0130649	3,4,5-trihydroxy-6-[2-(7-hydroxy-5-methoxy-6,8-dimethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)phenoxy]oxane-2-carboxylic acid	C24H26O11	M+H	491.1548	2.5
	HMDB0130651	3,4,5-trihydroxy-6-[4-(7-hydroxy-5-methoxy-6,8-dimethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)phenoxy]oxane-2-carboxylic acid	C24H26O11	M+H	491.1548	2.5
	HMDB0145213	3,4,5-trihydroxy-6-({2-hydroxy-3-[2-(3-phenylpropanoyl)phenoxy]propanoyl}oxy)oxane-2-carboxylic acid	C24H26O11	M+H	491.1548	2.5
	HMDB0145212	6-{1-carboxy-2-[2-(3-phenylpropanoyl)phenoxy]ethoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H26O11	M+H	491.1548	2.5
	HMDB0149102	3,4,5-trihydroxy-6-{2-hydroxy-5-[5-(3-hydroxypropyl)-7-methoxy-1-benzofuran-2-yl]phenoxy}oxane-2-carboxylic acid	C24H26O11	M+H	491.1548	2.5
	HMDB0149103	3,4,5-trihydroxy-6-{2-hydroxy-4-[5-(3-hydroxypropyl)-7-methoxy-1-benzofuran-2-yl]phenoxy}oxane-2-carboxylic acid	C24H26O11	M+H	491.1548	2.5
	HMDB0149504	3,4,5-trihydroxy-6-[(2-hydroxy-5-methoxy-5-oxo-3,4-diphenylpentanoyl)oxy]oxane-2-carboxylic acid	C24H26O11	M+H	491.1548	2.5
	HMDB0149503	6-(1-carboxy-4-methoxy-4-oxo-2,3-diphenylbutoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H26O11	M+H	491.1548	2.5
	HMDB0151691	6-[(3-benzyl-7,8-dimethoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-5-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H26O11	M+H	491.1548	2.5
	HMDB0130652	3,4,5-trihydroxy-6-{[2-(4-hydroxyphenyl)-5-methoxy-6,8-dimethyl-4-oxo-3,4-dihydro-2H-1-benzopyran-7-yl]oxy}oxane-2-carboxylic acid	C24H26O11	M+H	491.1548	2.5

HMDB0130647	3,4,5-trihydroxy-6-{{8-(hydroxymethyl)-5-methoxy-6-methyl-4-oxo-2-phenyl-3,4-dihydro-2H-1-benzopyran-7-yl}oxy}oxane-2-carboxylic acid	C24H26O11	M+H	491.1548	2.5
HMDB0130645	3,4,5-trihydroxy-6-{{6-(hydroxymethyl)-5-methoxy-8-methyl-4-oxo-2-phenyl-3,4-dihydro-2H-1-benzopyran-7-yl}oxy}oxane-2-carboxylic acid	C24H26O11	M+H	491.1548	2.5
HMDB0040512	4',5,6-Trimethylscutellarein 7-glucoside	C24H26O11	M+H	491.1548	2.5
HMDB0141695	5-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1-chloro-3-hydroxy-2-phenyl-decahydro-1-benzopyran-1-ium-7-id-7-olate	C21H26ClO10	M+NH4	491.1558	0.4
HMDB0141694	3-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1-chloro-5-hydroxy-2-phenyl-decahydro-1-benzopyran-1-ium-7-id-7-olate	C21H26ClO10	M+NH4	491.1558	0.4
HMDB0149294	3,4,5-trihydroxy-6-(3-{9-hydroxy-8-oxo-2H,8H-[1,3]dioxolo[4,5-g]chromen-6-yl}phenoxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0149292	3,4,5-trihydroxy-6-(2-{9-hydroxy-8-oxo-2H,8H-[1,3]dioxolo[4,5-g]chromen-6-yl}phenoxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0149295	3,4,5-trihydroxy-6-{{6-(3-hydroxyphenyl)-8-oxo-2H,8H-[1,3]dioxolo[4,5-g]chromen-9-yl}oxy}oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0147586	3,4,5-trihydroxy-6-({5-hydroxy-12-methoxy-9-oxo-8,17-dioxatetracyclo[8.7,,heptadeca-1(0),2(7),3,5,11,13,15-heptaen-14-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0147585	3,4,5-trihydroxy-6-({14-hydroxy-12-methoxy-9-oxo-8,17-dioxatetracyclo[8.7,,heptadeca-1(0),2(7),3,5,11,13,15-heptaen-5-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0146705	3,4,5-trihydroxy-6-{{3-(4-hydroxy-2H-1,3-benzodioxol-5-yl)-4-oxo-4H-chromen-7-yl}oxy}oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0174955	6-[(3-formyl-6-hydroxy-8-methoxy-9,-dioxo-9,-dihydroanthracen-1-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0146704	3,4,5-trihydroxy-6-{{5-(7-hydroxy-4-oxo-4H-chromen-3-yl)-2H-1,3-benzodioxol-4-yl}oxy}oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0146586	3,4,5-trihydroxy-6-{{7-(4-hydroxyphenyl)-8-oxo-2H,8H-[1,3]dioxolo[4,5-g]chromen-9-yl}oxy}oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0146587	3,4,5-trihydroxy-6-(4-{9-hydroxy-8-oxo-2H,8H-[1,3]dioxolo[4,5-g]chromen-7-yl}phenoxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0146160	3,4,5-trihydroxy-6-({6-hydroxy-5-methoxy-9-oxo-8,17-dioxatetracyclo[8.7,,heptadeca-1(0),2(7),3,5,11(16),12,14-heptaen-14-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0146161	3,4,5-trihydroxy-6-({14-hydroxy-5-methoxy-9-oxo-8,17-dioxatetracyclo[8.7,,heptadeca-1(0),2(7),3,5,11(16),12,14-heptaen-6-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0149293	3,4,5-trihydroxy-6-{{6-(2-hydroxyphenyl)-8-oxo-2H,8H-[1,3]dioxolo[4,5-g]chromen-9-yl}oxy}oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0149298	3,4,5-trihydroxy-6-{{6-(4-hydroxyphenyl)-8-oxo-2H,8H-[1,3]dioxolo[4,5-g]chromen-9-yl}oxy}oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0149297	3,4,5-trihydroxy-6-(4-{9-hydroxy-8-oxo-2H,8H-[1,3]dioxolo[4,5-g]chromen-6-yl}phenoxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0174956	6-[(7-formyl-5-hydroxy-4-methoxy-9,-dioxo-9,-dihydroanthracen-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9

HMDB0150615	6-{{3-(2H-1,3-benzodioxol-5-yl)-5-hydroxy-4-oxo-4H-chromen-7-yl}oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0150612	6-{{3-(2H-1,3-benzodioxol-5-yl)-7-hydroxy-4-oxo-4H-chromen-8-yl}oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0150614	6-{{3-(2H-1,3-benzodioxol-5-yl)-7-hydroxy-4-oxo-4H-chromen-5-yl}oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0150611	6-{{3-(2H-1,3-benzodioxol-5-yl)-6-hydroxy-4-oxo-4H-chromen-7-yl}oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0150613	6-{{3-(2H-1,3-benzodioxol-5-yl)-8-hydroxy-4-oxo-4H-chromen-7-yl}oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0150608	3,4,5-trihydroxy-6-{{6-(7-hydroxy-4-oxo-4H-chromen-3-yl)-2H-1,3-benzodioxol-5-yl}oxy}oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0150609	3,4,5-trihydroxy-6-{{3-(6-hydroxy-2H-1,3-benzodioxol-5-yl)-4-oxo-4H-chromen-7-yl}oxy}oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0150610	6-{{3-(2H-1,3-benzodioxol-5-yl)-7-hydroxy-4-oxo-4H-chromen-6-yl}oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0149765	3,4,5-trihydroxy-6-({14-hydroxy-3-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(),2,4,6,11(16),12,14-heptaen-5-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0149766	3,4,5-trihydroxy-6-({5-hydroxy-3-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(),2,4,6,11(16),12,14-heptaen-14-yl}oxy)oxane-2-	C22H18O12	M+NH4	492.1136	2.9
HMDB0140328	3,4,5-trihydroxy-6-({5-hydroxy-14-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(),2(7),3,5,11(16),12,14-heptaen-12-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0140329	3,4,5-trihydroxy-6-({12-hydroxy-14-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(),2(7),3,5,11,13,15-heptaen-5-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0140327	3,4,5-trihydroxy-6-({3-hydroxy-14-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(),2,4,6,11(16),12,14-heptaen-5-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0131396	2-(2H-1,3-benzodioxol-5-yl)-6-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1-benzofuran-5-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0128471	3,4,5-trihydroxy-6-({5-hydroxy-13-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(),2(7),3,5,11,13,15-heptaen-14-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0128469	3,4,5-trihydroxy-6-({5-hydroxy-14-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(),2(7),3,5,11,13,15-heptaen-13-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0128468	3,4,5-trihydroxy-6-({13-hydroxy-14-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(),2(7),3,5,11,13,15-heptaen-5-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0128470	3,4,5-trihydroxy-6-({14-hydroxy-13-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(),2(7),3,5,11,13,15-heptaen-5-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
HMDB0126143	6-({16,18-dioxo-6,8,19-trioxapentacyclo[.7.,nonadeca-1(12),2(9),4.,13(17)-pentaen-11-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9

	HMDB0002375	Chicoric acid	C22H18O12	M+NH4	492.1136	2.9
	HMDB0131397	6-[2-(2H-1,3-benzodioxol-5-yl)-6-hydroxy-1-benzofuran-5-carbonyloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
	HMDB0131401	2-{6-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-2H-1,3-benzodioxol-5-yl}-1-benzofuran-5-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
	HMDB0131402	3,4,5-trihydroxy-6-[2-(6-hydroxy-2H-1,3-benzodioxol-5-yl)-1-benzofuran-5-carbonyloxy]oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
	HMDB0140323	3,4,5-trihydroxy-6-({6-hydroxy-14-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(0),2(7),3,5,11(16),12,14-heptaen-5-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
	HMDB0140325	3,4,5-trihydroxy-6-({15-hydroxy-14-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(0),2(7),3,5,11(16),12,14-heptaen-5-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
	HMDB0140324	3,4,5-trihydroxy-6-({5-hydroxy-14-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(0),2(7),3,5,11(16),12,14-heptaen-15-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
	HMDB0140326	3,4,5-trihydroxy-6-({5-hydroxy-14-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(0),2(7),3,5,11(16),12,14-heptaen-3-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
	HMDB0140320	3,4,5-trihydroxy-6-({5-hydroxy-14-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(0),2,4,6,11(16),12,14-heptaen-4-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
	HMDB0140321	3,4,5-trihydroxy-6-({4-hydroxy-14-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(0),2,4,6,11(16),12,14-heptaen-5-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
	HMDB0140322	3,4,5-trihydroxy-6-({5-hydroxy-14-methoxy-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(0),2(7),3,5,11(16),12,14-heptaen-6-yl}oxy)oxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
	HMDB0131412	6-[2-(2H-1,3-benzodioxol-5-yl)-4-hydroxy-1-benzofuran-5-carbonyloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
	HMDB0131411	2-(2H-1,3-benzodioxol-5-yl)-4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1-benzofuran-5-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
	HMDB0131406	2-(2H-1,3-benzodioxol-5-yl)-7-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1-benzofuran-5-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
	HMDB0131407	6-[2-(2H-1,3-benzodioxol-5-yl)-7-hydroxy-1-benzofuran-5-carbonyloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H18O12	M+NH4	492.1136	2.9
	HMDB0033938	D-Chicoric acid	C22H18O12	M+NH4	492.1136	2.9
494.3231	HMDB0006510	Cervonyl carnitine	C29H45NO4	M+Na	494.3241	-2.0
	HMDB0010383	LysoPC(16:1(9Z))	C24H48NO7P	M+H	494.3241	-2.1
496.3389	HMDB0061702	2-Palmitoylglycerophosphocholine	C24H51NO7P	M+H	496.3403	-2.9
	HMDB0006321	Docosa-4,7,,13,16-pentaenoyl carnitine	C29H47NO4	M+Na	496.3397	-1.7
	HMDB0031402	23-Acetoxysoladulcidine	C29H47NO4	M+Na	496.3397	-1.7
	HMDB0006496	Clupanodonyl carnitine	C29H47NO4	M+Na	496.3397	-1.7
	HMDB0184256	2-oxo-3-(phosphonatoxy)propyl henicosanoate	C24H45O7P	M+NH4	496.3398	-1.7
	HMDB0183357	2-oxo-3-(phosphonatoxy)propyl 4,8,12,16-tetramethylheptadecanoate	C24H45O7P	M+NH4	496.3398	-1.7
	HMDB0010382	LysoPC(16)	C24H50NO7P	M+H	496.3398	-1.7
	HMDB0240262	LysoPC(16)	C24H50NO7P	M+H	496.3398	-1.7

	HMDB0062541	[3-(hexadecanoyloxy)-2-hydroxypropoxy][2-(trimethylazaniumyl)ethoxy]phosphinic acid	C24H51NO7P	M+H	496.3398	-1.7
498.5614	HMDB0041478	1-Tritriacontanol	C33H68O	M+NH4	498.5608	1.1
499.1579	HMDB0158102	3,4,5-trihydroxy-6-{[(15S)-8-hydroxy-15-methyl-13,14-dioxotetracyclo[8.7.,heptadeca-2(7),3,5-trien-5-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0158100	3,4,5-trihydroxy-6-{[(15S)-4-hydroxy-15-methyl-13,14-dioxotetracyclo[8.7.,heptadeca-2,4,6-trien-5-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0158096	3,4,5-trihydroxy-6-{[(15S)-15-(hydroxymethyl)-13,14-dioxotetracyclo[8.7.,heptadeca-2,4,6-trien-5-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0158099	3,4,5-trihydroxy-6-{[(15R)-5-hydroxy-15-methyl-13,14-dioxotetracyclo[8.7.,heptadeca-2,4,6-trien-4-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0158093	3,4,5-trihydroxy-6-{[(15S)-5-hydroxy-15-methyl-13,14-dioxotetracyclo[8.7.,heptadeca-2,4,6-trien-9-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0151527	3,4,5-trihydroxy-6-[3-hydroxy-5-methoxy-4,6-dimethyl-2-(3-phenylpropanoyl)phenoxy]oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0150337	3,4,5-trihydroxy-6-{[3-hydroxy-1,2-bis(4-methoxyphenyl)but-3-en-1-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0140242	3,4,5-trihydroxy-6-{[5-(2-hydroxyethyl)-2-(3-methoxyphenyl)-3-methyl-2,3-dihydro-1-benzofuran-7-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0158105	3,4,5-trihydroxy-6-{[(15S)-5-hydroxy-15-methyl-13,14-dioxotetracyclo[8.7.,heptadeca-2,4,6-trien-3-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0158106	3,4,5-trihydroxy-6-{[(15S)-3-hydroxy-15-methyl-13,14-dioxotetracyclo[8.7.,heptadeca-2,4,6-trien-5-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0158144	3,4,5-trihydroxy-6-{[(15S)-9-hydroxy-15-methyl-13,14-dioxotetracyclo[8.7.,heptadeca-2,4,6-trien-5-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0158120	3,4,5-trihydroxy-6-{[(15R)-16-hydroxy-15-methyl-13,14-dioxotetracyclo[8.7.,heptadeca-2,4,6-trien-5-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0158117	3,4,5-trihydroxy-6-{[(15S)-17-hydroxy-15-methyl-13,14-dioxotetracyclo[8.7.,heptadeca-2,4,6-trien-5-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0158115	3,4,5-trihydroxy-6-{[(15S)-1-hydroxy-15-methyl-13,14-dioxotetracyclo[8.7.,heptadeca-2,4,6-trien-5-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0158113	3,4,5-trihydroxy-6-{[(15S)-hydroxy-15-methyl-13,14-dioxotetracyclo[8.7.,heptadeca-2,4,6-trien-5-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0158108	3,4,5-trihydroxy-6-{[(15S)-12-hydroxy-15-methyl-13,14-dioxotetracyclo[8.7.,heptadeca-2,4,6-trien-5-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0158111	3,4,5-trihydroxy-6-{[(15S)-11-hydroxy-15-methyl-13,14-dioxotetracyclo[8.7.,heptadeca-2,4,6-trien-5-yl]oxy}oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0131236	6-[3,5-dimethoxy-2-methyl-6-(3-phenylpropanoyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
	HMDB0130654	3,4,5-trihydroxy-6-[(4-hydroxy-5-methoxy-6,8-dimethyl-2-phenyl-3,4-dihydro-2H-1-benzopyran-7-yl)oxy]oxane-2-carboxylic acid	C24H28O10	M+Na	499.1575	0.9
500.3062	HMDB0014936	Gentamicin	C21H43N5O7	M+Na	500.3055	1.5
	HMDB0172589	6-[(19-carboxynonadec-9-en-8-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H46O9	M+H	503.3215	2.9

503.3229	HMDB0172590	3,4,5-trihydroxy-6-[(13-hydroxyicos-11-enoyl)oxy]oxane-2-carboxylic acid	C26H46O9	M+H	503.3215	2.9
	HMDB0172592	6-[(1-carboxynonadec--en-9-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H46O9	M+H	503.3215	2.9
	HMDB0172593	3,4,5-trihydroxy-6-{[(11E)--hydroxyicos-11-enoyl]oxy}oxane-2-carboxylic acid	C26H46O9	M+H	503.3215	2.9
	HMDB0172595	6-{[(9E)-19-carboxynonadec-9-en-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H46O9	M+H	503.3215	2.9
	HMDB0172596	3,4,5-trihydroxy-6-{[(11E)-19-hydroxyicos-11-enoyl]oxy}oxane-2-carboxylic acid	C26H46O9	M+H	503.3215	2.9
	HMDB0172598	3,4,5-trihydroxy-6-{[-(3-octyloxiran-2-yl)decanoyl]oxy}oxane-2-carboxylic acid	C26H46O9	M+H	503.3215	2.9
	HMDB0172602	3,4,5-trihydroxy-6-{[(11E)--hydroxyicos-11-enoyl]oxy}oxane-2-carboxylic acid	C26H46O9	M+H	503.3215	2.9
	HMDB0172601	6-{[(9E)-19-carboxynonadec-9-en-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H46O9	M+H	503.3215	2.9
	HMDB0172604	6-{[(E)-1-carboxynonadec--en-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H46O9	M+H	503.3215	2.9
	HMDB0172605	3,4,5-trihydroxy-6-{[(11E)-2-hydroxyicos-11-enoyl]oxy}oxane-2-carboxylic acid	C26H46O9	M+H	503.3215	2.9
508.3387	HMDB0062306	Pa(22:2(13z,16z))	C25H47O7P	M+NH4	508.3398	-2.1
	HMDB0114751	LysoPA(22:2(13Z,16Z))	C25H47O7P	M+NH4	508.3398	-2.1
	HMDB0011512	LysoPE:(1(11Z))	C25H50NO7P	M+H	508.3398	-2.1
	HMDB0011482	LysoPE/:1(11Z))	C25H50NO7P	M+H	508.3398	-2.1
508.3747	HMDB0013122	LysoPC(P-18)	C26H54NO6P	M+H	508.3762	-2.9
509.3792	HMDB0035150	2'-Apo-beta-carotenal	C37H48O	M+H	509.3778	2.8
510.3548	HMDB0062304	Pa(22:1(11z))	C25H49O7P	M+NH4	510.3554	-1.2
	HMDB0114750	LysoPA(22:1(13Z))	C25H49O7P	M+NH4	510.3554	-1.2
	HMDB0011481	LysoPE/)	C25H52NO7P	M+H	510.3554	-1.2
	HMDB0011511	LysoPE()	C25H52NO7P	M+H	510.3554	-1.2
	HMDB0012108	LysoPC(17)	C25H52NO7P	M+H	510.3554	-1.2
	HMDB0147758	6-({14,15-dihydroxy-5,7,11,19-tetraoxapentacyclo[.8,?, 寶]icosa-2,4(8),9,13,15,17-hexaen-16-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
	HMDB0147760	6-({14,16-dihydroxy-5,7,11,19-tetraoxapentacyclo[.8,?, 寶]icosa-2,4(8),9,13(18),14,16-hexaen-15-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
	HMDB0150821	6-[5-(5,7-dihydroxy-6-methoxy-4-oxo-4H-chromen-2-yl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
	HMDB0150820	6-{[2-(3,4-dihydroxyphenyl)-7-hydroxy-6-methoxy-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
	HMDB0146155	6-({1,14-dihydroxy-5,7,11,19-tetraoxapentacyclo[.8,?, 寶]icosa-2,4(8),9,13,15,17-hexaen-16-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
	HMDB0150822	6-[4-(5,7-dihydroxy-6-methoxy-4-oxo-4H-chromen-2-yl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
	HMDB0150825	6-{[2-(3,4-dihydroxyphenyl)-7-hydroxy-5-methoxy-4-oxo-4H-chromen-6-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
	HMDB0151490	3,4,5-trihydroxy-6-{4-[3,5,6-trihydroxy-8-(hydroxymethyl)-4-oxo-4H-chromen-2-yl]phenoxy}oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5

HMDB0151492	6- {[3,6-dihydroxy-8-(hydroxymethyl)-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0151493	6- {[5,6-dihydroxy-8-(hydroxymethyl)-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0151463	3,4,5-trihydroxy-6- {[5,6,7-trihydroxy-2-(4-hydroxyphenyl)-8-methyl-4-oxo-4H-chromen-3-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0151462	3,4,5-trihydroxy-6- {[3,6,7-trihydroxy-2-(4-hydroxyphenyl)-8-methyl-4-oxo-4H-chromen-5-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0151461	3,4,5-trihydroxy-6- {[3,5,7-trihydroxy-2-(4-hydroxyphenyl)-8-methyl-4-oxo-4H-chromen-6-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0151459	3,4,5-trihydroxy-6- {[3,5,6-trihydroxy-2-(4-hydroxyphenyl)-8-methyl-4-oxo-4H-chromen-7-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0151460	3,4,5-trihydroxy-6-[4-(3,5,6,7-tetrahydroxy-8-methyl-4-oxo-4H-chromen-2-yl)phenoxy]oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0150827	6-[4-(6,7-dihydroxy-5-methoxy-4-oxo-4H-chromen-2-yl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0150824	6- {[2-(3,4-dihydroxyphenyl)-6-hydroxy-5-methoxy-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0150826	6-[5-(6,7-dihydroxy-5-methoxy-4-oxo-4H-chromen-2-yl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0151491	6- {[3,5-dihydroxy-8-(hydroxymethyl)-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-6-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0138832	6-(3-{2,12-dihydroxy-13-oxo-4,6,-trioxatricyclo[7.4, trideca-1,3(7),8-trien-11-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0138837	3,4,5-trihydroxy-6- {[12-hydroxy-11-(4-hydroxyphenyl)-13-oxo-4,6,-trioxatricyclo[7.4, trideca-1,3(7),8-trien-2-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0138836	6-(4-{2,12-dihydroxy-13-oxo-4,6,-trioxatricyclo[7.4, trideca-1,3(7),8-trien-11-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0138833	3,4,5-trihydroxy-6- {[12-hydroxy-11-(3-hydroxyphenyl)-13-oxo-4,6,-trioxatricyclo[7.4, trideca-1,3(7),8-trien-2-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0136028	6-[2,3-dihydroxy-4-(5-hydroxy-7-methoxy-4-oxo-4H-chromen-3-yl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0136026	6-[2,5-dihydroxy-4-(5-hydroxy-7-methoxy-4-oxo-4H-chromen-3-yl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0136025	6-[4-(5,6-dihydroxy-7-methoxy-4-oxo-4H-chromen-3-yl)-3-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0135938	3,4,5-trihydroxy-6- {[5-methoxy-4-oxo-3-(2,3,4-trihydroxyphenyl)-4H-chromen-7-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0135935	3,4,5-trihydroxy-6- {[5-methoxy-4-oxo-3-(2,4,5-trihydroxyphenyl)-4H-chromen-7-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0138841	3,4,5-trihydroxy-6- {[12-hydroxy-11-(2-hydroxyphenyl)-13-oxo-4,6,-trioxatricyclo[7.4, trideca-1,3(7),8-trien-2-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5

HMDB0138840	6-(2-{2,12-dihydroxy-13-oxo-4,6,-trioxatricyclo[7.4, trideca-1,3(7),8-trien-11-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0147759	6-({15,16-dihydroxy-5,7,11,19-tetraoxapentacyclo[.8,?, 寶 icoso-2,4(8),9,13(18),14,16-hexaen-14-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0146288	6-[4-(5,6-dihydroxy-7-methoxy-4-oxo-4H-chromen-3-yl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0146291	6-[2,6-dihydroxy-4-(5-hydroxy-7-methoxy-4-oxo-4H-chromen-3-yl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0146153	6-({1,17-dihydroxy-5,7,11,19-tetraoxapentacyclo[.8,?, 寶 icoso-2,4(8),9,13(18),14,16-hexaen-16-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0146154	6-({1,16-dihydroxy-5,7,11,19-tetraoxapentacyclo[.8,?, 寶 icoso-2,4(8),9,13(18),14,16-hexaen-14-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0146152	6-({1,16-dihydroxy-5,7,11,19-tetraoxapentacyclo[.8,?, 寶 icoso-2,4(8),9,13(18),14,16-hexaen-17-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0146151	6-({1,15-dihydroxy-5,7,11,19-tetraoxapentacyclo[.8,?, 寶 icoso-2,4(8),9,13,15,17-hexaen-16-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0146150	6-({1,16-dihydroxy-5,7,11,19-tetraoxapentacyclo[.8,?, 寶 icoso-2,4(8),9,13,15,17-hexaen-15-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0135937	6-[2,3-dihydroxy-4-(7-hydroxy-5-methoxy-4-oxo-4H-chromen-3-yl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0151504	6-{[2-(3,4-dihydroxyphenyl)-3,5-dihydroxy-8-methyl-4-oxo-4H-chromen-6-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0151503	3,4,5-trihydroxy-6-[2-hydroxy-4-(3,5,6-trihydroxy-8-methyl-4-oxo-4H-chromen-2-yl)phenoxy]oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0153048	3-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-5,7-dihydroxy-2-(1-hydroxy-3-methoxy-4-oxocyclohexa-2,5-dien-1-yl)-1 位?chromen-1-ylum	C22H21O13	M+Na	515.0796	2.5
HMDB0153050	5-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-3,7-dihydroxy-2-(1-hydroxy-3-methoxy-4-oxocyclohexa-2,5-dien-1-yl)-1 位?chromen-1-ylum	C22H21O13	M+Na	515.0796	2.5
HMDB0174957	6-{[1,6-dihydroxy-3-(hydroxymethyl)-8-methoxy-9,-dioxo-9,-dihydroanthracen-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0174958	6-{[2,6-dihydroxy-3-(hydroxymethyl)-8-methoxy-9,-dioxo-9,-dihydroanthracen-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0174961	6-{[3,8-dihydroxy-6-(hydroxymethyl)-1-methoxy-9,-dioxo-9,-dihydroanthracen-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0174959	6-{[5,6-dihydroxy-7-(hydroxymethyl)-4-methoxy-9,-dioxo-9,-dihydroanthracen-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0174962	6-{[6,7-dihydroxy-3-(hydroxymethyl)-8-methoxy-9,-dioxo-9,-dihydroanthracen-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0174963	6-{[3,5-dihydroxy-7-(hydroxymethyl)-4-methoxy-9,-dioxo-9,-dihydroanthracen-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0175005	3,4,5-trihydroxy-6-(4,7,9-trihydroxy-5-methoxy--oxo-9,-dihydroanthracene-2-carbonyloxy)oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5

HMDB0175004	6-[(7-carboxy-5,9-dihydroxy-4-methoxy--oxo-9,-dihydroanthracen-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0175003	6-[(3-carboxy-6,-dihydroxy-8-methoxy-9-oxo-9,-dihydroanthracen-1-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0175008	6-[(7-carboxy-5,-dihydroxy-4-methoxy-9-oxo-9,-dihydroanthracen-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0175007	6-[(3-carboxy-6,9-dihydroxy-8-methoxy--oxo-9,-dihydroanthracen-1-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0175009	3,4,5-trihydroxy-6-(4,7,-trihydroxy-5-methoxy-9-oxo-9,-dihydroanthracene-2-carbonyloxy)oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0177038	6-(5-carboxy-2-{[(1Z)-1-carboxy-2-(3-hydroxyphenyl)eth-1-en-1-yl]oxy}phenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0177037	6-{3-[(1Z)-2-carboxy-2-(4-carboxy-2-hydroxyphenoxy)eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0177039	6-{[(2Z)-2-(4-carboxy-2-hydroxyphenoxy)-3-(3-hydroxyphenyl)prop-2-enoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0153049	(6-carboxy-3,4,5-trihydroxyoxan-2-yl)[3,5-dihydroxy-2-(1-hydroxy-3-methoxy-4-oxocyclohexa-2,5-dien-1-yl)-7H-chromen-7-ylidene]oxidanium	C22H21O13	M+Na	515.0796	2.5
HMDB0153046	2-{4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-3-methoxyphenyl}-3,5,6,7-tetrahydroxy-1H-chromen-1-ylum	C22H21O13	M+Na	515.0796	2.5
HMDB0153042	6-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-3,5,7-trihydroxy-2-(4-hydroxy-3-methoxyphenyl)-1H-chromen-1-ylum	C22H21O13	M+Na	515.0796	2.5
HMDB0151502	3,4,5-trihydroxy-6-[2-hydroxy-5-(3,5,6-trihydroxy-8-methyl-4-oxo-4H-chromen-2-yl)phenoxy]oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0151505	6-{[2-(3,4-dihydroxyphenyl)-3,6-dihydroxy-8-methyl-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0151506	6-{[2-(3,4-dihydroxyphenyl)-5,6-dihydroxy-8-methyl-4-oxo-4H-chromen-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0152041	6-{[7,8-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0152042	6-{[5,8-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0152043	3,4,5-trihydroxy-6-[2-methoxy-5-(5,7,8-trihydroxy-4-oxo-4H-chromen-2-yl)phenoxy]oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0152233	3,4,5-trihydroxy-6-[2-(hydroxymethyl)-5-(3,5,7-trihydroxy-4-oxo-4H-chromen-2-yl)phenoxy]oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0152236	6-({3,7-dihydroxy-2-[3-hydroxy-4-(hydroxymethyl)phenyl]-4-oxo-4H-chromen-5-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0152235	6-({3,5-dihydroxy-2-[3-hydroxy-4-(hydroxymethyl)phenyl]-4-oxo-4H-chromen-7-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0152234	6-({5,7-dihydroxy-2-[3-hydroxy-4-(hydroxymethyl)phenyl]-4-oxo-4H-chromen-3-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0152319	6-({[3,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5

HMDB0152318	SCHEMBL37298	C22H20O13	M+Na	515.0796	2.5
HMDB0152320	SCHEMBL37349	C22H20O13	M+Na	515.0796	2.5
HMDB0152321	SCHEMBL372875	C22H20O13	M+Na	515.0796	2.5
HMDB0153045	5-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-3,6,7-trihydroxy-2-(4-hydroxy-3-methoxyphenyl)-1H-chromen-1-ylum	C22H21O13	M+Na	515.0796	2.5
HMDB0153043	3-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-5,6,7-trihydroxy-2-(4-hydroxy-3-methoxyphenyl)-1H-chromen-1-ylum	C22H21O13	M+Na	515.0796	2.5
HMDB0153044	(6-carboxy-3,4,5-trihydroxyoxan-2-yl)[3,5,6-trihydroxy-2-(4-hydroxy-3-methoxyphenyl)-7H-chromen-7-ylidene]oxidanium	C22H21O13	M+Na	515.0796	2.5
HMDB0177040	6-(4-{[(1Z)-1-carboxy-2-(3-hydroxyphenyl)eth-1-en-1-yl]oxy}-3-hydroxybenzoyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0135934	6-[2,5-dihydroxy-4-(7-hydroxy-5-methoxy-4-oxo-4H-chromen-3-yl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0038772	8-Hydroxyluteolin 4'-methyl ether 8-glucuronide	C22H20O13	M+Na	515.0796	2.5
HMDB0126574	6-{[3,5-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0126577	3,4,5-trihydroxy-6-[2-methoxy-4-(3,5,7-trihydroxy-4-oxo-4H-chromen-2-yl)phenoxy]oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0124879	6-{[2-(3,4-dihydroxy-5-methoxyphenyl)-7-hydroxy-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0124882	6-{[2-(3,5-dihydroxy-4-methoxyphenyl)-5-hydroxy-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0124881	6-[5-(5,7-dihydroxy-4-oxo-4H-chromen-2-yl)-2-hydroxy-3-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0124880	6-[4-(5,7-dihydroxy-4-oxo-4H-chromen-2-yl)-2-hydroxy-6-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0124883	6-{[2-(3,5-dihydroxy-4-methoxyphenyl)-7-hydroxy-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0124884	6-[5-(5,7-dihydroxy-4-oxo-4H-chromen-2-yl)-3-hydroxy-2-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0126046	3,4,5-trihydroxy-6-({5-hydroxy-16,18-dioxo-6,8,19-trioxapentacyclo[7,,,nonadeca-1(12),2(9),,13(17)-tetraen-11-yl]oxy}oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0126575	6-{[3,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0127506	3,4,5-trihydroxy-6-{[3,5,7-trihydroxy-2-(4-methoxyphenyl)-4-oxo-4H-chromen-6-yl]oxy}oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0127508	3,4,5-trihydroxy-6-{[3,6,7-trihydroxy-2-(4-methoxyphenyl)-4-oxo-4H-chromen-5-yl]oxy}oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0127507	3,4,5-trihydroxy-6-{[3,5,6-trihydroxy-2-(4-methoxyphenyl)-4-oxo-4H-chromen-7-yl]oxy}oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0127509	3,4,5-trihydroxy-6-{[5,6,7-trihydroxy-2-(4-methoxyphenyl)-4-oxo-4H-chromen-3-yl]oxy}oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0128797	3,4,5-trihydroxy-6-{[3,6,7-trihydroxy-2-(3-methoxyphenyl)-4-oxo-4H-chromen-5-yl]oxy}oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5

HMDB0128799	3,4,5-trihydroxy-6-{{[3,5,6-trihydroxy-2-(3-methoxyphenyl)-4-oxo-4H-chromen-7-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0039904	3'-Methoxytricetin 7-glucuronide	C22H20O13	M+Na	515.0796	2.5
HMDB0126576	6-{{[5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-4-oxo-4H-chromen-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0030658	Carmine red	C22H20O13	M+Na	515.0796	2.5
HMDB0037459	6-Methoxyluteolin 7-glucuronide	C22H20O13	M+Na	515.0796	2.5
HMDB0041757	Isorhamnetin 4'-O-glucuronide	C22H20O13	M+Na	515.0796	2.5
HMDB0240536	Isorhamnetin 3-glucuronide	C22H20O13	M+Na	515.0796	2.5
HMDB0128798	3,4,5-trihydroxy-6-{{[3,5,7-trihydroxy-2-(3-methoxyphenyl)-4-oxo-4H-chromen-6-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0128800	3,4,5-trihydroxy-6-{{[5,6,7-trihydroxy-2-(3-methoxyphenyl)-4-oxo-4H-chromen-3-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0128821	6-{{[3,7-dihydroxy-2-(3-hydroxyphenyl)-6-methoxy-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0131938	6-{{[2-(3,4-dihydroxyphenyl)-6-hydroxy-7-methoxy-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0131939	6-{{[2-(3,4-dihydroxyphenyl)-5-hydroxy-7-methoxy-4-oxo-4H-chromen-6-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0132012	6-[3-(5,6-dihydroxy-7-methoxy-4-oxo-4H-chromen-2-yl)-5-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0132013	6-{{[2-(3,5-dihydroxyphenyl)-6-hydroxy-7-methoxy-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0132014	6-{{[2-(3,5-dihydroxyphenyl)-5-hydroxy-7-methoxy-4-oxo-4H-chromen-6-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0132144	3,4,5-trihydroxy-6-{{[3,7,8-trihydroxy-2-(4-methoxyphenyl)-4-oxo-4H-chromen-5-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0132143	3,4,5-trihydroxy-6-{{[3,5,8-trihydroxy-2-(4-methoxyphenyl)-4-oxo-4H-chromen-7-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0132147	6-{{[3,7-dihydroxy-2-(4-hydroxyphenyl)-8-methoxy-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0132148	6-{{[5,7-dihydroxy-2-(4-hydroxyphenyl)-8-methoxy-4-oxo-4H-chromen-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0132145	3,4,5-trihydroxy-6-{{[5,7,8-trihydroxy-2-(4-methoxyphenyl)-4-oxo-4H-chromen-3-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0132146	6-{{[3,5-dihydroxy-2-(4-hydroxyphenyl)-8-methoxy-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0132149	3,4,5-trihydroxy-6-[4-(3,5,7-trihydroxy-8-methoxy-4-oxo-4H-chromen-2-yl)phenoxy]oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0133826	6-[5-(3,5-dihydroxy-7-methoxy-4-oxo-4H-chromen-2-yl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0133825	6-[4-(3,5-dihydroxy-7-methoxy-4-oxo-4H-chromen-2-yl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0133827	6-{{[2-(3,4-dihydroxyphenyl)-5-hydroxy-7-methoxy-4-oxo-4H-chromen-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5

HMDB0133828	6- {[2-(3,4-dihydroxyphenyl)-3-hydroxy-7-methoxy-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0135930	6-[4-(6,7-dihydroxy-5-methoxy-4-oxo-4H-chromen-3-yl)-3-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0131936	6-[4-(5,6-dihydroxy-7-methoxy-4-oxo-4H-chromen-2-yl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0131937	6-[5-(5,6-dihydroxy-7-methoxy-4-oxo-4H-chromen-2-yl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0131446	2-{3-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-4-hydroxy-5-methoxyphenyl}-3,5,7-trihydroxy-1H-chromen-1-ylum	C22H21O13	M+Na	515.0796	2.5
HMDB0128822	6- {[3,5-dihydroxy-2-(3-hydroxyphenyl)-6-methoxy-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0128823	6- {[5,7-dihydroxy-2-(3-hydroxyphenyl)-6-methoxy-4-oxo-4H-chromen-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0128824	3,4,5-trihydroxy-6-[3-(3,5,7-trihydroxy-6-methoxy-4-oxo-4H-chromen-2-yl)phenoxy]oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0130186	3,4,5-trihydroxy-6- {[5,7,8-trihydroxy-2-(4-methoxyphenyl)-4-oxo-4H-chromen-6-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0130187	3,4,5-trihydroxy-6- {[6,7,8-trihydroxy-2-(4-methoxyphenyl)-4-oxo-4H-chromen-5-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0130188	3,4,5-trihydroxy-6- {[5,6,8-trihydroxy-2-(4-methoxyphenyl)-4-oxo-4H-chromen-7-yl]oxy} oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0130688	3,4,5-trihydroxy-6-[4-(5,7,8-trihydroxy-6-methoxy-4-oxo-4H-chromen-2-yl)phenoxy]oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0130689	6- {[7,8-dihydroxy-2-(4-hydroxyphenyl)-6-methoxy-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0130693	6- {[5,6-dihydroxy-2-(4-hydroxyphenyl)-8-methoxy-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0130690	6- {[5,8-dihydroxy-2-(4-hydroxyphenyl)-6-methoxy-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0130692	6- {[6,7-dihydroxy-2-(4-hydroxyphenyl)-8-methoxy-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0130691	3,4,5-trihydroxy-6-[4-(5,6,7-trihydroxy-8-methoxy-4-oxo-4H-chromen-2-yl)phenoxy]oxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0130694	6- {[5,7-dihydroxy-2-(4-hydroxyphenyl)-8-methoxy-4-oxo-4H-chromen-6-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
HMDB0131443	(6-carboxy-3,4,5-trihydroxyoxan-2-yl)[2-(3,4-dihydroxy-5-methoxyphenyl)-3,5-dihydroxy-7H-chromen-7-ylidene]oxidanium	C22H21O13	M+Na	515.0796	2.5
HMDB0131442	3-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-2-(3,4-dihydroxy-5-methoxyphenyl)-5,7-dihydroxy-1H-chromen-1-ylum	C22H21O13	M+Na	515.0796	2.5
HMDB0131445	2-{4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-3-hydroxy-5-methoxyphenyl}-3,5,7-trihydroxy-1H-chromen-1-ylum	C22H21O13	M+Na	515.0796	2.5
HMDB0131444	5-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-2-(3,4-dihydroxy-5-methoxyphenyl)-3,7-dihydroxy-1H-chromen-1-ylum	C22H21O13	M+Na	515.0796	2.5

	HMDB0135931	6-([3-(2,4-dihydroxyphenyl)-6-hydroxy-5-methoxy-4-oxo-4H-chromen-7-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H20O13	M+Na	515.0796	2.5
	HMDB0140255	6-({5,7'-dihydroxy-2H,2'H-[6,8'-bichromene]-2,2'-diyl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H18O13	M+H	515.0820	-2.2
	HMDB0140253	6-({7',8'-dihydroxy-2H,2'H-[6,8'-bichromene]-2,2'-diyl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H18O13	M+H	515.0820	-2.2
	HMDB0140250	6-({6',7'-dihydroxy-2H,2'H-[6,8'-bichromene]-2,2'-diyl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H18O13	M+H	515.0820	-2.2
	HMDB0140254	6-({5,7-dihydroxy-2H,2'H-[6,8'-bichromene]-2,2'-diyl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H18O13	M+H	515.0820	-2.2
	HMDB0140249	6-({7,7'-dihydroxy-2H,2'H-[6,8'-bichromene]-2,2'-diyl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H18O13	M+H	515.0820	-2.2
	HMDB0140251	6-({6',7'-dihydroxy-2H,2'H-[6,8'-bichromene]-2,2'-diyl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H18O13	M+H	515.0820	-2.2
	HMDB0140252	6-({7,8-dihydroxy-2H,2'H-[6,8'-bichromene]-2,2'-diyl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H18O13	M+H	515.0820	-2.2
516.3366	HMDB0185592	[(2-{3-[(2R)-6-hydroxy-2,8-dimethyl-3,4-dihydro-2H-1-benzopyran-2-yl]propyl}-6,-dimethylundecyl)oxy]sulfonic acid	C27H46O6S	M+NH4	516.3353	2.5
	HMDB0185594	({9-[(2R)-6-hydroxy-2,8-dimethyl-3,4-dihydro-2H-1-benzopyran-2-yl]-6-methyl-2-(4-methylpentyl)nonyl}oxy)sulfonic acid	C27H46O6S	M+NH4	516.3353	2.5
	HMDB0185590	[(2R)-6-hydroxy-2,8-dimethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-1-benzopyran-4-yl]oxidanesulfonic acid	C27H46O6S	M+NH4	516.3353	2.5
	HMDB0185588	{[(2R)-6-hydroxy-2-methyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-1-benzopyran-8-yl]methoxy}sulfonic acid	C27H46O6S	M+NH4	516.3353	2.5
	HMDB0185581	{[(2R)-6-hydroxy-8-methyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-1-benzopyran-2-yl]methoxy}sulfonic acid	C27H46O6S	M+NH4	516.3353	2.5
	HMDB0172295	{[13-(6-hydroxy-2,7-dimethyl-3,4-dihydro-2H-1-benzopyran-2-yl)-2,6,-trimethyltridecyl]oxy}sulfonic acid	C27H46O6S	M+NH4	516.3353	2.5
	HMDB0172293	{[9-(6-hydroxy-2,7-dimethyl-3,4-dihydro-2H-1-benzopyran-2-yl)-6-methyl-2-(4-methylpentyl)nonyl]oxy}sulfonic acid	C27H46O6S	M+NH4	516.3353	2.5
	HMDB0172291	({2-[3-(6-hydroxy-2,7-dimethyl-3,4-dihydro-2H-1-benzopyran-2-yl)propyl]-6,-dimethylundecyl}oxy)sulfonic acid	C27H46O6S	M+NH4	516.3353	2.5
	HMDB0172285	[6-hydroxy-2,7-dimethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-1-benzopyran-4-yl]oxidanesulfonic acid	C27H46O6S	M+NH4	516.3353	2.5
	HMDB0172283	{[6-hydroxy-2-methyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-1-benzopyran-7-yl]methoxy}sulfonic acid	C27H46O6S	M+NH4	516.3353	2.5
	HMDB0172278	{[6-hydroxy-7-methyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-1-benzopyran-2-yl]methoxy}sulfonic acid	C27H46O6S	M+NH4	516.3353	2.5
	HMDB0185596	({13-[(2R)-6-hydroxy-2,8-dimethyl-3,4-dihydro-2H-1-benzopyran-2-yl]-2,6,-trimethyltridecyl}oxy)sulfonic acid	C27H46O6S	M+NH4	516.3353	2.5
	HMDB0186729	3,4,5-trihydroxy-6-[(2S,17R,18S)-16-hydroxy-2,17,18-trimethyl-6,7-diazapentacyclo[11.7,??]icoso-4,7-dien-17-yl]oxy}oxane-2-carboxylic acid	C27H40N2O8	M+H	521.2857	2.8
	HMDB0186732	3,4,5-trihydroxy-6-[(2S,17S,18S)-17-hydroxy-18-(hydroxymethyl)-2,17-dimethyl-6,7-diazapentacyclo[11.7,??]icoso-4,7-dien-6-yl]oxane-2-carboxylic acid	C27H40N2O8	M+H	521.2857	2.8
	HMDB0186734	3,4,5-trihydroxy-6-[(2S,17S,18S)-17-hydroxy-17-(hydroxymethyl)-2,18-dimethyl-6,7-diazapentacyclo[11.7,??]icoso-4,7-dien-6-yl]oxane-2-carboxylic acid	C27H40N2O8	M+H	521.2857	2.8

521.2872	HMDB0186733	3,4,5-trihydroxy-6-[(2S,17S,18S)-18-(hydroxymethyl)-2,17-dimethyl-6,7-diazapentacyclo[11.7.?? icososa-4,7-dien-17-yl]oxy}oxane-2-carboxylic acid	C27H40N2O8	M+H	521.2857	2.8
	HMDB0186930	6-[(1S,2S,S,13R,14S,17R,18S)-16,17-dihydroxy-2,17,18-trimethyl-6,7-diazapentacyclo[11.7.?? icososa-4(8),5-dien-7-yl]-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H40N2O8	M+H	521.2857	2.8
	HMDB0187482	6-[(1S,2R,R,13R,14S,17S,18S)-9,17-dihydroxy-2,17,18-trimethyl-6,7-diazapentacyclo[11.7.?? icososa-4(8),5-dien-7-yl]-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H40N2O8	M+H	521.2857	2.8
	HMDB0187483	3,4,5-trihydroxy-6-[(1S,2R,R,13R,14S,17S,18S)-9-hydroxy-2,17,18-trimethyl-6,7-diazapentacyclo[11.7.?? icososa-4,7-dien-17-yl]oxy}oxane-2-carboxylic acid	C27H40N2O8	M+H	521.2857	2.8
	HMDB0186730	3,4,5-trihydroxy-6-[(2R,17S,18S)-17-hydroxy-2-(hydroxymethyl)-17,18-dimethyl-6,7-diazapentacyclo[11.7.?? icososa-4,7-dien-6-yl]oxane-2-carboxylic acid	C27H40N2O8	M+H	521.2857	2.8
	HMDB0186728	6-[(2S,17R,18S)-16,17-dihydroxy-2,17,18-trimethyl-6,7-diazapentacyclo[11.7.?? icososa-4,7-dien-6-yl]-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H40N2O8	M+H	521.2857	2.8
	HMDB0186731	3,4,5-trihydroxy-6-[(2R,17S,18S)-2-(hydroxymethyl)-17,18-dimethyl-6,7-diazapentacyclo[11.7.?? icososa-4,7-dien-17-yl]oxy}oxane-2-carboxylic acid	C27H40N2O8	M+H	521.2857	2.8
	HMDB0186726	6-[(2R,17S,18S)-11,17-dihydroxy-2,17,18-trimethyl-6,7-diazapentacyclo[11.7.?? icososa-4,7-dien-6-yl]-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H40N2O8	M+H	521.2857	2.8
	HMDB0186725	3,4,5-trihydroxy-6-[(2S,17S,18S)-hydroxy-2,17,18-trimethyl-6,7-diazapentacyclo[11.7.?? icososa-4,7-dien-17-yl]oxy}oxane-2-carboxylic acid	C27H40N2O8	M+H	521.2857	2.8
	HMDB0186724	6-[(2S,17S,18S)-17-dihydroxy-2,17,18-trimethyl-6,7-diazapentacyclo[11.7.?? icososa-4,7-dien-6-yl]-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H40N2O8	M+H	521.2857	2.8
	HMDB0186727	3,4,5-trihydroxy-6-[(2R,17S,18S)-11-hydroxy-2,17,18-trimethyl-6,7-diazapentacyclo[11.7.?? icososa-4,7-dien-17-yl]oxy}oxane-2-carboxylic acid	C27H40N2O8	M+H	521.2857	2.8
521.3356	HMDB0011485	LysoPE/:3(5Z,8Z,11Z))	C25H46NO7P	M+NH4	521.3350	1.1
	HMDB0011486	LysoPE/:3(8Z,11Z,14Z))	C25H46NO7P	M+NH4	521.3350	1.1
	HMDB0011484	LysoPE/:3(11Z,14Z,17Z))	C25H46NO7P	M+NH4	521.3350	1.1
	HMDB0011514	LysoPE(:3(11Z,14Z,17Z))	C25H46NO7P	M+NH4	521.3350	1.1
	HMDB0011516	LysoPE(:3(8Z,11Z,14Z))	C25H46NO7P	M+NH4	521.3350	1.1
	HMDB0011515	LysoPE(:3(5Z,8Z,11Z))	C25H46NO7P	M+NH4	521.3350	1.1
	HMDB0006599	3-Galactosyllactose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0039706	4-O-beta-Laminaribiosyl-D-glucose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0034072	Gentianose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0039703	3-beta-Gentiobiosylglucose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0029937	Panose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0035322	Fagopyritol B2	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0029922	Galactotriose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0033673	6-Kestose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0038853	beta-D-Galactopyranosyl-(1->3)-beta-D-galactopyranosyl-(1->6)-D-galactose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0029929	6-O-Glucosylmaltose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0039708	3-beta-Cellobiosylglucose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0029910	Gentiotriose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0038852	beta-D-Galactopyranosyl-(1->4)-beta-D-galactopyranosyl-(1->4)-D-galactose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0001262	Maltotriose	C18H32O16	M+NH4	522.2029	-1.8

522.2019	HMDB0003539	Levan	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0006857	Dextrin	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0011729	1-Kestose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0011730	Melezitose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0038851	beta-D-Galactopyranosyl-(1->2)-[beta-D-galactopyranosyl-(1->4)]-D-galactose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0040984	Sophorotriose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0029930	beta-D-Fructofuranosyl alpha-D-glucopyranosyl-(1->4)-D-glucopyranoside	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0041948	Nephritogenoside	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0060468	D-Gal alpha 1->6D-Gal alpha 1->6D-Glucose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0003213	Raffinose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0040181	Fagopyritol A2	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0029921	Neokestose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0033748	Umbelliferose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0039707	alpha-D-Glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->6)-D-glucose	C18H32O16	M+NH4	522.2029	-1.8
	HMDB0039704	alpha-D-Glucopyranosyl-(1->6)-alpha-D-glucopyranosyl-(1->2)-D-glucose	C18H32O16	M+NH4	522.2029	-1.8
522.3545	HMDB0002815	LysoPC(18:1(9Z))	C26H52NO7P	M+H	522.3554	-1.8
	HMDB0061701	2-oleoyl-sn-glycero-3-phosphocholine	C26H52NO7P	M+H	522.3554	-1.8
	HMDB0062651	2-oleoyl-sn-glycero-3-phosphocholine	C26H52NO7P	M+H	522.3554	-1.8
	HMDB0010385	LysoPC(18:1(11Z))	C26H52NO7P	M+H	522.3554	-1.8
524.3711	HMDB0062195	2-acetyl-1-alkyl-sn-glycero-3-phosphocholine	C26H54NO7P	M+H	524.3711	0.1
	HMDB0010384	LysoPC(18)	C26H54NO7P	M+H	524.3711	0.1
	HMDB0011128	LysoPC(18)	C26H54NO7P	M+H	524.3711	0.1
526.3377	HMDB0185169	6-[(13Z,16Z,19Z)-docosa-13,16,19,21-tetraenoyloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H44O8	M+NH4	526.3374	0.5
	HMDB0158857	6-[[11-carboxy-6-,dimethyl-2-(4-methylpentyl)undecyl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
	HMDB0158852	3,4,5-trihydroxy-6-[[3-(hydroxymethyl)-7,11,15-trimethylhexadecanoyl]oxy]oxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
	HMDB0158858	3,4,5-trihydroxy-6-[[11-(hydroxymethyl)-3,7,15-trimethylhexadecanoyl]oxy]oxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
	HMDB0158854	6-[[7-carboxy-2-(4,8-dimethylnonyl)-6-methylheptyl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
	HMDB0158855	3,4,5-trihydroxy-6-[[7-(hydroxymethyl)-3,11,15-trimethylhexadecanoyl]oxy]oxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
	HMDB0158860	6-[(15-carboxy-2,6,,14-tetramethylpentadecyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
	HMDB0158861	3,4,5-trihydroxy-6-[(16-hydroxy-3,7,11,15-tetramethylhexadecanoyl)oxy]oxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
	HMDB0158863	6-[(1-carboxy-2,6,,14-tetramethylpentadecyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
	HMDB0158864	3,4,5-trihydroxy-6-[(2-hydroxy-3,7,11,15-tetramethylhexadecanoyl)oxy]oxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
	HMDB0158851	6-[3-carboxy-2-(4,8,12-trimethyltridecyl)propoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
	HMDB0158847	6-[(15-carboxy-2,6,,14-tetramethylpentadecan-6-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
	HMDB0158843	6-[(1-carboxy-2,6,,14-tetramethylpentadecan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
	HMDB0158846	3,4,5-trihydroxy-6-[(7-hydroxy-3,7,11,15-tetramethylhexadecanoyl)oxy]oxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
	HMDB0158844	3,4,5-trihydroxy-6-[(3-hydroxy-3,7,11,15-tetramethylhexadecanoyl)oxy]oxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6

527.3204

HMDB0158845	6-[(1-carboxy-2,6,,14-tetramethylpentadecan-6-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
HMDB0158848	3,4,5-trihydroxy-6-[(11-hydroxy-3,7,11,15-tetramethylhexadecanoyl)oxy]oxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
HMDB0158850	3,4,5-trihydroxy-6-[(15-hydroxy-3,7,11,15-tetramethylhexadecanoyl)oxy]oxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
HMDB0158849	6-[(15-carboxy-2,6,,14-tetramethylpentadecan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H48O9	M+Na	527.3191	2.6
HMDB0185170	6-{[(12Z,15Z,18Z)-1-carboxyhenicosa-12,15,18-trien-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185142	6-{[(3Z)-21-carboxyhenicosa-3,6,9-trien-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185140	3,4,5-trihydroxy-6-{[(13Z,16Z,19Z)-15-hydroxydocosa-13,16,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185146	3,4,5-trihydroxy-6-{[(13Z,15E,19Z)-17-hydroxydocosa-13,15,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185145	6-{[(3Z,9Z)-21-carboxyhenicosa-3,7,9-trien-6-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185148	6-{[(3Z,6Z)-21-carboxyhenicosa-3,6,8-trien-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185149	3,4,5-trihydroxy-6-{[(16Z,19Z)-13-hydroxydocosa-14,16,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185151	6-{[(6Z,9Z)-21-carboxyhenicosa-4,6,9-trien-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185155	3,4,5-trihydroxy-6-{[(13Z,19Z)-16-hydroxydocosa-13,17,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185154	6-{[(3Z,9Z)-21-carboxyhenicosa-3,5,9-trien-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185152	3,4,5-trihydroxy-6-{[(13Z,16Z,18E)-hydroxydocosa-13,16,18-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185157	3,4,5-trihydroxy-6-[(12-{3-[(2Z,5Z)-octa-2,5-dien-1-yl]oxiran-2-yl}dodecanoyl)oxy]oxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185163	6-{[(13Z,16Z)-18-(3-ethyloxiran-2-yl)octadeca-13,16-dienoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185160	3,4,5-trihydroxy-6-{[(13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadec-13-enoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185167	3,4,5-trihydroxy-6-{[(13Z,16Z,19Z)-22-hydroxydocosa-13,16,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185166	6-{[(3Z,6Z,9Z)-21-carboxyhenicosa-3,6,9-trien-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185171	3,4,5-trihydroxy-6-{[(13Z,16Z,19Z)-2-hydroxydocosa-13,16,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185143	3,4,5-trihydroxy-6-{[(13Z,16Z,19Z)-18-hydroxydocosa-13,16,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185139	6-{[(6Z,9Z)-21-carboxyhenicosa-3,6,9-trien-8-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185133	6-{[(3Z,6Z,9Z)-21-carboxyhenicosa-3,6,9-trien-11-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185137	3,4,5-trihydroxy-6-{[(13Z,16Z,19Z)-21-hydroxydocosa-13,16,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185134	3,4,5-trihydroxy-6-{[(13Z,16Z,19Z)-12-hydroxydocosa-13,16,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0185136	6-{[(6Z,9Z)-21-carboxyhenicosa-3,6,9-trien-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+H	527.3215	-2.0
HMDB0178787	2-amino-4-(1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(8Z)-4-hydroxy-1-methoxy-1-oxodec-8-en-5-yl]sulfanyl)ethyl)-C-hydroxycarbonimidoyl)butanoic acid	C21H35N3O9S	M+Na	528.1986	-0.8

528.1982	HMDB0179408	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{(4Z)-6-hydroxy-1-methoxy-1-oxodec-4-en-3-yl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H35N3O9S	M+Na	528.1986	-0.8
	HMDB0179413	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{(4Z)-3-hydroxy-1-methoxy-1-oxodec-4-en-2-yl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H35N3O9S	M+Na	528.1986	-0.8
	HMDB0179411	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{(4Z)-9-hydroxy-1-methoxy-1-oxodec-4-en-3-yl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H35N3O9S	M+Na	528.1986	-0.8
	HMDB0179419	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{(4Z)--hydroxy-1-methoxy-1-oxodec-4-en-3-yl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H35N3O9S	M+Na	528.1986	-0.8
	HMDB0179414	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{(4Z)-2-hydroxy-1-methoxy-1-oxodec-4-en-3-yl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H35N3O9S	M+Na	528.1986	-0.8
	HMDB0179415	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{(2E)-5-hydroxy-1-methoxy-1-oxodec-2-en-4-yl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H35N3O9S	M+Na	528.1986	-0.8
	HMDB0179416	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(4-hydroxy-1-methoxy-1-oxodec-2-en-5-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H35N3O9S	M+Na	528.1986	-0.8
	HMDB0179417	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{3-methoxy-3-oxo-1-(3-pentylloxiran-2-yl)propyl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H35N3O9S	M+Na	528.1986	-0.8
	HMDB0178788	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{(8Z)-5-hydroxy-1-methoxy-1-oxodec-8-en-4-yl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H35N3O9S	M+Na	528.1986	-0.8
	HMDB0178785	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{(6Z)-3-hydroxy--methoxy-oxodec-6-en-2-yl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H35N3O9S	M+Na	528.1986	-0.8
	HMDB0178786	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{(6Z)-2-hydroxy--methoxy-oxodec-6-en-3-yl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H35N3O9S	M+Na	528.1986	-0.8
	HMDB0163311	(2E)-6-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-5-hydroxyundec-2-enoic acid	C21H35N3O9S	M+Na	528.1986	-0.8
	HMDB0163310	(2E)-5-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-6-hydroxyundec-2-enoic acid	C21H35N3O9S	M+Na	528.1986	-0.8
	HMDB0163308	3-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-2-hydroxyundec-5-enoic acid	C21H35N3O9S	M+Na	528.1986	-0.8
	HMDB0163307	(5Z)-2-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-3-hydroxyundec-5-enoic acid	C21H35N3O9S	M+Na	528.1986	-0.8
	HMDB0180171	[4-hydroxy-2-(6-{{(2E)-4-hydroxy-3-methylbut-2-en-1-yl}amino}-9H-purin-9-yl)-5-[(phosphonoxy)methyl]oxolan-3-yl]oxidanesulfonic acid	C15H22N5O11PS	M+NH4	529.1112	1.1

529.1118	HMDB0180172	[4-hydroxy-5-(6-((2E)-4-hydroxy-3-methylbut-2-en-1-yl)amino)-9H-purin-9-yl)-2-[(phosphonooxy)methyl]oxolan-3-yl]oxidanesulfonic acid	C15H22N5O11PS	M+NH4	529.1112	1.1
	HMDB0180170	{[(2E)-4-[(9-{3,4-dihydroxy-5-[(phosphonooxy)methyl]oxolan-2-yl)-9H-purin-6-yl]amino]-2-methylbut-2-en-1-yl]oxy}sulfonic acid	C15H22N5O11PS	M+NH4	529.1112	1.1
530.3516	HMDB0172243	{[6-hydroxy-5,7-dimethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-1-benzopyran-2-yl]methoxy}sulfonic acid	C28H48O6S	M+NH4	530.3510	1.2
	HMDB0174602	[18-hydroxy-12-(hydroxymethyl)-16-methyl-15-(6-methylheptan-2-yl)pentacyclo[9.7,,,octadecan-6-yl]oxidanesulfonic acid	C28H48O6S	M+NH4	530.3510	1.2
	HMDB0174600	[18-hydroxy-16-(hydroxymethyl)-12-methyl-15-(6-methylheptan-2-yl)pentacyclo[9.7,,,octadecan-6-yl]oxidanesulfonic acid	C28H48O6S	M+NH4	530.3510	1.2
	HMDB0174598	[18-hydroxy-15-(1-hydroxy-6-methylheptan-2-yl)-12,16-dimethylpentacyclo[9.7,,,octadecan-6-yl]oxidanesulfonic acid	C28H48O6S	M+NH4	530.3510	1.2
	HMDB0174596	[14,18-dihydroxy-12,16-dimethyl-15-(6-methylheptan-2-yl)pentacyclo[9.7,,,octadecan-6-yl]oxidanesulfonic acid	C28H48O6S	M+NH4	530.3510	1.2
	HMDB0174594	[9,18-dihydroxy-12,16-dimethyl-15-(6-methylheptan-2-yl)pentacyclo[9.7,,,octadecan-6-yl]oxidanesulfonic acid	C28H48O6S	M+NH4	530.3510	1.2
	HMDB0174591	[5,18-dihydroxy-12,16-dimethyl-15-(6-methylheptan-2-yl)pentacyclo[9.7,,,octadecan-6-yl]oxidanesulfonic acid	C28H48O6S	M+NH4	530.3510	1.2
	HMDB0172258	{[13-(6-hydroxy-2,5,7-trimethyl-3,4-dihydro-2H-1-benzopyran-2-yl)-2,6,-trimethyltridecyl]oxy}sulfonic acid	C28H48O6S	M+NH4	530.3510	1.2
	HMDB0172256	{[9-(6-hydroxy-2,5,7-trimethyl-3,4-dihydro-2H-1-benzopyran-2-yl)-6-methyl-2-(4-methylpentyl)nonyl]oxy}sulfonic acid	C28H48O6S	M+NH4	530.3510	1.2
	HMDB0172254	[(2-[3-(6-hydroxy-2,5,7-trimethyl-3,4-dihydro-2H-1-benzopyran-2-yl)propyl]-6,-dimethylundecyl]oxy)sulfonic acid	C28H48O6S	M+NH4	530.3510	1.2
	HMDB0172250	{[6-hydroxy-2,7-dimethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-1-benzopyran-5-yl]methoxy}sulfonic acid	C28H48O6S	M+NH4	530.3510	1.2
	HMDB0172252	[6-hydroxy-2,5,7-trimethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-1-benzopyran-4-yl]oxidanesulfonic acid	C28H48O6S	M+NH4	530.3510	1.2
	HMDB0172248	{[6-hydroxy-2,5-dimethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-1-benzopyran-7-yl]methoxy}sulfonic acid	C28H48O6S	M+NH4	530.3510	1.2
	HMDB0174604	[18-hydroxy-15-(7-hydroxy-6-methylheptan-2-yl)-12,16-dimethylpentacyclo[9.7,,,octadecan-6-yl]oxidanesulfonic acid	C28H48O6S	M+NH4	530.3510	1.2
531.0553	HMDB0127338	{2-[5,7-dihydroxy-2-(3-methoxyphenyl)-4-oxo-4H-chromen-6-yl]-4-hydroxy-6-methyl-5-oxooxan-3-yl}oxidanesulfonic acid	C22H20O12S	M+Na	531.0568	-2.8
	HMDB0127339	{2-[5,7-dihydroxy-2-(3-methoxyphenyl)-4-oxo-4H-chromen-6-yl]-3-hydroxy-6-methyl-5-oxooxan-4-yl}oxidanesulfonic acid	C22H20O12S	M+Na	531.0568	-2.8
	HMDB0139047	{[15-formyl-7,14-dihydroxy-6-methoxy-12-methyl-5-(3-methylbut-2-enoyl)--oxo-2,9-dioxatricyclo[9.4, 實 pentadeca-1(11),3(8),4,6,12,14-hexaen-4-yl]methoxy}sulfonic acid	C22H20O12S	M+Na	531.0568	-2.8
	HMDB0139050	{[15-formyl-7,14-dihydroxy-6-methoxy-4-methyl-5-(3-methylbut-2-enoyl)--oxo-2,9-dioxatricyclo[9.4, 實 pentadeca-1(11),3(8),4,6,12,14-hexaen-12-yl]methoxy}sulfonic acid	C22H20O12S	M+Na	531.0568	-2.8
532.2907	HMDB0174901	2-amino-N-[(Z)-5,8-dihydroxy-7-[(1H-indol-3-yl)methyl]-3-(propan-2-yl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,,12,15-hexaen-4-yl]-3-methylbutanimidic acid	C30H37N5O4	M+H	532.2918	-2.1

	HMDB0036435	Cyclodehydroisolibimin	C29H38O8	M+NH4	532.2905	0.4
	HMDB0037036	Glycinoeclepin C	C29H38O8	M+NH4	532.2905	0.4
532.3314	HMDB0160871	[(2S,15R)-16-hydroxy-14-(6-hydroxy-6-methylheptan-2-yl)-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-9-yl]oxidanesulfonic acid	C27H46O7S	M+NH4	532.3302	2.2
	HMDB0160872	[(2S,15R)-9-hydroxy-14-(6-hydroxy-6-methylheptan-2-yl)-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-16-yl]oxidanesulfonic acid	C27H46O7S	M+NH4	532.3302	2.2
	HMDB0160874	[(2S,15R)-16-hydroxy-14-(6-hydroxy-6-methylheptan-2-yl)-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C27H46O7S	M+NH4	532.3302	2.2
	HMDB0160875	[(2S,15R)-5-hydroxy-14-(6-hydroxy-6-methylheptan-2-yl)-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-16-yl]oxidanesulfonic acid	C27H46O7S	M+NH4	532.3302	2.2
	HMDB0160924	[(2S,15S)-9,16-dihydroxy-14-(6-hydroxy-6-methylhept-1-en-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C27H46O7S	M+NH4	532.3302	2.2
	HMDB0160925	[(2S,15S)-5,16-dihydroxy-14-(6-hydroxy-6-methylhept-1-en-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadecan-9-yl]oxidanesulfonic acid	C27H46O7S	M+NH4	532.3302	2.2
	HMDB0160926	[(2S,15S)-5,9-dihydroxy-14-(6-hydroxy-6-methylhept-1-en-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadecan-16-yl]oxidanesulfonic acid	C27H46O7S	M+NH4	532.3302	2.2
533.3356	HMDB0010389	LysoPC(18:4(6Z,9Z,12Z,15Z))	C26H46NO7P	M+NH4	533.3350	1.1
535.1217	HMDB0126126	6-({12,12-dimethyl-4-oxo-6-phenyl-3,11,14-trioxatetracyclo[8.5.,pentadeca-1(),2(7),5,8-tetraen-8-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H24O11	M+Na	535.1211	1.2
	HMDB0126123	3,4,5-trihydroxy-6-(4-{5-hydroxy-8,8-dimethyl-2-oxo-2H,8H-pyrano[2,3-f]chromen-4-yl}phenoxy)oxane-2-carboxylic acid	C26H24O11	M+Na	535.1211	1.2
	HMDB0126124	3,4,5-trihydroxy-6-{[4-(4-hydroxyphenyl)-8,8-dimethyl-2-oxo-2H,8H-pyrano[2,3-f]chromen-5-yl]oxy}oxane-2-carboxylic acid	C26H24O11	M+Na	535.1211	1.2
	HMDB0126129	3,4,5-trihydroxy-6-{[8-(hydroxymethyl)-8-methyl-2-oxo-4-phenyl-2H,8H-pyrano[2,3-f]chromen-5-yl]oxy}oxane-2-carboxylic acid	C26H24O11	M+Na	535.1211	1.2
	HMDB0127415	3,4,5-trihydroxy-6-({5-hydroxy-8,8-dimethyl-4-oxo-2-phenyl-4H,8H-pyrano[2,3-f]chromen-3-yl}oxy)oxane-2-carboxylic acid	C26H24O11	M+Na	535.1211	1.2
	HMDB0127416	3,4,5-trihydroxy-6-({3-hydroxy-8,8-dimethyl-4-oxo-2-phenyl-4H,8H-pyrano[2,3-f]chromen-5-yl}oxy)oxane-2-carboxylic acid	C26H24O11	M+Na	535.1211	1.2
	HMDB0135725	6-(4-{8,8-dimethyl-2-oxo-2H,8H-pyrano[2,3-f]chromen-3-yl}-3-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H24O11	M+Na	535.1211	1.2
	HMDB0135724	6-(2-{8,8-dimethyl-2-oxo-2H,8H-pyrano[2,3-f]chromen-3-yl}-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H24O11	M+Na	535.1211	1.2
	HMDB0148084	6-({17,17-dimethyl-3-oxo-4,12,18-trioxapentacyclo[11.8.??]henicosa-1(13),2(11),5(),6,8,14(19),-heptaen-7-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H24O11	M+Na	535.1211	1.2
	HMDB0148241	3,4,5-trihydroxy-6-{[5-hydroxy-4-(3-methylbut-2-en-1-yl)-9-oxo-8,17-dioxatetracyclo[8.7.,heptadeca-1(),2(7),3,5,11(16),12,14-heptaen-14-yl]oxy}oxane-2-carboxylic acid	C26H24O11	M+Na	535.1211	1.2
	HMDB0126120	3,4,5-trihydroxy-6-(3-{5-hydroxy-8,8-dimethyl-2-oxo-2H,8H-pyrano[2,3-f]chromen-4-yl}phenoxy)oxane-2-carboxylic acid	C26H24O11	M+Na	535.1211	1.2
	HMDB0126121	3,4,5-trihydroxy-6-{[4-(3-hydroxyphenyl)-8,8-dimethyl-2-oxo-2H,8H-pyrano[2,3-f]chromen-5-yl]oxy}oxane-2-carboxylic acid	C26H24O11	M+Na	535.1211	1.2

	HMDB0126118	3,4,5-trihydroxy-6-(2-{5-hydroxy-8,8-dimethyl-2-oxo-2H,8H-pyrano[2,3-f]chromen-4-yl}phenoxy)oxane-2-carboxylic acid	C26H24O11	M+Na	535.1211	1.2
	HMDB0126119	3,4,5-trihydroxy-6-{{4-(2-hydroxyphenyl)-8,8-dimethyl-2-oxo-2H,8H-pyrano[2,3-f]chromen-5-yl}oxy}oxane-2-carboxylic acid	C26H24O11	M+Na	535.1211	1.2
	HMDB0148240	3,4,5-trihydroxy-6-{{14-hydroxy-4-(3-methylbut-2-en-1-yl)-9-oxo-8,17-dioxatetracyclo[8.7.,,heptadeca-10,2(7),3,5,11(16),12,14-heptaen-5-yl]oxy}oxane-2-carboxylic acid	C26H24O11	M+Na	535.1211	1.2
535.2993	HMDB0061697	1-Stearoylglycerophosphoglycerol	C24H49O9P	M+Na	535.3006	-2.5
	HMDB0061703	2-Stearoylglycerophosphoglycerol	C24H49O9P	M+Na	535.3006	-2.5
538.2576	HMDB0014538	Beclometasone dipropionate	C28H37ClO7	M+NH4	538.2566	1.9
	HMDB0030142	Physalolactone C	C28H37ClO7	M+NH4	538.2566	1.9
	HMDB0041366	24,25-Diacetylvulgaroside	C29H44O8	M+NH4	538.3374	-1.4
538.3367	HMDB0060819	Sorafenib N-oxide	C29H44O8	M+NH4	538.3374	-1.4
	HMDB0165567	4-{5-[(4,5-dihydroxy-6-methyloxan-2-yl)oxy]-11,17-dihydroxy-2,15-dimethyltetracyclo[8.7.,,heptadecan-14-yl]-2,5-dihydrofuran-2-one	C29H44O8	M+NH4	538.3374	-1.4
538.5189	HMDB0004949	Cer(d18:1/16)	C34H67NO3	M+H	538.5194	-0.9
	HMDB0000790	N-Palmitoylsphingosine	C34H67NO3	M+H	538.5194	-0.9
541.9989	HMDB0156364	[5-(2,6-dihydroxy-9H-purin-9-yl)-4-hydroxy-2-({[hydroxy(phosphonooxy)phosphoryl]oxy}methyl)oxolan-3-yl]oxidanesulfonic acid	C10H14N4O15P2S	M+NH4	541.9990	-0.2
	HMDB0156363	[2-(2,6-dihydroxy-9H-purin-9-yl)-4-hydroxy-5-({[hydroxy(phosphonooxy)phosphoryl]oxy}methyl)oxolan-3-yl]oxidanesulfonic acid	C10H14N4O15P2S	M+NH4	541.9990	-0.2
544.0005	HMDB0060781	6-Thioguanosine-5'-O- triphosphate	C11H18N5O13P3	M+Na	544.0006	-0.2
	HMDB0002815	LysoPC(18:1(9Z))	C26H52NO7P	M+Na	544.3374	1.4
544.3381	HMDB0061701	2-oleoyl-sn-glycero-3-phosphocholine	C26H52NO7P	M+Na	544.3374	1.4
	HMDB0062651	2-oleoyl-sn-glycero-3-phosphocholine	C26H52NO7P	M+Na	544.3374	1.4
	HMDB0010385	LysoPC(18:1(11Z))	C26H52NO7P	M+Na	544.3374	1.4
	HMDB0030794	(E)-Methyl 1-propenyl disulfide	C33H36O7	M+H	545.2534	2.8
545.2549	HMDB0164988	{15-[(3E)-5,6-dimethylhept-3-en-2-yl]-2,16-dimethyl-5-oxo-8,19-dioxahexacyclo[9.7.1.,,nonadecan-yl]oxidanesulfonic acid	C28H42O7S	M+Na	545.2543	1.0
545.9613	HMDB0061267	{[hydroxy({[hydroxy({[(2R,3S,5R)-3-hydroxy-5-(2-imino-6-sulfany-3,9-dihydro-2H-purin-9-yl)oxolan-2-yl]methoxy})phosphoryl]oxy})phosphoryl]oxy}phosphonic acid	C10H16N5O12P3S	M+Na	545.9621	-1.5
	HMDB0164023	[18'-hydroxy-19'-(hydroxymethyl)-5,7',9',13'-tetramethyl-5'-oxaspiro[oxane-2,6'-pentacyclo[.7,?, 實 nonadecane]-16'-yl]oxidanesulfonic acid	C27H44O8S	M+NH4	546.3095	2.9
546.3111	HMDB0164022	({16',18'-dihydroxy-5,7',9',13'-tetramethyl-5'-oxaspiro[oxane-2,6'-pentacyclo[.7,?, 實 nonadecane]-19'-yl]methoxy)sulfonic acid	C27H44O8S	M+NH4	546.3095	2.9
	HMDB0172531	{5,19'-dihydroxy-5,7',9',13'-tetramethyl-5'-oxaspiro[oxane-2,6'-pentacyclo[.8,?, 實 icosane]-16'-yl]oxidanesulfonic acid	C27H44O8S	M+NH4	546.3095	2.9
	HMDB0168867	[(2S,15S)-14-(3,4-dihydroxy-5,6-dimethylheptan-2-yl)-2,15-dimethyl-4-oxotetracyclo[8.7.,,heptadecan-5-yl]oxidanesulfonic acid	C28H48O7S	M+NH4	546.3459	2.0
546.3470	HMDB0173071	[14-(3,4-dihydroxy-6-methyl-5-methylideneheptan-2-yl)-4-hydroxy-2,15-dimethyltetracyclo[8.7.,,heptadecan-5-yl]oxidanesulfonic acid	C28H48O7S	M+NH4	546.3459	2.0
	HMDB0174691	[14-(3,4-dihydroxy-5,6-dimethylheptan-2-yl)-2,15-dimethyl-8-oxotetracyclo[8.7.,,heptadecan-5-yl]oxidanesulfonic acid	C28H48O7S	M+NH4	546.3459	2.0

546.3833	HMDB0159535	[(2S,15R)-14-(5-ethyl-6-methylheptan-2-yl)-4,5-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-9-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159567	[(2S,15R)-9-hydroxy-14-[7-hydroxy-5-(propan-2-yl)heptan-2-yl]-2,15-dimethyltetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159563	[(2S,15R)-14-(5-ethyl-7-hydroxy-6-methylheptan-2-yl)-9-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159564	[(2S,15R)-14-(5-ethyl-7-hydroxy-6-methylheptan-2-yl)-5-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-9-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159559	[(2S,15R)-9-hydroxy-14-[6-hydroxy-5-(propan-2-yl)heptan-2-yl]-2,15-dimethyltetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159560	[(2S,15R)-5-hydroxy-14-[6-hydroxy-5-(propan-2-yl)heptan-2-yl]-2,15-dimethyltetracyclo[8.7.,heptadecan-9-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159555	[(2R,15R)-14-(5-ethyl-6-methylheptan-2-yl)-9-hydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159556	[(2R,15R)-14-(5-ethyl-6-methylheptan-2-yl)-5-hydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-9-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159552	[(2S,15S)-14-(5-ethyl-6-methylheptan-2-yl)-5-hydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadecan-9-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159551	[(2S,15S)-14-(5-ethyl-6-methylheptan-2-yl)-9-hydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159548	[(2S,15R)-14-(5-ethyl-1-hydroxy-6-methylheptan-2-yl)-5-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-9-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159547	[(2S,15R)-14-(5-ethyl-1-hydroxy-6-methylheptan-2-yl)-9-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159544	[(2S,15S)-14-(5-ethyl-6-methylheptan-2-yl)-5,13-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-9-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159543	[(2S,15S)-14-(5-ethyl-6-methylheptan-2-yl)-9,13-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159540	[(2R,15R)-14-(5-ethyl-6-methylheptan-2-yl)-5,8-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-9-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159539	[(2R,15R)-14-(5-ethyl-6-methylheptan-2-yl)-8,9-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159534	[(2S,15R)-14-(5-ethyl-6-methylheptan-2-yl)-4,9-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
	HMDB0159568	[(2S,15R)-5-hydroxy-14-[7-hydroxy-5-(propan-2-yl)heptan-2-yl]-2,15-dimethyltetracyclo[8.7.,heptadecan-9-yl]oxidanesulfonic acid	C29H52O6S	M+NH4	546.3823	1.9
547.3504	HMDB0011493	LysoPE/22:4(7Z,Z,13Z,16Z))	C27H48NO7P	M+NH4	547.3507	-0.5

547.3507	HMDB0011523	LysoPE(22:4(7Z,Z,13Z,16Z))	C27H48NO7P	M+NH4	547.3507	-0.5
548.1796	HMDB0181410	2-amino-3-(1-{1-[3-(2-amino-2-carboxyethyl)-1H-indol-1-yl]-2-(sulfooxyethyl)}-1H-indol-3-yl)propanoic acid	C24H26N4O8S	M+NH4	548.1810	-2.5
	HMDB0181412	2-amino-3-(1-{1-[3-(2-amino-2-carboxyethyl)-1H-indol-1-yl]ethyl}-1H-indol-3-yl)-3-(sulfooxy)propanoic acid	C24H26N4O8S	M+NH4	548.1810	-2.5
548.3446	HMDB0030392	Kukoamine A	C28H42N4O6	M+NH4	548.3443	0.6
	HMDB0060526	Kukoamine C	C28H42N4O6	M+NH4	548.3443	0.6
	HMDB0060525	Kukoamine B	C28H42N4O6	M+NH4	548.3443	0.6
	HMDB0060527	Kukoamine D	C28H42N4O6	M+NH4	548.3443	0.6
549.4650	HMDB0161107	(8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraen-1-yl (9Z,12Z)-octadeca-9,12-dienoate	C38H60O2	M+H	549.4666	-2.9
550.2161	HMDB0015414	Rolitetracycline	C27H33N3O8	M+Na	550.2160	0.2
	HMDB0145364	1-[(6S,12aS)-4-(dimethylamino)-6,12,12a-tetrahydroxy-6-methyl-1,3,11-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracen-2-yl](hydroxy)methylidene}amino)methyl]-3,4-dihydro-2H-pyrrol-1-ium	C27H34N3O8	M+Na	550.2160	0.2
	HMDB0145365	1-[(6S,12aR)-4-(dimethylamino)-3,6,12a-tetrahydroxy-6-methyl-1,11,12-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracen-2-yl](hydroxy)methylidene}amino)methyl]-3,4-dihydro-2H-pyrrol-1-ium	C27H34N3O8	M+Na	550.2160	0.2
	HMDB0145349	(6S,12aS)-4-(dimethylamino)-6,12a-trihydroxy-6-methyl-1,3,11,12-tetraoxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C27H33N3O8	M+Na	550.2160	0.2
	HMDB0145306	1-[(6S,12aS)-4-(dimethylamino)-3,6,12,12a-pentahydroxy-6-methyl-1,11-dioxo-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracen-2-yl](hydroxy)methylidene}amino)methyl]-3,4-dihydro-2H-pyrrol-1-ium	C27H34N3O8	M+Na	550.2160	0.2
	HMDB0145291	1-[(6S,12aR)-4-(dimethylamino)-3,6,11,12a-pentahydroxy-6-methyl-1,12-dioxo-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracen-2-yl](hydroxy)methylidene}amino)methyl]-3,4-dihydro-2H-pyrrol-1-ium	C27H34N3O8	M+Na	550.2160	0.2
	HMDB0145274	(4aS,5aS,6S,12aS)-4-(dimethylamino)-3,6,12a-tetrahydroxy-6-methyl-1,11,12-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O8	M+Na	550.2160	0.2
	HMDB0145273	(4aS,5aS,6S,12aS)-4-(dimethylamino)-6,12,12a-tetrahydroxy-6-methyl-1,3,11-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O8	M+Na	550.2160	0.2
	HMDB0055960	DG(14/16:1n7)	C33H62O5	M+NH4	556.4935	-1.0
556.4930	HMDB0056014	DG(16/14:1n5)	C33H62O5	M+NH4	556.4935	-1.0
	HMDB0007124	DG(16:1(9Z)/14)	C33H62O5	M+NH4	556.4935	-1.0
	HMDB0007096	DG(16/14:1(9Z))	C33H62O5	M+NH4	556.4935	-1.0
	HMDB0007040	DG(14:1(9Z)/16)	C33H62O5	M+NH4	556.4935	-1.0
	HMDB0007012	DG(14/16:1(9Z))	C33H62O5	M+NH4	556.4935	-1.0
	HMDB0093090	DG(i-12/18)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093004	DG(/i-)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093002	DG(/)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0092952	DG(8/22)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0092954	DG(8/i-22)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093087	DG(12/18)	C33H64O5	M+NH4	558.5092	-0.7

HMDB0093894	DG(18/12)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093001	DG(/)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0094121	DG(/)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0094409	DG(22/8)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0092951	DG(8/22)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093003	DG(/i-)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093092	DG(i-12/i-18)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093236	DG(13/i-17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093230	DG(i-13/a-17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093228	DG(a-13/i-17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093238	DG(13/a-17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093234	DG(i-13/i-17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093226	DG(i-13/17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093240	DG(a-13/a-17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093232	DG(a-13/17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093094	DG(12/i-18)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0092953	DG(8/i-22)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0094123	DG(i-/)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0094411	DG(i-22/8)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093734	DG(a-17/i-13)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093089	DG(i-12/18)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093091	DG(i-12/i-18)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093225	DG(i-13/17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093229	DG(i-13/a-17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093233	DG(i-13/i-17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093363	DG(i-14/16)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093365	DG(i-14/i-16)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093480	DG(i-15/15)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093484	DG(i-15/a-15)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093488	DG(i-15/i-15)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093625	DG(i-16/14)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093627	DG(i-16/i-14)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093732	DG(i-17/13)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093736	DG(i-17/a-13)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093740	DG(i-17/i-13)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093896	DG(i-18/12)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093746	DG(a-17/a-13)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093738	DG(a-17/13)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093482	DG(a-15/i-15)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093093	DG(12/i-18)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093223	DG(13/17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093237	DG(13/a-17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093235	DG(13/i-17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093367	DG(14/i-16)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093492	DG(15/a-15)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093490	DG(15/i-15)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093629	DG(16/i-14)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093730	DG(17/13)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093744	DG(17/a-13)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093742	DG(17/i-13)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093900	DG(18/i-12)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093231	DG(a-13/17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093239	DG(a-13/a-17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093227	DG(a-13/i-17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093486	DG(a-15/15)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093494	DG(a-15/a-15)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093898	DG(i-18/i-12)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093224	DG(13/17)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0007011	DG(14/16)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0094124	DG(i-/)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0094122	DG(/)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093901	DG(18/i-12)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093899	DG(i-18/i-12)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093897	DG(i-18/12)	C33H64O5	M+NH4	558.5092	-0.7
HMDB0093743	DG(17/i-13)	C33H64O5	M+NH4	558.5092	-0.7

	HMDB0093731	DG(17/13)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0094412	DG(i-22/8)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0094410	DG(22/8)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0007068	DG(15/15)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0007095	DG(16/14)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0055981	DG(15/15)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093895	DG(12/18)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093624	DG(14/16)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0055954	DG(14/16)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093088	DG(18/12)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093735	DG(a-17/i-13)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093737	DG(i-17/a-13)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093493	DG(15/a-15)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093483	DG(a-15/i-15)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093489	DG(i-15/i-15)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093481	DG(i-15/15)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093487	DG(a-15/15)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093495	DG(a-15/a-15)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093368	DG(14/i-16)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093364	DG(i-14/16)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093366	DG(i-14/i-16)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093485	DG(i-15/a-15)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093733	DG(i-17/13)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093739	DG(a-17/13)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093741	DG(i-17/i-13)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093745	DG(17/a-13)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093747	DG(a-17/a-13)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093491	DG(15/i-15)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093628	DG(i-16/i-14)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093626	DG(i-16/14)	C33H64O5	M+NH4	558.5092	-0.7
	HMDB0093630	DG(16/i-14)	C33H64O5	M+NH4	558.5092	-0.7
560.0776	HMDB0012276	1-(5-phosphoribosyl)-5'-AMP	C15H23N5O14P2	M+H	560.0789	-2.4
	HMDB0001178	Adenosine diphosphate ribose	C15H23N5O14P2	M+H	560.0789	-2.4
560.3630	HMDB0174756	{14-[(5E)-3,4-dihydroxy-5-(propan-2-yl)hept-5-en-2-yl]-4-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C29H50O7S	M+NH4	560.3615	2.6
564.3580	HMDB0168869	[(2S,15S)-4-hydroxy-2,15-dimethyl-14-(1,3,4-trihydroxy-5,6-dimethylheptan-2-yl)tetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C28H50O8S	M+NH4	564.3565	2.7
	HMDB0168871	[(2S,15S)-14-(3,4-dihydroxy-5,6-dimethylheptan-2-yl)-4,17-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C28H50O8S	M+NH4	564.3565	2.7
574.3786	HMDB0183066	[1,6,6,11,15-pentamethyl-14-(4,5,6-trihydroxy-6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-yl]oxidanesulfonic acid	C30H52O7S	M+NH4	574.3772	2.4
582.5086	HMDB0056137	DG(14:1n5/18:1n9)	C35H64O5	M+NH4	582.5092	-1.0
	HMDB0056136	DG(14:1n5/18:1n7)	C35H64O5	M+NH4	582.5092	-1.0
	HMDB0056156	DG(16:1n7/16:1n7)	C35H64O5	M+NH4	582.5092	-1.0
	HMDB0032094	Panatellin	C35H64O5	M+NH4	582.5092	-1.0
	HMDB0032732	cis-Solamin	C35H64O5	M+NH4	582.5092	-1.0
	HMDB0031390	Annotemoyin 1	C35H64O5	M+NH4	582.5092	-1.0
	HMDB0007240	DG(18:2(9Z,12Z)/14)	C35H64O5	M+NH4	582.5092	-1.0
	HMDB0007212	DG(18:1(9Z)/14:1(9Z))	C35H64O5	M+NH4	582.5092	-1.0
	HMDB0007183	DG(18:1(11Z)/14:1(9Z))	C35H64O5	M+NH4	582.5092	-1.0
	HMDB0007128	DG(16:1(9Z)/16:1(9Z))	C35H64O5	M+NH4	582.5092	-1.0
	HMDB0007043	DG(14:1(9Z)/18:1(11Z))	C35H64O5	M+NH4	582.5092	-1.0
	HMDB0007044	DG(14:1(9Z)/18:1(9Z))	C35H64O5	M+NH4	582.5092	-1.0
	HMDB0007016	DG(14/18:2(9Z,12Z))	C35H64O5	M+NH4	582.5092	-1.0
584.0878	HMDB0000286	Uridine diphosphate glucose	C15H24N2O17P2	M+NH4	584.0888	-1.8
	HMDB0000302	Uridine diphosphategalactose	C15H24N2O17P2	M+NH4	584.0888	-1.8

	HMDB0062573	Uridine diphosphategalactose	C15H24N2O17P2	M+NH4	584.0888	-1.8
	HMDB0060079	Uridine diphosphate glucose	C15H24N2O17P2	M+NH4	584.0888	-1.8
584.5241	HMDB0056040	DG(18/14:1n5)	C35H66O5	M+NH4	584.5248	-1.3
	HMDB0056015	DG(16/16:1n7)	C35H66O5	M+NH4	584.5248	-1.3
	HMDB0055961	DG(14/18:1n7)	C35H66O5	M+NH4	584.5248	-1.3
	HMDB0055962	DG(14/18:1n9)	C35H66O5	M+NH4	584.5248	-1.3
	HMDB0007211	DG(18:1(9Z)/14)	C35H66O5	M+NH4	584.5248	-1.3
	HMDB0007182	DG(18:1(11Z)/14)	C35H66O5	M+NH4	584.5248	-1.3
	HMDB0007154	DG(18/14:1(9Z))	C35H66O5	M+NH4	584.5248	-1.3
	HMDB0007127	DG(16:1(9Z)/16)	C35H66O5	M+NH4	584.5248	-1.3
	HMDB0007099	DG(16/16:1(9Z))	C35H66O5	M+NH4	584.5248	-1.3
	HMDB0007042	DG(14:1(9Z)/18)	C35H66O5	M+NH4	584.5248	-1.3
	HMDB0007014	DG(14/18:1(11Z))	C35H66O5	M+NH4	584.5248	-1.3
	HMDB0007015	DG(14/18:1(9Z))	C35H66O5	M+NH4	584.5248	-1.3
	HMDB0094415	DG(i-22/)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093012	DG(22/)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093014	DG(/i-22)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093108	DG(i-12/i-)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093106	DG(i-12/)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0092956	DG(8/i-24)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093011	DG(22/)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0094129	DG(i-/i-12)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0094127	DG(i-/12)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0092955	DG(8/i-24)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0094131	DG(/i-12)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093013	DG(/i-22)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0094413	DG(22/)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0094125	DG(12/)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093103	DG(12/)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093110	DG(12/i-)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093254	DG(13/19)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093382	DG(i-14/18)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093384	DG(i-14/i-18)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093386	DG(14/i-18)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093264	DG(13/i-19)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093262	DG(i-13/i-19)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093104	DG(12/)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093260	DG(a-13/19)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093256	DG(i-13/19)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093258	DG(a-13/i-19)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0094522	DG(i-24/8)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0094019	DG(i-19/i-13)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093508	DG(i-15/17)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093383	DG(i-14/i-18)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093381	DG(i-14/18)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093261	DG(i-13/i-19)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093255	DG(i-13/19)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093107	DG(i-12/i-)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093105	DG(i-12/)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093764	DG(a-17/i-15)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093512	DG(i-15/a-17)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093516	DG(i-15/i-17)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093642	DG(i-16/16)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0094017	DG(i-19/a-13)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0094015	DG(i-19/13)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093917	DG(i-18/i-14)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093915	DG(i-18/14)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093770	DG(i-17/i-15)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093766	DG(i-17/a-15)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093762	DG(i-17/15)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093644	DG(i-16/i-16)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093776	DG(a-17/a-15)	C35H68O5	M+NH4	586.5405	1.0
	HMDB0093768	DG(a-17/15)	C35H68O5	M+NH4	586.5405	1.0

586.5411

HMDB0093760	DG(17/15)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093646	DG(16/i-16)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093518	DG(15/i-17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093520	DG(15/a-17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093506	DG(15/17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093385	DG(14/i-18)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093263	DG(13/i-19)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093253	DG(13/19)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093774	DG(17/a-15)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093772	DG(17/i-15)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093919	DG(18/i-14)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093510	DG(a-15/i-17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093522	DG(a-15/a-17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093514	DG(a-15/17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093257	DG(a-13/i-19)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093259	DG(a-13/19)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094021	DG(19/i-13)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094023	DG(19/a-13)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094013	DG(19/13)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093109	DG(12/i-)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093523	DG(a-15/a-17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094018	DG(i-19/a-13)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094014	DG(19/13)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094130	DG(i-/i-12)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094128	DG(i-/12)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094022	DG(19/i-13)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093920	DG(18/i-14)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094016	DG(i-19/13)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094020	DG(i-19/i-13)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094024	DG(19/a-13)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094132	DG(i-/12)	C35H68O5	M+NH4	586.5405	1.0
HMDB0031011	DG(16/16)	C35H68O5	M+NH4	586.5405	1.0
HMDB0056009	DG(16/16)	C35H68O5	M+NH4	586.5405	1.0
HMDB0007153	DG(18/14)	C35H68O5	M+NH4	586.5405	1.0
HMDB0007098	DG(16/16)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093914	DG(14/18)	C35H68O5	M+NH4	586.5405	1.0
HMDB0055955	DG(14/18)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094126	DG(/12)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094416	DG(i-22/)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094414	DG(22/)	C35H68O5	M+NH4	586.5405	1.0
HMDB0094523	DG(i-24/8)	C35H68O5	M+NH4	586.5405	1.0
HMDB0007013	DG(14/18)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093918	DG(i-18/i-14)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093519	DG(15/i-17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093507	DG(15/17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093645	DG(i-16/i-16)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093643	DG(i-16/16)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093511	DG(a-15/i-17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093513	DG(i-15/a-17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093765	DG(i-15/a-17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093509	DG(i-15/17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093515	DG(a-15/17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093521	DG(15/a-17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093517	DG(i-15/i-17)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093647	DG(16/i-16)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093767	DG(i-17/a-15)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093773	DG(17/i-15)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093761	DG(17/15)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093775	DG(17/a-15)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093769	DG(a-17/15)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093777	DG(a-17/a-15)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093763	DG(i-17/15)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093771	DG(i-17/i-15)	C35H68O5	M+NH4	586.5405	1.0
HMDB0093916	DG(i-18/14)	C35H68O5	M+NH4	586.5405	1.0

590.3367	HMDB0167809	{[(5E)-2-{4,5-dihydroxy-2,16-dimethyl-8-oxo-9-oxatetracyclo[9.7.,octadecan-15-yl]-4-hydroxy-5-(propan-2-yl)hept-5-en-3-yl}oxy} sulfonic acid	C29H48O9S	M+NH4	590.3357	1.6
	HMDB0167808	{15-[(5E)-3,4-dihydroxy-5-(propan-2-yl)hept-5-en-2-yl]-4-hydroxy-2,16-dimethyl-8-oxo-9-oxatetracyclo[9.7.,octadecan-5-yl]oxidanesulfonic acid	C29H48O9S	M+NH4	590.3357	1.6
	HMDB0167807	{15-[(5E)-3,4-dihydroxy-5-(propan-2-yl)hept-5-en-2-yl]-5-hydroxy-2,16-dimethyl-8-oxo-9-oxatetracyclo[9.7.,octadecan-4-yl]oxidanesulfonic acid	C29H48O9S	M+NH4	590.3357	1.6
	HMDB0167810	{[(2E)-6-{4,5-dihydroxy-2,16-dimethyl-8-oxo-9-oxatetracyclo[9.7.,octadecan-15-yl]-5-hydroxy-3-(propan-2-yl)hept-2-en-4-yl}oxy} sulfonic acid	C29H48O9S	M+NH4	590.3357	1.6
	HMDB0170393	{4-hydroxy-2,15-dimethyl-8-oxo-14-[(5E)-1,3,4-trihydroxy-5-(propan-2-yl)hept-5-en-2-yl]tetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C29H48O9S	M+NH4	590.3357	1.6
	HMDB0170395	{14-[(5E)-3,4-dihydroxy-5-(propan-2-yl)hept-5-en-2-yl]-4,17-dihydroxy-2,15-dimethyl-8-oxotetracyclo[8.7.,heptadecan-5-yl]oxidanesulfonic acid	C29H48O9S	M+NH4	590.3357	1.6
598.0668	HMDB0153551	(5-{4-[(2-aminoethyl)sulfanyl]-5,7-dihydroxy-3-(3,4,5-trihydroxybenzoyloxy)-3,4-dihydro-2H-1-benzopyran-2-yl]-2-hydroxyphenyl)oxidanesulfonic acid	C24H23NO13S2	M+H	598.0684	-2.6
	HMDB0000935	Uridine diphosphate glucuronic acid	C15H22N2O18P2	M+NH4	598.0681	-2.2
	HMDB0012302	UDP-D-galacturonate	C15H22N2O18P2	M+NH4	598.0681	-2.2
	HMDB0012304	UDP-L-iduronate	C15H22N2O18P2	M+NH4	598.0681	-2.2
	HMDB0156315	3,4,5-trihydroxy-6-([4-hydroxy-2-({[hydroxy(phosphonooxy)phosphoryl]oxy}methyl)-5-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)oxolan-3-yl]oxy}oxane-2-carboxylic acid	C15H22N2O18P2	M+NH4	598.0681	-2.2
	HMDB0156314	3,4,5-trihydroxy-6-([4-hydroxy-5-({[hydroxy(phosphonooxy)phosphoryl]oxy}methyl)-2-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)oxolan-3-yl]oxy}oxane-2-carboxylic acid	C15H22N2O18P2	M+NH4	598.0681	-2.2
598.5403	HMDB0055989	DG(15/18:1n7)	C36H68O5	M+NH4	598.5405	-0.3
	HMDB0055990	DG(15/18:1n9)	C36H68O5	M+NH4	598.5405	-0.3
	HMDB0007213	DG(18:1(9Z)/15)	C36H68O5	M+NH4	598.5405	-0.3
	HMDB0007184	DG(18:1(11Z)/15)	C36H68O5	M+NH4	598.5405	-0.3
	HMDB0007072	DG(15/18:1(11Z))	C36H68O5	M+NH4	598.5405	-0.3
	HMDB0007073	DG(15/18:1(9Z))	C36H68O5	M+NH4	598.5405	-0.3
604.3520	HMDB0175874	[3,5,-trihydroxy-4a,9-bis(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-4-yl]oxidanesulfonic acid	C30H50O9S	M+NH4	604.3514	1.0
	HMDB0175873	[4,5,-trihydroxy-4a,9-bis(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-3-yl]oxidanesulfonic acid	C30H50O9S	M+NH4	604.3514	1.0
	HMDB0175876	[8,9,-trihydroxy-4,8a-bis(hydroxymethyl)-4,6a,6b,11,11,14b-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-3-yl]oxidanesulfonic acid	C30H50O9S	M+NH4	604.3514	1.0
	HMDB0175875	[3,4,-trihydroxy-4a,9-bis(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-5-yl]oxidanesulfonic acid	C30H50O9S	M+NH4	604.3514	1.0
	HMDB0175872	{[3,8,9,-tetrahydroxy-8a-(hydroxymethyl)-4,6a,6b,11,11,14b-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-4-yl]methoxy} sulfonic acid	C30H50O9S	M+NH4	604.3514	1.0

	HMDB0175871	{[3,4,5,-tetrahydroxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-4a-yl]methoxy}sulfonic acid	C30H50O9S	M+NH4	604.3514	1.0
	HMDB0012188	All-trans-hexaprenyl diphosphate	C30H52O7P2	M+NH4	604.3527	-1.1
	HMDB0001278	Presqualene diphosphate	C30H52O7P2	M+NH4	604.3527	-1.1
608.0873	HMDB0060522	UDP-N-acetyl-alpha-D-galactosamine	C17H27N3O17P2	M+H	608.0888	-2.5
	HMDB0000290	Uridine diphosphate-N-acetylglucosamine	C17H27N3O17P2	M+H	608.0888	-2.5
	HMDB0062760	Uridine diphosphate-N-acetylgalactosamine	C17H27N3O17P2	M+H	608.0888	-2.5
	HMDB0000304	Uridine diphosphate-N-acetylgalactosamine	C17H27N3O17P2	M+H	608.0888	-2.5
	HMDB0013112	UDP-N-acetyl-D-mannosamine	C17H27N3O17P2	M+H	608.0888	-2.5
608.5242	HMDB0056144	DG(14:1n5/:2n6)	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0056030	DG(16/18:3n3)	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0056023	DG(16/18:3n6)	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0055970	DG(14/:3n6)	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0055964	DG(14/:3n9)	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0007472	DG(3(8Z,11Z,14Z)/14)	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0007443	DG(3(5Z,8Z,11Z)/14)	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0007415	DG(2(11Z,14Z)/14:1(9Z))	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0007301	DG(18:3(9Z,12Z,15Z)/16)	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0007272	DG(18:3(6Z,9Z,12Z)/16)	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0007244	DG(18:2(9Z,12Z)/16:1(9Z))	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0007132	DG(16:1(9Z)/18:2(9Z,12Z))	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0007104	DG(16/18:3(6Z,9Z,12Z))	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0007105	DG(16/18:3(9Z,12Z,15Z))	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0007051	DG(14:1(9Z)/:2(11Z,14Z))	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0007024	DG(14/:3(8Z,11Z,14Z))	C37H66O5	M+NH4	608.5248	-1.1
	HMDB0007023	DG(14/:3(5Z,8Z,11Z))	C37H66O5	M+NH4	608.5248	-1.1
610.5397	HMDB0055969	DG(14/:2n6)	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0056157	DG(16:1n7/18:1n7)	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0056158	DG(16:1n7/18:1n9)	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0056138	DG(14:1n5/:1n9)	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0055995	DG(15/18:2n6)	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0034560	cis-Uvariamicin IV	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0032714	cis-Uvariamicin IB	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0034302	Reticulatin 2	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0034924	Neoreticulatin A	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0007414	DG(2(11Z,14Z)/14)	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0007386	DG(1(11Z)/14:1(9Z))	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0007243	DG(18:2(9Z,12Z)/16)	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0007215	DG(18:1(9Z)/16:1(9Z))	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0007186	DG(18:1(11Z)/16:1(9Z))	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0007131	DG(16:1(9Z)/18:1(9Z))	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0007130	DG(16:1(9Z)/18:1(11Z))	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0007103	DG(16/18:2(9Z,12Z))	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0007050	DG(14:1(9Z)/:1(11Z))	C37H68O5	M+NH4	610.5405	-1.3
	HMDB0007022	DG(14/:2(11Z,14Z))	C37H68O5	M+NH4	610.5405	-1.3
612.5557	HMDB0181787	3-{15-hydroxy-15-[5-(1-hydroxytridecyl)oxolan-2-yl]pentadecyl}-5-methyloxolan-2-one	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0176309	3-{11-hydroxy-11-[5-(1-hydroxyheptadecyl)oxolan-2-yl]undecyl}-5-methyloxolan-2-one	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0172633	3-(16-{[5-(1-hydroxyundecyl)oxolan-2-yl]methoxy}hexadecyl)-5-methyloxolan-2-one	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0056041	DG(18/16:1n7)	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0056016	DG(16/18:1n7)	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0055963	DG(14/:1n9)	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0056065	DG(/14:1n5)	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0007385	DG(1(11Z)/14)	C37H70O5	M+NH4	612.5561	-0.7

	HMDB0007357	DG(14:1(9Z))	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0007214	DG(18:1(9Z)/16)	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0007185	DG(18:1(11Z)/16)	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0007157	DG(18/16:1(9Z))	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0007129	DG(16:1(9Z)/18)	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0007102	DG(16/18:1(9Z))	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0007101	DG(16/18:1(11Z))	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0007049	DG(14:1(9Z)/)	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0056017	DG(16/18:1n9)	C37H70O5	M+NH4	612.5561	-0.7
	HMDB0007021	DG(14/:1(11Z))	C37H70O5	M+NH4	612.5561	-0.7
613.1766	HMDB0176722	6-[2,6-dihydroxy-4-({[3,4,5-trihydroxy-6-(2-phenylethoxy)oxan-2-yl]methoxy}carbonyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H32O16	M+H	613.1763	0.5
	HMDB0128224	5,6-dihydroxy-4-[hydroxy(3,4,5-trihydroxyoxan-2-yl)methyl]-2-[(2E)-3-(4-hydroxyphenyl)prop-2-enoyl]-6-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]cyclohex-4-ene-1,3-dione	C27H32O16	M+H	613.1763	0.5
	HMDB0126731	3,4,5-trihydroxy-6-(3-{3,5,7-trihydroxy-8-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-3,4-dihydro-2H-1-benzopyran-2-yl}phenoxy)oxane-2-carboxylic acid	C27H32O16	M+H	613.1763	0.5
	HMDB0126732	6-{[3,5-dihydroxy-2-(3-hydroxyphenyl)-8-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-3,4-dihydro-2H-1-benzopyran-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H32O16	M+H	613.1763	0.5
	HMDB0126697	6-{[3,5-dihydroxy-2-(3-hydroxyphenyl)-6-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-3,4-dihydro-2H-1-benzopyran-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H32O16	M+H	613.1763	0.5
	HMDB0126696	3,4,5-trihydroxy-6-(3-{3,5,7-trihydroxy-6-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-3,4-dihydro-2H-1-benzopyran-2-yl}phenoxy)oxane-2-carboxylic acid	C27H32O16	M+H	613.1763	0.5
	HMDB0128225	5,6-dihydroxy-2-[hydroxy(3,4,5-trihydroxyoxan-2-yl)methyl]-4-[(2E)-3-(4-hydroxyphenyl)prop-2-enoyl]-6-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]cyclohex-4-ene-1,3-dione	C27H32O16	M+H	613.1763	0.5
	HMDB0132682	6-[3,5-dihydroxy-2-[3-(3-hydroxyphenyl)propanoyl]-6-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H32O16	M+H	613.1763	0.5
	HMDB0132684	6-[3,5-dihydroxy-2-[3-(3-hydroxyphenyl)propanoyl]-4-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H32O16	M+H	613.1763	0.5
	HMDB0176721	6-[2,3-dihydroxy-5-({[3,4,5-trihydroxy-6-(2-phenylethoxy)oxan-2-yl]methoxy}carbonyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H32O16	M+H	613.1763	0.5
	HMDB0153790	6-{4-[3-(2,6-dihydroxy-4-{{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}phenyl)-3-oxopropyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H32O16	M+H	613.1763	0.5
	HMDB0153789	3,4,5-trihydroxy-6-{3-hydroxy-2-[3-(4-hydroxyphenyl)propanoyl]-5-{{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}phenoxy}oxane-2-carboxylic acid	C27H32O16	M+H	613.1763	0.5
	HMDB0150833	3,4,5-trihydroxy-6-{5-hydroxy-2-[3-(4-hydroxyphenyl)propanoyl]-3-{{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}phenoxy}oxane-2-carboxylic acid	C27H32O16	M+H	613.1763	0.5
	HMDB0150834	3,4,5-trihydroxy-6-{3-hydroxy-4-[3-(4-hydroxyphenyl)propanoyl]-5-{{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}phenoxy}oxane-2-carboxylic acid	C27H32O16	M+H	613.1763	0.5

	HMDB0150832	6-{4-[3-(2,4-dihydroxy-6-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}phenyl)-3-oxopropyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H32O16	M+H	613.1763	0.5
	HMDB0132685	6-{3,5-dihydroxy-4-[3-(3-hydroxyphenyl)propanoyl]-2-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H32O16	M+H	613.1763	0.5
	HMDB0132683	3,4,5-trihydroxy-6-[3-(3-oxo-3-{2,4,6-trihydroxy-3-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]phenyl}propyl)phenoxy]oxane-2-carboxylic acid	C27H32O16	M+H	613.1763	0.5
	HMDB0030558	Safflomin A	C27H32O16	M+H	613.1763	0.5
	HMDB0040677	Hydroxysafflor yellow A	C27H32O16	M+H	613.1763	0.5
	HMDB0040559	Aromadendrin 3,7-diglucoside	C27H32O16	M+H	613.1763	0.5
	HMDB0040125	Carthamidin 6,7-diglucoside	C27H32O16	M+H	613.1763	0.5
615.1730	HMDB0133713	(3-hydroxy-16,17-dimethoxy-9-oxo-15-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}tricyclo[12.3.1.1,nonadeca-1(17),2,4,6(19),14(18),15-hexaen-8-yl)oxidanesulfonic acid	C27H34O14S	M+H	615.1742	-2.0
616.1763	HMDB0003178	Heme	C34H32FeN4O4	M+H	616.1773	-1.6
624.5557	HMDB0056022	DG(16/18:2n6)	C38H70O5	M+NH4	624.5561	-0.7
	HMDB0055997	DG(15/:2n6)	C38H70O5	M+NH4	624.5561	-0.7
	HMDB0007416	DG(:2(11Z,14Z)/15)	C38H70O5	M+NH4	624.5561	-0.7
	HMDB0007080	DG(15/:2(11Z,14Z))	C38H70O5	M+NH4	624.5561	-0.7
625.1139	HMDB0060522	UDP-N-acetyl-alpha-D-galactosamine	C17H27N3O17P2	M+NH4	625.1154	-2.4
	HMDB0000290	Uridine diphosphate-N-acetylglucosamine	C17H27N3O17P2	M+NH4	625.1154	-2.4
	HMDB0062760	Uridine diphosphate-N-acetylgalactosamine	C17H27N3O17P2	M+NH4	625.1154	-2.4
	HMDB0000304	Uridine diphosphate-N-acetylgalactosamine	C17H27N3O17P2	M+NH4	625.1154	-2.4
	HMDB0013112	UDP-N-acetyl-D-mannosamine	C17H27N3O17P2	M+NH4	625.1154	-2.4
634.5403	HMDB0056203	DG(18:1n9/18:3n6)	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0056210	DG(18:1n9/18:3n3)	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007113	DG(16/:4(8Z,11Z,14Z,17Z))	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0056191	DG(18:1n7/18:3n3)	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0056184	DG(18:1n7/18:3n6)	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0056166	DG(16:1n7/:3n6)	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0055973	DG(14/22:4n6)	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0056026	DG(16/:4n6)	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0056032	DG(16/:4n3)	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0056057	DG(18/18:4n3)	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0056160	DG(16:1n7/:3n9)	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007031	DG(14/22:4(7Z,Z,13Z,16Z))	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007305	DG(18:3(9Z,12Z,15Z)/18:1(9Z))	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007304	DG(18:3(9Z,12Z,15Z)/18:1(11Z))	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007332	DG(18:4(6Z,9Z,12Z,15Z)/18)	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007447	DG(:3(5Z,8Z,11Z)/16:1(9Z))	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007476	DG(:3(8Z,11Z,14Z)/16:1(9Z))	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007504	DG(:4(5Z,8Z,11Z,14Z)/16)	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007533	DG(:4(8Z,11Z,14Z,17Z)/16)	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007675	DG(22:4(7Z,Z,13Z,16Z)/14)	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007276	DG(18:3(6Z,9Z,12Z)/18:1(9Z))	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007275	DG(18:3(6Z,9Z,12Z)/18:1(11Z))	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007248	DG(18:2(9Z,12Z)/18:2(9Z,12Z))	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007112	DG(16/:4(5Z,8Z,11Z,14Z))	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007140	DG(16:1(9Z)/:3(8Z,11Z,14Z))	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007139	DG(16:1(9Z)/:3(5Z,8Z,11Z))	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007164	DG(18/18:4(6Z,9Z,12Z,15Z))	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007191	DG(18:1(11Z)/18:3(6Z,9Z,12Z))	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007192	DG(18:1(11Z)/18:3(9Z,12Z,15Z))	C39H68O5	M+NH4	634.5405	-0.3
	HMDB0007220	DG(18:1(9Z)/18:3(6Z,9Z,12Z))	C39H68O5	M+NH4	634.5405	-0.3

	HMDB0007221	DG(18:1(9Z)/18:3(9Z,12Z,15Z))	C39H68O5	M+NH4	634.5405	-0.3
636.5557	HMDB0240593	(2S)-1-(hexadecanoyloxy)-3-hydroxypropan-2-yl (11Z,14Z,17Z)-icosa-11,14,17-trienoate	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0056165	DG(16:1n7/:2n6)	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0056147	DG(14:1n5/22:2n6)	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0056056	DG(18/18:3n3)	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0056049	DG(18/18:3n6)	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0056025	DG(16/:3n6)	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0056019	DG(16/:3n9)	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007475	DG(:3(8Z,11Z,14Z)/16)	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007446	DG(:3(5Z,8Z,11Z)/16)	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007418	DG(:2(11Z,14Z)/16:1(9Z))	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007303	DG(18:3(9Z,12Z,15Z)/18)	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007274	DG(18:3(6Z,9Z,12Z)/18)	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007246	DG(18:2(9Z,12Z)/18:1(11Z))	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007247	DG(18:2(9Z,12Z)/18:1(9Z))	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007219	DG(18:1(9Z)/18:2(9Z,12Z))	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007190	DG(18:1(11Z)/18:2(9Z,12Z))	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007162	DG(18/18:3(6Z,9Z,12Z))	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007163	DG(18/18:3(9Z,12Z,15Z))	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007138	DG(16:1(9Z):2(11Z,14Z))	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007111	DG(16/:3(8Z,11Z,14Z))	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007110	DG(16/:3(5Z,8Z,11Z))	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007647	DG(22:2(13Z,16Z)/14:1(9Z))	C39H70O5	M+NH4	636.5561	-0.7
	HMDB0007059	DG(14:1(9Z)/22:2(13Z,16Z))	C39H70O5	M+NH4	636.5561	-0.7
637.1564	HMDB0133713	(3-hydroxy-16,17-dimethoxy-9-oxo-15-[[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}tricyclo[12.3.1.1,nonadeca-1(17),2,4,6(19),14(18),15-hexaen-8-yl]oxidanesulfonic acid	C27H34O14S	M+Na	637.1561	0.4
638.5711	HMDB0056024	DG(16/:2n6)	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0055972	DG(14/22:2n6)	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0056140	DG(14:1n5/22:1n9)	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0056159	DG(16:1n7/:1n9)	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0007030	DG(14/22:2(13Z,16Z))	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0007417	DG(:2(11Z,14Z)/16)	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0007618	DG(22:1(13Z)/14:1(9Z))	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0007646	DG(22:2(13Z,16Z)/14)	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0007389	DG(:1(11Z)/16:1(9Z))	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0007245	DG(18:2(9Z,12Z)/18)	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0007058	DG(14:1(9Z)/22:1(13Z))	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0007109	DG(16/:2(11Z,14Z))	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0007137	DG(16:1(9Z):1(11Z))	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0007161	DG(18/18:2(9Z,12Z))	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0007188	DG(18:1(11Z)/18:1(11Z))	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0007189	DG(18:1(11Z)/18:1(9Z))	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0007217	DG(18:1(9Z)/18:1(11Z))	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0007218	DG(18:1(9Z)/18:1(9Z))	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0056177	DG(18:1n7/18:1n7)	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0056197	DG(18:1n9/18:1n9)	C39H72O5	M+NH4	638.5718	-1.1
	HMDB0056178	DG(18:1n7/18:1n9)	C39H72O5	M+NH4	638.5718	-1.1
640.6008	HMDB0166469	2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-yl (3Z)-hexadec-3-enoate	C43H74O2	M+NH4	640.6027	-3.0
	HMDB0062460	cholesteryl palmitoleate	C43H74O2	M+NH4	640.6027	-3.0
	HMDB0000658	cholesteryl palmitoleate	C43H74O2	M+NH4	640.6027	-3.0
	HMDB0061374	(1S,2R,5S,11R,14R,15R)-2,15-dimethyl-14-[(2R)-6-methylheptan-2-yl]tetracyclo[8.7.,]heptadeca-7,9-dien-5-yl hexadecanoate	C43H74O2	M+NH4	640.6027	-3.0
	HMDB0187005	2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-yl (9Z)-hexadec-9-enoate	C43H74O2	M+NH4	640.6027	-3.0
642.6184	HMDB0000885	CE(16)	C43H76O2	M+NH4	642.6184	0.1
	HMDB0155889	2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,]heptadec-7-en-5-yl hexadecanoate	C43H76O2	M+NH4	642.6184	0.1

642.0107	HMDB0184329	2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-yl 4,8,12-trimethyltridecanoate	C43H76O2	M+NH4	642.6184	0.1
648.6287	HMDB0004953	Cer(d18:1/24:1(15Z))	C42H81NO3	M+H	648.6289	-0.3
650.6449	HMDB0000831	N-Lignoceroylsphingosine	C42H83NO3	M+H	650.6446	0.5
	HMDB0011769	Cer(d18/24:1(15Z))	C42H83NO3	M+H	650.6446	0.5
	HMDB0004956	Ceramide (d18:1/24)	C42H83NO3	M+H	650.6446	0.5
653.1296	HMDB0012206	CMP-N-glycoloylneuraminate	C20H31N4O17P	M+Na	653.1314	-2.8
	HMDB0062569	AC1MMORG	C20H31N4O17P	M+Na	653.1314	-2.8
656.5243	HMDB0056368	DG(18:3n3/4n3)	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0056336	DG(4n6/18:3n3)	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0056327	DG(3n6/18:4n3)	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0056305	DG(18:3n6/4n3)	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0056299	DG(18:3n6/4n6)	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0056246	DG(3n9/18:4n3)	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0056176	DG(16:1n7/22:6n3)	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007567	DG(5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007539	DG(4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007540	DG(4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007511	DG(4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007510	DG(4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007483	DG(3(8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007454	DG(3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007342	DG(18:4(6Z,9Z,12Z,15Z)/3(5Z,8Z,11Z))	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007343	DG(18:4(6Z,9Z,12Z,15Z)/3(8Z,11Z,14Z))	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007315	DG(18:3(9Z,12Z,15Z)/4(5Z,8Z,11Z,14Z))	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007316	DG(18:3(9Z,12Z,15Z)/4(8Z,11Z,14Z,17Z))	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007286	DG(18:3(6Z,9Z,12Z)/4(5Z,8Z,11Z,14Z))	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007287	DG(18:3(6Z,9Z,12Z)/4(8Z,11Z,14Z,17Z))	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007259	DG(18:2(9Z,12Z)/5(5Z,8Z,11Z,14Z,17Z))	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007766	DG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C41H66O5	M+NH4	656.5248	-0.8
	HMDB0007150	DG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C41H66O5	M+NH4	656.5248	-0.8
658.5401	HMDB0056326	DG(3n6/18:3n3)	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0056316	DG(2n6/18:4n3)	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0056298	DG(18:3n6/3n6)	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0056245	DG(3n9/18:3n3)	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0056238	DG(3n9/18:3n6)	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0056035	DG(16/22:6n3)	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0056170	DG(16:1n7/22:5n6)	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0056175	DG(16:1n7/22:5n3)	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0056194	DG(18:1n7/5n3)	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0056213	DG(18:1n9/5n3)	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007121	DG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007453	DG(3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007481	DG(3(8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007482	DG(3(8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007509	DG(4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007538	DG(4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007565	DG(5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007566	DG(5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007708	DG(22:5(4Z,7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007737	DG(22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007765	DG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/16)	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007452	DG(3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007425	DG(2(11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007341	DG(18:4(6Z,9Z,12Z,15Z)/2(11Z,14Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007148	DG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007149	DG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007201	DG(18:1(11Z)/5(5Z,8Z,11Z,14Z,17Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007230	DG(18:1(9Z)/5(5Z,8Z,11Z,14Z,17Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007257	DG(18:2(9Z,12Z)/4(5Z,8Z,11Z,14Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007258	DG(18:2(9Z,12Z)/4(8Z,11Z,14Z,17Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007284	DG(18:3(6Z,9Z,12Z)/3(5Z,8Z,11Z))	C41H68O5	M+NH4	658.5405	-0.6

	HMDB0007285	DG(18:3(6Z,9Z,12Z)/:3(8Z,11Z,14Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007313	DG(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C41H68O5	M+NH4	658.5405	-0.6
	HMDB0007314	DG(18:3(9Z,12Z,15Z)/:3(8Z,11Z,14Z))	C41H68O5	M+NH4	658.5405	-0.6
660.5559	HMDB0056212	DG(18:1n9/:4n3)	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0056229	DG(:1n9/18:4n3)	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0056297	DG(18:3n6/:2n6)	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0056315	DG(:2n6/18:3n3)	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0158438	14-{[2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-yl]oxy}-12-hydroxy-14-oxotetradecanoic acid	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0056206	DG(18:1n9/:4n6)	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0056193	DG(18:1n7/:4n3)	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0056029	DG(16/22:5n6)	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0056034	DG(16/22:5n3)	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0056059	DG(18/:5n3)	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0056169	DG(16:1n7/22:4n6)	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0056187	DG(18:1n7/:4n6)	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0158435	14-{[2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-yl]oxy}-3-hydroxy-14-oxotetradecanoic acid	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007119	DG(16/22:5(4Z,7Z,Z,13Z,16Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007423	DG(:2(11Z,14Z)/18:3(6Z,9Z,12Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007424	DG(:2(11Z,14Z)/18:3(9Z,12Z,15Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007451	DG(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007480	DG(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007508	DG(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007507	DG(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007536	DG(:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007537	DG(:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007564	DG(:5(5Z,8Z,11Z,14Z,17Z)/18)	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007679	DG(22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007707	DG(22:5(4Z,7Z,Z,13Z,16Z)/16)	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007396	DG(:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007340	DG(18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007120	DG(16/22:5(7Z,Z,13Z,16Z,19Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007147	DG(16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007172	DG(18/:5(5Z,8Z,11Z,14Z,17Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007200	DG(18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007199	DG(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007228	DG(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007229	DG(18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007256	DG(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007255	DG(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007283	DG(18:3(6Z,9Z,12Z)/:2(11Z,14Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007312	DG(18:3(9Z,12Z,15Z)/:2(11Z,14Z))	C41H70O5	M+NH4	660.5561	-0.4
	HMDB0007736	DG(22:5(7Z,Z,13Z,16Z,19Z)/16)	C41H70O5	M+NH4	660.5561	-0.4
662.5718	HMDB0056282	DG(18:2n6/18:2n6)	C41H72O5	M+NH4	662.5718	0.0
	HMDB0056221	DG(:1n9/18:3n6)	C41H72O5	M+NH4	662.5718	0.0
	HMDB0056228	DG(:1n9/18:3n3)	C41H72O5	M+NH4	662.5718	0.0
	HMDB0056205	DG(18:1n9/:3n6)	C41H72O5	M+NH4	662.5718	0.0
	HMDB0056199	DG(18:1n9/:3n9)	C41H72O5	M+NH4	662.5718	0.0
	HMDB0056186	DG(18:1n7/:3n6)	C41H72O5	M+NH4	662.5718	0.0
	HMDB0056028	DG(16/22:4n6)	C41H72O5	M+NH4	662.5718	0.0
	HMDB0056052	DG(18/:4n6)	C41H72O5	M+NH4	662.5718	0.0
	HMDB0056058	DG(18/:4n3)	C41H72O5	M+NH4	662.5718	0.0
	HMDB0056082	DG(/18:4n3)	C41H72O5	M+NH4	662.5718	0.0
	HMDB0056180	DG(18:1n7/:3n9)	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007118	DG(16/22:4(7Z,Z,13Z,16Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007449	DG(:3(5Z,8Z,11Z)/18:1(11Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007450	DG(:3(5Z,8Z,11Z)/18:1(9Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007479	DG(:3(8Z,11Z,14Z)/18:1(9Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007478	DG(:3(8Z,11Z,14Z)/18:1(11Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007506	DG(:4(5Z,8Z,11Z,14Z)/18)	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007535	DG(:4(8Z,11Z,14Z,17Z)/18)	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007678	DG(22:4(7Z,Z,13Z,16Z)/16)	C41H72O5	M+NH4	662.5718	0.0

	HMDB0007422	DG:(2(11Z,14Z)/18:2(9Z,12Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007395	DG:(1(11Z)/18:3(9Z,12Z,15Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007394	DG:(1(11Z)/18:3(6Z,9Z,12Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007171	DG(18:/4(8Z,11Z,14Z,17Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007170	DG(18:/4(5Z,8Z,11Z,14Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007198	DG(18:1(11Z)/:3(8Z,11Z,14Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007227	DG(18:1(9Z)/:3(8Z,11Z,14Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007226	DG(18:1(9Z)/:3(5Z,8Z,11Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007254	DG(18:2(9Z,12Z)/:2(11Z,14Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007282	DG(18:3(6Z,9Z,12Z)/:1(11Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007311	DG(18:3(9Z,12Z,15Z)/:1(11Z))	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007339	DG(18:4(6Z,9Z,12Z,15Z)/)	C41H72O5	M+NH4	662.5718	0.0
	HMDB0007367	DG(/18:4(6Z,9Z,12Z,15Z))	C41H72O5	M+NH4	662.5718	0.0
664.1153	HMDB0039421	Fenugreekine	C21H27N7O1 4P2	M+H	664.1164	-1.7
	HMDB0000902	NAD+	C21H27N7O1 4P2	M+H	664.1164	-1.7
	HMDB0155854	1-{5-[(1-((5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy}(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)methyl]-3,4-dihydroxyoxolan-2-yl}-3-(C-hydroxycarbonimidoyl)-1-pyridin-1-ylum	C21H28N7O1 4P2	M+H	664.1164	-1.7
664.5870	HMDB0056204	DG(18:1n9/:2n6)	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0056185	DG(18:1n7/:2n6)	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0056168	DG(16:1n7/22:2n6)	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0056081	DG(/18:3n3)	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0056074	DG(/18:3n6)	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0056051	DG(18:/3n6)	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0056045	DG(18:/3n9)	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007650	DG(22:2(13Z,16Z)/16:1(9Z))	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007477	DG(:3(8Z,11Z,14Z)/18)	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007448	DG(:3(5Z,8Z,11Z)/18)	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007420	DG:(2(11Z,14Z)/18:1(11Z))	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007421	DG:(2(11Z,14Z)/18:1(9Z))	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007393	DG:(1(11Z)/18:2(9Z,12Z))	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007366	DG(/18:3(9Z,12Z,15Z))	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007365	DG(/18:3(6Z,9Z,12Z))	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007310	DG(18:3(9Z,12Z,15Z)/)	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007281	DG(18:3(6Z,9Z,12Z)/)	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007253	DG(18:2(9Z,12Z)/:1(11Z))	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007225	DG(18:1(9Z)/:2(11Z,14Z))	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007196	DG(18:1(11Z)/:2(11Z,14Z))	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007168	DG(18:/3(5Z,8Z,11Z))	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007169	DG(18:/3(8Z,11Z,14Z))	C41H74O5	M+NH4	664.5874	-0.7
	HMDB0007146	DG(16:1(9Z)/22:2(13Z,16Z))	C41H74O5	M+NH4	664.5874	-0.7
665.5342	HMDB0168953	6-(dotriacontan-2-yloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C38H74O7	M+Na	665.5327	2.3
	HMDB0168955	6-(dotriacontyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C38H74O7	M+Na	665.5327	2.3
666.6187	HMDB0000610	CE(18:2(9Z,12Z))	C45H76O2	M+NH4	666.6184	0.5
	HMDB0161106	2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-yl (9Z,12Z)-octadeca-9,12-dienoate	C45H76O2	M+NH4	666.6184	0.5
	HMDB0093873	DG(17/i-22)	C42H82O5	M+H	667.6235	-2.8
	HMDB0093587	DG(i-15/i-24)	C42H82O5	M+H	667.6235	-2.8
	HMDB0093424	DG(i-14/a-25)	C42H82O5	M+H	667.6235	-2.8
	HMDB0093426	DG(14/a-25)	C42H82O5	M+H	667.6235	-2.8
	HMDB0055986	DG(15/24)	C42H82O5	M+H	667.6235	-2.8
	HMDB0094189	DG(/19)	C42H82O5	M+H	667.6235	-2.8
	HMDB0094081	DG(19/)	C42H82O5	M+H	667.6235	-2.8
	HMDB0094331	DG(21/18)	C42H82O5	M+H	667.6235	-2.8
	HMDB0094462	DG(22/17)	C42H82O5	M+H	667.6235	-2.8
	HMDB0094087	DG(19/i-)	C42H82O5	M+H	667.6235	-2.8
	HMDB0094195	DG(/i-19)	C42H82O5	M+H	667.6235	-2.8
	HMDB0094341	DG(21/i-18)	C42H82O5	M+H	667.6235	-2.8

667.6216

HMDB0094472	DG(22/a-17)	C42H82O5	M+H	667.6235	-2.8
HMDB0093585	DG(a-15/i-24)	C42H82O5	M+H	667.6235	-2.8
HMDB0093863	DG(17/22)	C42H82O5	M+H	667.6235	-2.8
HMDB0093867	DG(a-17/i-22)	C42H82O5	M+H	667.6235	-2.8
HMDB0093871	DG(i-17/i-22)	C42H82O5	M+H	667.6235	-2.8
HMDB0093869	DG(a-17/22)	C42H82O5	M+H	667.6235	-2.8
HMDB0093865	DG(i-17/22)	C42H82O5	M+H	667.6235	-2.8
HMDB0093589	DG(15/i-24)	C42H82O5	M+H	667.6235	-2.8
HMDB0094470	DG(22/i-17)	C42H82O5	M+H	667.6235	-2.8
HMDB0094337	DG(a-21/18)	C42H82O5	M+H	667.6235	-2.8
HMDB0094335	DG(a-21/i-18)	C42H82O5	M+H	667.6235	-2.8
HMDB0093862	DG(17/22)	C42H82O5	M+H	667.6235	-2.8
HMDB0093872	DG(17/i-22)	C42H82O5	M+H	667.6235	-2.8
HMDB0093971	DG(18/21)	C42H82O5	M+H	667.6235	-2.8
HMDB0093981	DG(18/a-21)	C42H82O5	M+H	667.6235	-2.8
HMDB0093979	DG(18/i-21)	C42H82O5	M+H	667.6235	-2.8
HMDB0093584	DG(a-15/i-24)	C42H82O5	M+H	667.6235	-2.8
HMDB0093868	DG(a-17/22)	C42H82O5	M+H	667.6235	-2.8
HMDB0093866	DG(a-17/i-22)	C42H82O5	M+H	667.6235	-2.8
HMDB0093423	DG(i-14/a-25)	C42H82O5	M+H	667.6235	-2.8
HMDB0093586	DG(i-15/i-24)	C42H82O5	M+H	667.6235	-2.8
HMDB0093864	DG(i-17/22)	C42H82O5	M+H	667.6235	-2.8
HMDB0093870	DG(i-17/i-22)	C42H82O5	M+H	667.6235	-2.8
HMDB0093973	DG(i-18/21)	C42H82O5	M+H	667.6235	-2.8
HMDB0093975	DG(i-18/a-21)	C42H82O5	M+H	667.6235	-2.8
HMDB0093588	DG(15/i-24)	C42H82O5	M+H	667.6235	-2.8
HMDB0093425	DG(14/a-25)	C42H82O5	M+H	667.6235	-2.8
HMDB0094598	DG(a-25/14)	C42H82O5	M+H	667.6235	-2.8
HMDB0094596	DG(a-25/i-14)	C42H82O5	M+H	667.6235	-2.8
HMDB0094083	DG(i-19/)	C42H82O5	M+H	667.6235	-2.8
HMDB0094085	DG(i-19/i-)	C42H82O5	M+H	667.6235	-2.8
HMDB0094191	DG(i-/19)	C42H82O5	M+H	667.6235	-2.8
HMDB0094193	DG(i-/i-19)	C42H82O5	M+H	667.6235	-2.8
HMDB0094333	DG(i-21/18)	C42H82O5	M+H	667.6235	-2.8
HMDB0094339	DG(i-21/i-18)	C42H82O5	M+H	667.6235	-2.8
HMDB0094464	DG(i-22/17)	C42H82O5	M+H	667.6235	-2.8
HMDB0094466	DG(i-22/a-17)	C42H82O5	M+H	667.6235	-2.8
HMDB0094468	DG(i-22/i-17)	C42H82O5	M+H	667.6235	-2.8
HMDB0094540	DG(i-24/15)	C42H82O5	M+H	667.6235	-2.8
HMDB0094542	DG(i-24/a-15)	C42H82O5	M+H	667.6235	-2.8
HMDB0094544	DG(i-24/i-15)	C42H82O5	M+H	667.6235	-2.8
HMDB0093977	DG(i-18/i-21)	C42H82O5	M+H	667.6235	-2.8
HMDB0093974	DG(i-18/21)	C42H82O5	M+H	667.6235	-2.8
HMDB0007093	DG(15/24)	C42H82O5	M+H	667.6235	-2.8
HMDB0094471	DG(22/i-17)	C42H82O5	M+H	667.6235	-2.8
HMDB0094467	DG(i-22/a-17)	C42H82O5	M+H	667.6235	-2.8
HMDB0094473	DG(22/a-17)	C42H82O5	M+H	667.6235	-2.8
HMDB0094469	DG(i-22/i-17)	C42H82O5	M+H	667.6235	-2.8
HMDB0094465	DG(i-22/17)	C42H82O5	M+H	667.6235	-2.8
HMDB0094332	DG(21/18)	C42H82O5	M+H	667.6235	-2.8
HMDB0094342	DG(21/i-18)	C42H82O5	M+H	667.6235	-2.8
HMDB0094463	DG(22/17)	C42H82O5	M+H	667.6235	-2.8
HMDB0007793	DG(24/15)	C42H82O5	M+H	667.6235	-2.8
HMDB0094597	DG(a-25/i-14)	C42H82O5	M+H	667.6235	-2.8
HMDB0094599	DG(a-25/14)	C42H82O5	M+H	667.6235	-2.8
HMDB0094543	DG(i-24/a-15)	C42H82O5	M+H	667.6235	-2.8
HMDB0094545	DG(i-24/i-15)	C42H82O5	M+H	667.6235	-2.8
HMDB0094541	DG(i-24/15)	C42H82O5	M+H	667.6235	-2.8
HMDB0094336	DG(a-21/i-18)	C42H82O5	M+H	667.6235	-2.8
HMDB0094340	DG(i-21/i-18)	C42H82O5	M+H	667.6235	-2.8
HMDB0094088	DG(19/i-)	C42H82O5	M+H	667.6235	-2.8
HMDB0094086	DG(i-19/i-)	C42H82O5	M+H	667.6235	-2.8
HMDB0094084	DG(i-19/)	C42H82O5	M+H	667.6235	-2.8
HMDB0093972	DG(18/21)	C42H82O5	M+H	667.6235	-2.8
HMDB0093976	DG(i-18/a-21)	C42H82O5	M+H	667.6235	-2.8

	HMDB0093980	DG(18/i-21)	C42H82O5	M+H	667.6235	-2.8
	HMDB0093982	DG(18/a-21)	C42H82O5	M+H	667.6235	-2.8
	HMDB0093978	DG(i-18/i-21)	C42H82O5	M+H	667.6235	-2.8
	HMDB0094082	DG(19/)	C42H82O5	M+H	667.6235	-2.8
	HMDB0094334	DG(i-21/18)	C42H82O5	M+H	667.6235	-2.8
	HMDB0094338	DG(a-21/18)	C42H82O5	M+H	667.6235	-2.8
	HMDB0094196	DG(/i-19)	C42H82O5	M+H	667.6235	-2.8
	HMDB0094190	DG(/19)	C42H82O5	M+H	667.6235	-2.8
	HMDB0094194	DG(i-/i-19)	C42H82O5	M+H	667.6235	-2.8
	HMDB0094192	DG(i-/19)	C42H82O5	M+H	667.6235	-2.8
668.6332	HMDB0160384	Cholesteryl elaidate	C45H78O2	M+NH4	668.6340	-1.2
	HMDB0155797	Cholesterol, oleate	C45H78O2	M+NH4	668.6340	-1.2
	HMDB0000918	CE(18:1(9Z))	C45H78O2	M+NH4	668.6340	-1.2
	HMDB0034420	Palmitoylstigmasterol	C45H78O2	M+NH4	668.6340	-1.2
	HMDB0005189	Barium	C45H78O2	M+NH4	668.6340	-1.2
	HMDB0187018	2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-yl (11Z)-octadec-11-enoate	C45H78O2	M+NH4	668.6340	-1.2
675.5427	HMDB0012097	SM(d18:1/14)	C37H75N2O6P	M+H	675.5436	-1.3
	HMDB0240616	N-(hexadecanoyl)hexadecasphingosine-1-phosphocholine	C37H75N2O6P	M+H	675.5436	-1.3
676.4918	HMDB0038620	Acidissiminin epoxide	C43H65NO5	M+H	676.4936	-2.6
	HMDB0113840	PE-NMe2(14:1(9Z)/15)	C36H70NO8P	M+H	676.4912	0.9
	HMDB0112941	PE-NMe(14:1(9Z)/16)	C36H70NO8P	M+H	676.4912	0.9
	HMDB0112940	PE-NMe(14/16:1(9Z))	C36H70NO8P	M+H	676.4912	0.9
	HMDB0113918	PE-NMe2(15/14:1(9Z))	C36H70NO8P	M+H	676.4912	0.9
	HMDB0113061	PE-NMe(16:1(9Z)/14)	C36H70NO8P	M+H	676.4912	0.9
	HMDB0113040	PE-NMe(16/14:1(9Z))	C36H70NO8P	M+H	676.4912	0.9
	HMDB0008955	PE(16:1(9Z)/15)	C36H70NO8P	M+H	676.4912	0.9
	HMDB0008891	PE(15/16:1(9Z))	C36H70NO8P	M+H	676.4912	0.9
	HMDB0007899	PC(14:1(9Z)/14)	C36H70NO8P	M+H	676.4912	0.9
	HMDB0007867	PC(14/14:1(9Z))	C36H70NO8P	M+H	676.4912	0.9
	HMDB0114948	PA(18:2(9Z,12Z)/15)	C36H67O8P	M+NH4	676.4912	0.9
	HMDB0114815	PA(15/18:2(9Z,12Z))	C36H67O8P	M+NH4	676.4912	0.9
	HMDB0114898	PA(18:1(11Z)/15)	C36H69O8P	M+NH4	678.5068	-0.6
678.5064	HMDB0114923	PA(18:1(9Z)/15)	C36H69O8P	M+NH4	678.5068	-0.6
	HMDB0113917	PE-NMe2(15/14)	C36H72NO8P	M+H	678.5068	-0.6
	HMDB0008922	PE(16/15)	C36H72NO8P	M+H	678.5068	-0.6
	HMDB0008890	PE(15/16)	C36H72NO8P	M+H	678.5068	-0.6
	HMDB0113039	PE-NMe(16/14)	C36H72NO8P	M+H	678.5068	-0.6
	HMDB0113838	PE-NMe2(14/15)	C36H72NO8P	M+H	678.5068	-0.6
	HMDB0112944	PE-NMe(14/16)	C36H72NO8P	M+H	678.5068	-0.6
	HMDB0112939	PE-NMe(15/15)	C36H72NO8P	M+H	678.5068	-0.6
	HMDB0007866	PC(14/14)	C36H72NO8P	M+H	678.5068	-0.6
	HMDB0056196	DG(18:1n7/22:6n3)	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0056318	DG(:2n6/:5n3)	C43H70O5	M+NH4	684.5561	-0.7

684.5557	HMDB0056215	DG(18:1n9/22:6n3)	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0056241	DG(:3n9/:4n6)	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0056247	DG(:3n9/:4n3)	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0056301	DG(18:3n6/22:4n6)	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0056322	DG(:3n6/:4n6)	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0056328	DG(:3n6/:4n3)	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0056353	DG(22:4n6/18:3n3)	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007208	DG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007545	DG(:4(8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007546	DG(:4(8Z,11Z,14Z,17Z)/:3(8Z,11Z,14Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007573	DG(:5(5Z,8Z,11Z,14Z,17Z)/:2(11Z,14Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007685	DG(22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007684	DG(22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007712	DG(22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007741	DG(22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007769	DG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007768	DG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007517	DG(:4(5Z,8Z,11Z,14Z)/:3(8Z,11Z,14Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007516	DG(:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007490	DG(:3(8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007237	DG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007264	DG(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007265	DG(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007292	DG(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007321	DG(18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007433	DG(:2(11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007460	DG(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007461	DG(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C43H70O5	M+NH4	684.5561	-0.7
	HMDB0007489	DG(:3(8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C43H70O5	M+NH4	684.5561	-0.7
685.1438	HMDB0014678	Gadoversetamide	C20H34GdN5O10	M+Na	685.1439	-0.1
685.2812	HMDB0171549	6-(1-{1,6-dimethyl-2-oxo-3,7-dioxabicyclo[4.1]heptan-4-yl}-1-{6-hydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7.?,octadec-4-en-15-yl]ethoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H46O13	M+Na	685.2831	-2.7
	HMDB0171548	6-([15-(1-{1,6-dimethyl-2-oxo-3,7-dioxabicyclo[4.1]heptan-4-yl}-1-hydroxyethyl)-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7.?,octadec-4-en-6-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H46O13	M+Na	685.2831	-2.7
	HMDB0168827	6-([15-[1-(4,5-dimethyl-6-oxo-3,6-dihydro-2H-pyran-2-yl)ethyl]-12,13-dihydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7.?,octadec-4-en-6-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H46O13	M+Na	685.2831	-2.7
	HMDB0168826	6-([15-[1-(4,5-dimethyl-6-oxo-3,6-dihydro-2H-pyran-2-yl)ethyl]-6,12-dihydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7.?,octadec-4-en-13-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H46O13	M+Na	685.2831	-2.7
	HMDB0168828	6-([15-[1-(4,5-dimethyl-6-oxo-3,6-dihydro-2H-pyran-2-yl)ethyl]-6,13-dihydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7.?,octadec-4-en-12-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H46O13	M+Na	685.2831	-2.7
	HMDB0174562	6-([14-[1-(4,5-dimethyl-6-oxo-3,6-dihydro-2H-pyran-2-yl)-1-hydroxyethyl]-7,9-dihydroxy-2,15-dimethyl-3-oxotetracyclo[8.7.,heptadeca-4,8-dien-8-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H46O13	M+Na	685.2831	-2.7
	HMDB0056234	DG(:3n9/:3n9)	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0056321	DG(:3n6/:3n6)	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0056195	DG(18:1n7/22:5n3)	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0056209	DG(18:1n9/22:5n6)	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0056214	DG(18:1n9/22:5n3)	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0056231	DG(:1n9/:5n3)	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0056240	DG(:3n9/:3n6)	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0056346	DG(22:2n6/18:4n3)	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0056317	DG(:2n6/:4n3)	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0056311	DG(:2n6/:4n6)	C43H72O5	M+NH4	686.5718	-0.9

686.5712	HMDB0056190	DG(18:1n7/22:5n6)	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0056061	DG(18/22:6n3)	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007179	DG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007487	DG(:3(8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007515	DG(:4(5Z,8Z,11Z,14Z)/:2(11Z,14Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007544	DG(:4(8Z,11Z,14Z,17Z)/:2(11Z,14Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007572	DG(:5(5Z,8Z,11Z,14Z,17Z)/:1(11Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007657	DG(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007683	DG(22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007711	DG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007710	DG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007739	DG(22:5(7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007488	DG(:3(8Z,11Z,14Z)/:3(8Z,11Z,14Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007458	DG(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007459	DG(:3(5Z,8Z,11Z)/:3(8Z,11Z,14Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007207	DG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007206	DG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007236	DG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007235	DG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007263	DG(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007349	DG(18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007404	DG(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007431	DG(:2(11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007432	DG(:2(11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007740	DG(22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C43H72O5	M+NH4	686.5718	-0.9
	HMDB0007767	DG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18)	C43H72O5	M+NH4	686.5718	-0.9
688.4931	HMDB0113844	PE-NMe2(14:1(9Z)/16:1(9Z))	C37H70NO8P	M+H	688.4912	2.8
	HMDB0113963	PE-NMe2(16:1(9Z)/14:1(9Z))	C37H70NO8P	M+H	688.4912	2.8
	HMDB0009085	PE(18:2(9Z,12Z)/14)	C37H70NO8P	M+H	688.4912	2.8
	HMDB0009053	PE(18:1(9Z)/14:1(9Z))	C37H70NO8P	M+H	688.4912	2.8
	HMDB0009020	PE(18:1(11Z)/14:1(9Z))	C37H70NO8P	M+H	688.4912	2.8
	HMDB0008957	PE(16:1(9Z)/16:1(9Z))	C37H70NO8P	M+H	688.4912	2.8
	HMDB0008861	PE(14:1(9Z)/18:1(9Z))	C37H70NO8P	M+H	688.4912	2.8
	HMDB0008860	PE(14:1(9Z)/18:1(11Z))	C37H70NO8P	M+H	688.4912	2.8
	HMDB0008829	PE(14/18:2(9Z,12Z))	C37H70NO8P	M+H	688.4912	2.8
	HMDB0115118	PA(:3(5Z,8Z,11Z)/14)	C37H67O8P	M+NH4	688.4912	2.8
	HMDB0115506	PA(14:1(9Z)/:2(11Z,14Z))	C37H67O8P	M+NH4	688.4912	2.8
	HMDB0115505	PA(14/:3(8Z,11Z,14Z))	C37H67O8P	M+NH4	688.4912	2.8
	HMDB0115533	PA(:2(11Z,14Z)/14:1(9Z))	C37H67O8P	M+NH4	688.4912	2.8
	HMDB0115003	PA(18:3(9Z,12Z,15Z)/16)	C37H67O8P	M+NH4	688.4912	2.8
	HMDB0114976	PA(18:3(6Z,9Z,12Z)/16)	C37H67O8P	M+NH4	688.4912	2.8
	HMDB0114950	PA(18:2(9Z,12Z)/16:1(9Z))	C37H67O8P	M+NH4	688.4912	2.8
	HMDB0114856	PA(16:1(9Z)/18:2(9Z,12Z))	C37H67O8P	M+NH4	688.4912	2.8
	HMDB0114836	PA(16/18:3(6Z,9Z,12Z))	C37H67O8P	M+NH4	688.4912	2.8
	HMDB0114837	PA(16/18:3(9Z,12Z,15Z))	C37H67O8P	M+NH4	688.4912	2.8
	HMDB0114784	PA(14/:3(5Z,8Z,11Z))	C37H67O8P	M+NH4	688.4912	2.8
	HMDB0115561	PA(:3(8Z,11Z,14Z)/14)	C37H67O8P	M+NH4	688.4912	2.8
688.5269	HMDB0007928	PC(14:1(9Z)/P-16)	C38H74NO7P	M+H	688.5276	-1.0
	HMDB0013410	PC(O-16:1(9Z)/14:1(9Z))	C38H74NO7P	M+H	688.5276	-1.0
	HMDB0008919	PE(15/P-18:1(9Z))	C38H74NO7P	M+H	688.5276	-1.0
	HMDB0008918	PE(15/P-18:1(11Z))	C38H74NO7P	M+H	688.5276	-1.0

	HMDB0011204	PC(P-16/14:1(9Z))	C38H74NO7P	M+H	688.5276	-1.0
	HMDB0011403	PE(P-18:1(11Z)/15)	C38H74NO7P	M+H	688.5276	-1.0
	HMDB0011436	PE(P-18:1(9Z)/15)	C38H74NO7P	M+H	688.5276	-1.0
689.0952	HMDB0162227	[(6-hydroxy-7-{6-hydroxy-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl}-5,8-dimethoxy-4-oxo-4H-benzo[g]chromen-2-yl)methoxy]sulfonic acid	C32H26O14S	M+Na	689.0935	2.4
	HMDB0162230	[(6-hydroxy--{6-hydroxy-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-7-yl}-5,8-dimethoxy-4-oxo-4H-benzo[g]chromen-2-yl)methoxy]sulfonic acid	C32H26O14S	M+Na	689.0935	2.4
	HMDB0162278	[(5-hydroxy--{5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl}-6,8-dimethoxy-4-oxo-4H-benzo[g]chromen-2-yl)methoxy]sulfonic acid	C32H26O14S	M+Na	689.0935	2.4
	HMDB0162342	[(5-hydroxy-6-{5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl}-8,-dimethoxy-4-oxo-4H-benzo[h]chromen-2-yl)methoxy]sulfonic acid	C32H26O14S	M+Na	689.0935	2.4
	HMDB0162345	[(5-hydroxy--{5-hydroxy-8,-dimethoxy-2-methyl-4-oxo-4H-benzo[h]chromen-6-yl}-6,8-dimethoxy-4-oxo-4H-benzo[g]chromen-2-yl)methoxy]sulfonic acid	C32H26O14S	M+Na	689.0935	2.4
	HMDB0168115	[(5-hydroxy-7-{5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl}-6,8-dimethoxy-4-oxo-4H-benzo[g]chromen-2-yl)methoxy]sulfonic acid	C32H26O14S	M+Na	689.0935	2.4
	HMDB0168118	[(5-hydroxy--{5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-7-yl}-6,8-dimethoxy-4-oxo-4H-benzo[g]chromen-2-yl)methoxy]sulfonic acid	C32H26O14S	M+Na	689.0935	2.4
	HMDB0150856	{[4-(2,4-dihydroxyphenyl)-,18-dihydroxy-8-(6-hydroxy-1-benzofuran-2-yl)-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-14-yl]methoxy} sulfonic acid	C34H24O14S	M+H	689.0960	-1.1
689.5601	HMDB0240608	N-pentadecanoylsphingosine-1-phosphocholine	C38H77N2O6P	M+H	689.5592	1.3
	HMDB0240617	N-(heptadecanoyl)hexadecaspingosine-1-phosphocholine	C38H77N2O6P	M+H	689.5592	1.3
690.4350	HMDB0183781	15-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl} sulfanyl)-16-hydroxytetracosanoic acid	C34H63N3O9S	M+H	690.4358	-1.1
	HMDB0183782	16-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl} sulfanyl)-15-hydroxytetracosanoic acid	C34H63N3O9S	M+H	690.4358	-1.1
690.5066	HMDB0114900	PA(18:1(11Z)/16:1(9Z))	C37H69O8P	M+NH4	690.5068	-0.3
	HMDB0114925	PA(18:1(9Z)/16:1(9Z))	C37H69O8P	M+NH4	690.5068	-0.3
	HMDB0007860	PA(16/18:2(9Z,12Z))	C37H69O8P	M+NH4	690.5068	-0.3
	HMDB0115532	PA(:2(11Z,14Z)/14)	C37H69O8P	M+NH4	690.5068	-0.3
	HMDB0115504	PA(14/:2(11Z,14Z))	C37H69O8P	M+NH4	690.5068	-0.3
	HMDB0115092	PA(:1(11Z)/14:1(9Z))	C37H69O8P	M+NH4	690.5068	-0.3
	HMDB0114949	PA(18:2(9Z,12Z)/16)	C37H69O8P	M+NH4	690.5068	-0.3
	HMDB0113843	PE-NMe2(14:1(9Z)/16)	C37H72NO8P	M+H	690.5068	-0.3
	HMDB0113842	PE-NMe2(14/16:1(9Z))	C37H72NO8P	M+H	690.5068	-0.3
	HMDB0009019	PE(18:1(11Z)/14)	C37H72NO8P	M+H	690.5068	-0.3
	HMDB0113063	PE-NMe(16:1(9Z)/15)	C37H72NO8P	M+H	690.5068	-0.3
	HMDB0113962	PE-NMe2(16:1(9Z)/14)	C37H72NO8P	M+H	690.5068	-0.3
	HMDB0113941	PE-NMe2(16/14:1(9Z))	C37H72NO8P	M+H	690.5068	-0.3
	HMDB0009052	PE(18:1(9Z)/14)	C37H72NO8P	M+H	690.5068	-0.3

	HMDB0008987	PE(18/14:1(9Z))	C37H72NO8P	M+H	690.5068	-0.3
	HMDB0008956	PE(16:1(9Z)/16)	C37H72NO8P	M+H	690.5068	-0.3
	HMDB0008924	PE(16/16:1(9Z))	C37H72NO8P	M+H	690.5068	-0.3
	HMDB0008859	PE(14:1(9Z)/18)	C37H72NO8P	M+H	690.5068	-0.3
	HMDB0008828	PE(14/18:1(9Z))	C37H72NO8P	M+H	690.5068	-0.3
	HMDB0008827	PE(14/18:1(11Z))	C37H72NO8P	M+H	690.5068	-0.3
	HMDB0007933	PC(15/14:1(9Z))	C37H72NO8P	M+H	690.5068	-0.3
	HMDB0112945	PE-NMe(15/16:1(9Z))	C37H72NO8P	M+H	690.5068	-0.3
	HMDB0007901	PC(14:1(9Z)/15)	C37H72NO8P	M+H	690.5068	-0.3
690.5433	HMDB0013403	PC(O-16/14:1(9Z))	C38H76NO7P	M+H	690.5432	0.1
	HMDB0013402	PC(O-14/16:1(9Z))	C38H76NO7P	M+H	690.5432	0.1
	HMDB0011370	PE(P-18/15)	C38H76NO7P	M+H	690.5432	0.1
	HMDB0011203	PC(P-16/14)	C38H76NO7P	M+H	690.5432	0.1
	HMDB0008917	PE(15/P-18)	C38H76NO7P	M+H	690.5432	0.1
	HMDB0007895	PC(14/P-16)	C38H76NO7P	M+H	690.5432	0.1
690.6186	HMDB0010371	CE(:4(8Z,11Z,14Z,17Z))	C47H76O2	M+NH4	690.6184	0.4
	HMDB0006726	CE(:4(5Z,8Z,11Z,14Z))	C47H76O2	M+NH4	690.6184	0.4
691.0856	HMDB0240283	Gadobenic acid	C22H31GdN3O11	M+Na	691.0857	-0.2
691.2858	HMDB0176927	2-amino-4-[(2-{[3,5-bis(acetyloxy)-2-hydroxy-4-(3-hydroxy-6-methylhepta-1,5-dien-2-yl)-1-methyl-6-oxocyclohexyl]sulfanyl}-1-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl)-C-hydroxycarbonimidoyl]butanoic acid	C29H43N3O13S	M+NH4	691.2855	0.5
691.6215	HMDB0056097	DG(22/18:2n6)	C44H82O5	M+H	691.6235	-2.9
692.5226	HMDB0113041	PE-NMe(16/15)	C37H74NO8P	M+H	692.5225	0.2
	HMDB0113940	PE-NMe2(16/14)	C37H74NO8P	M+H	692.5225	0.2
	HMDB0008986	PE(18/14)	C37H74NO8P	M+H	692.5225	0.2
	HMDB0008923	PE(16/16)	C37H74NO8P	M+H	692.5225	0.2
	HMDB0008826	PE(14/18)	C37H74NO8P	M+H	692.5225	0.2
	HMDB0029174	3-Sn-phosphatidylethanolamine	C37H74NO8P	M+H	692.5225	0.2
	HMDB0112964	PE-NMe(15/16)	C37H74NO8P	M+H	692.5225	0.2
	HMDB0007932	PC(15/14)	C37H74NO8P	M+H	692.5225	0.2
	HMDB0007868	PC(14/15)	C37H74NO8P	M+H	692.5225	0.2
	HMDB0113845	PE-NMe2(14/16)	C37H74NO8P	M+H	692.5225	0.2
	HMDB0113841	PE-NMe2(15/15)	C37H74NO8P	M+H	692.5225	0.2
	HMDB0007858	PA(16/18:1(11Z))	C37H71O8P	M+NH4	692.5225	0.2
	HMDB0007859	PA(16/18:1(9Z))	C37H71O8P	M+NH4	692.5225	0.2

	HMDB0031130	9-Octadecenoic acid 1-[[[(1-oxohexadecyl)oxy]methyl]-2-(phosphonoxy)ethyl ester	C37H71O8P	M+NH4	692.5225	0.2
	HMDB0114877	PA(18/16:1(9Z))	C37H71O8P	M+NH4	692.5225	0.2
	HMDB0115091	PA(:1(11Z)/14)	C37H71O8P	M+NH4	692.5225	0.2
	HMDB0115062	PA(/14:1(9Z))	C37H71O8P	M+NH4	692.5225	0.2
	HMDB0114899	PA(18:1(11Z)/16)	C37H71O8P	M+NH4	692.5225	0.2
	HMDB0114924	PA(18:1(9Z)/16)	C37H71O8P	M+NH4	692.5225	0.2
692.5588	HMDB0013341	PC(O-14/16)	C38H78NO7P	M+H	692.5589	-0.1
692.6341	HMDB0006736	CE(:3(8Z,11Z,14Z))	C47H78O2	M+NH4	692.6340	0.1
	HMDB0185652	2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-yl (8Z,11Z,14Z)-icosa-8,11,14-trienoate	C47H78O2	M+NH4	692.6340	0.1
	HMDB0010373	CE(:3(5Z,8Z,11Z))	C47H78O2	M+NH4	692.6340	0.1
694.4539	HMDB0169017	((5,12-dihydroxy-1-[5-(1-hydroxytridecyl)oxolan-2-yl]-13-(5-methyl-2-oxo-2,5-dihydrofuran-3-yl)tridecyl}oxy)sulfonic acid	C35H64O10S	M+NH4	694.4558	-2.8
	HMDB0169018	[(1-{5-[1,5,12-trihydroxy-13-(5-methyl-2-oxo-2,5-dihydrofuran-3-yl)tridecyl]oxolan-2-yl}tridecyl)oxy]sulfonic acid	C35H64O10S	M+NH4	694.4558	-2.8
	HMDB0169016	((1,12-dihydroxy-1-[5-(1-hydroxytridecyl)oxolan-2-yl]-13-(5-methyl-2-oxo-2,5-dihydrofuran-3-yl)tridecan-5-yl}oxy)sulfonic acid	C35H64O10S	M+NH4	694.4558	-2.8
	HMDB0169015	((9,13-dihydroxy-13-[5-(1-hydroxytridecyl)oxolan-2-yl]-1-(5-methyl-2-oxo-2,5-dihydrofuran-3-yl)tridecan-2-yl}oxy)sulfonic acid	C35H64O10S	M+NH4	694.4558	-2.8
	HMDB0164715	[(1-{5-[1,6,12-trihydroxy-13-(5-methyl-2-oxo-2,5-dihydrofuran-3-yl)tridecyl]oxolan-2-yl}tridecyl)oxy]sulfonic acid	C35H64O10S	M+NH4	694.4558	-2.8
	HMDB0164712	((8,13-dihydroxy-13-[5-(1-hydroxytridecyl)oxolan-2-yl]-1-(5-methyl-2-oxo-2,5-dihydrofuran-3-yl)tridecan-2-yl}oxy)sulfonic acid	C35H64O10S	M+NH4	694.4558	-2.8
	HMDB0164714	((6,12-dihydroxy-1-[5-(1-hydroxytridecyl)oxolan-2-yl]-13-(5-methyl-2-oxo-2,5-dihydrofuran-3-yl)tridecyl}oxy)sulfonic acid	C35H64O10S	M+NH4	694.4558	-2.8
	HMDB0164713	((1,12-dihydroxy-1-[5-(1-hydroxytridecyl)oxolan-2-yl]-13-(5-methyl-2-oxo-2,5-dihydrofuran-3-yl)tridecan-6-yl}oxy)sulfonic acid	C35H64O10S	M+NH4	694.4558	-2.8
694.6481	HMDB0006734	Lactosylceramide (d18:1/16)	C47H80O2	M+NH4	694.6497	-2.2
	HMDB0062455	:2 cholesterol ester	C47H80O2	M+NH4	694.6497	-2.2
696.6649	HMDB0005193	CE(:1(11Z))	C47H82O2	M+NH4	696.6653	-0.6
	HMDB0172585	2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-yl (11E)-icos-11-enoate	C47H82O2	M+NH4	696.6653	-0.6
	HMDB0030508	Cyclolaudenyl palmitate	C47H82O2	M+NH4	696.6653	-0.6
	HMDB0169635	6-[1-(4,5-dimethyl-6-oxo-3,6-dihydro-2H-pyran-2-yl)-1-{6,12,15-trihydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7.,?,octadecan-15-yl]ethoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
	HMDB0169639	6-({15-[1-(4,5-dimethyl-6-oxooxan-2-yl)-1-hydroxyethyl]-6,12-dihydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7.,?,octadec-4-en-15-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
	HMDB0169640	6-[1-(4,5-dimethyl-6-oxooxan-2-yl)-1-{6,12,15-trihydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7.,?,octadec-4-en-15-yl]ethoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
	HMDB0173105	6-({14-[1-(4,5-dimethyl-6-oxooxan-2-yl)-1-hydroxyethyl]-7,9,11-trihydroxy-2,15-dimethyl-3-oxotetracyclo[8.7.,heptadeca-4,8-dien-8-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
	HMDB0173129	6-{8,18-dihydroxy-3',4',8,,14-pentamethyl-5,-dioxaspiro[hexacyclo[11.9,???]docosane-6,2'-oxolane]-5',15-dioneoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0

698.3375

HMDB0173130	6-{7,18-dihydroxy-3',4',8,,14-pentamethyl-5,-dioxaspiro[hexacyclo[11.9,???]docosane-6,2'-oxolane]-5',15-dioneoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
HMDB0173131	6-{7,8-dihydroxy-3',4',8,,14-pentamethyl-5,-dioxaspiro[hexacyclo[11.9,???]docosane-6,2'-oxolane]-5',15-dioneoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
HMDB0174229	6-(2-{6,14-dihydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7,?,octadec-4-en-15-yl]-1-(3,4-dimethyl-5-oxooxolan-2-yl)-2-hydroxypropoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
HMDB0174228	6-[(2-{6,14-dihydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7,?,octadec-4-en-15-yl]-1-(3,4-dimethyl-5-oxooxolan-2-yl)-1-hydroxypropan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
HMDB0174226	6-({15-[1-(3,4-dimethyl-5-oxooxolan-2-yl)-1,2-dihydroxypropan-2-yl]-14-hydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7,?,octadec-4-en-6-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
HMDB0174227	6-({15-[1-(3,4-dimethyl-5-oxooxolan-2-yl)-1,2-dihydroxypropan-2-yl]-6-hydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7,?,octadec-4-en-14-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
HMDB0174293	6-({7-[1-(4,5-dimethyl-6-oxooxan-2-yl)-1-hydroxyethyl]-7,17-dihydroxy-8,12-dimethyl-13-oxo-18-oxapentacyclo[13.2.1,?,octadec-4-en-16-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
HMDB0174294	6-({7-[1-(4,5-dimethyl-6-oxooxan-2-yl)-1-hydroxyethyl]-7,16-dihydroxy-8,12-dimethyl-13-oxo-18-oxapentacyclo[13.2.1,?,octadec-4-en-17-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
HMDB0174296	6-[1-(4,5-dimethyl-6-oxooxan-2-yl)-1-{7,16,17-trihydroxy-8,12-dimethyl-13-oxo-18-oxapentacyclo[13.2.1,?,octadec-4-en-7-yl]ethoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
HMDB0169637	6-({15-[1-(4,5-dimethyl-6-oxooxan-2-yl)-1-hydroxyethyl]-12,15-dihydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7,?,octadec-4-en-6-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
HMDB0169638	6-({15-[1-(4,5-dimethyl-6-oxooxan-2-yl)-1-hydroxyethyl]-6,15-dihydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7,?,octadec-4-en-12-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
HMDB0168411	6-({16-[1-(4,5-dimethyl-6-oxooxan-2-yl)-1-hydroxyethyl]-16-hydroxy-2,17-dimethyl-3-oxo-5,9-dioxahexacyclo[.7,??,nonadecan-13-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
HMDB0168412	6-({16-[1-(4,5-dimethyl-6-oxooxan-2-yl)-1-hydroxyethyl]-13-hydroxy-2,17-dimethyl-3-oxo-5,9-dioxahexacyclo[.7,??,nonadecan-16-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
HMDB0168413	6-(1-{13,16-dihydroxy-2,17-dimethyl-3-oxo-5,9-dioxahexacyclo[.7,??,nonadecan-16-yl]-1-(4,5-dimethyl-6-oxooxan-2-yl)ethoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
HMDB0169633	6-({15-[1-(4,5-dimethyl-6-oxo-3,6-dihydro-2H-pyran-2-yl)-1-hydroxyethyl]-6,15-dihydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7,?,octadecan-12-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
HMDB0169632	6-({15-[1-(4,5-dimethyl-6-oxo-3,6-dihydro-2H-pyran-2-yl)-1-hydroxyethyl]-12,15-dihydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7,?,octadecan-6-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0

	HMDB0169634	6-({15-[1-(4,5-dimethyl-6-oxo-3,6-dihydro-2H-pyran-2-yl)-1-hydroxyethyl]-6,12-dihydroxy-2,16-dimethyl-3-oxo-8-oxapentacyclo[9.7.?,octadecan-15-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
	HMDB0174295	6-({7-[1-(4,5-dimethyl-6-oxooxan-2-yl)-1-hydroxyethyl]-16,17-dihydroxy-8,12-dimethyl-13-oxo-18-oxapentacyclo[13.2.1.?,octadec-4-en-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H48O14	M+NH4	698.3382	-1.0
699.2546	HMDB0125481	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(4-{3-[2-(2,4-dihydroxyphenyl)-2-oxoethyl]-4,6-dihydroxy-2-methoxyphenyl}-3-hydroxy-2-methylbutan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C30H39N3O13S	M+NH4	699.2542	0.6
	HMDB0148655	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(4-{2,6-dihydroxy-3-[1-oxo-1-(2,4,6-trihydroxyphenyl)propan-2-yl]phenyl}-3-hydroxy-2-methylbutan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C30H39N3O13S	M+NH4	699.2542	0.6
	HMDB0148654	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1-{2,6-dihydroxy-3-[1-oxo-1-(2,4,6-trihydroxyphenyl)propan-2-yl]phenyl}-3-hydroxy-3-methylbutan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C30H39N3O13S	M+NH4	699.2542	0.6
	HMDB0150572	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(4-{3-[2-(2,4-dihydroxyphenyl)propanoyl]-2,4,6-trihydroxyphenyl}-3-hydroxy-2-methylbutan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C30H39N3O13S	M+NH4	699.2542	0.6
	HMDB0150571	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1-{3-[2-(2,4-dihydroxyphenyl)propanoyl]-2,4,6-trihydroxyphenyl}-3-hydroxy-3-methylbutan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C30H39N3O13S	M+NH4	699.2542	0.6
700.5261	HMDB0008984	PE(16:1(9Z)/P-18:1(11Z))	C39H74NO7P	M+H	700.5276	-2.1
	HMDB0008985	PE(16:1(9Z)/P-18:1(9Z))	C39H74NO7P	M+H	700.5276	-2.1
	HMDB0009114	PE(18:2(9Z,12Z)/P-16)	C39H74NO7P	M+H	700.5276	-2.1
	HMDB0011343	PE(P-16/18:2(9Z,12Z))	C39H74NO7P	M+H	700.5276	-2.1
	HMDB0011405	PE(P-18:1(11Z)/16:1(9Z))	C39H74NO7P	M+H	700.5276	-2.1
	HMDB0011438	PE(P-18:1(9Z)/16:1(9Z))	C39H74NO7P	M+H	700.5276	-2.1
701.5583	HMDB0240613	N-(9Z-hexadecenoyl)sphingosine-1-phosphocholine	C39H77N2O6P	M+H	701.5592	-1.3
	HMDB0240638	Sm(d18:2/16)	C39H77N2O6P	M+H	701.5592	-1.3
702.5066	HMDB0115120	PA(:3(5Z,8Z,11Z)/15)	C38H69O8P	M+NH4	702.5068	-0.3
	HMDB0114820	PA(15/:3(5Z,8Z,11Z))	C38H69O8P	M+NH4	702.5068	-0.3
	HMDB0115509	PA(15/:3(8Z,11Z,14Z))	C38H69O8P	M+NH4	702.5068	-0.3
	HMDB0115563	PA(:3(8Z,11Z,14Z)/15)	C38H69O8P	M+NH4	702.5068	-0.3
	HMDB0112979	PE-NMe(14/18:2(9Z,12Z))	C38H72NO8P	M+H	702.5068	-0.3
	HMDB0113138	PE-NMe(18:1(9Z)/14:1(9Z))	C38H72NO8P	M+H	702.5068	-0.3
	HMDB0113164	PE-NMe(18:2(9Z,12Z)/14)	C38H72NO8P	M+H	702.5068	-0.3
	HMDB0113111	PE-NMe(18:1(11Z)/14:1(9Z))	C38H72NO8P	M+H	702.5068	-0.3
	HMDB0009087	PE(18:2(9Z,12Z)/15)	C38H72NO8P	M+H	702.5068	-0.3

	HMDB0008895	PE(15/18:2(9Z,12Z))	C38H72NO8P	M+H	702.5068	-0.3
	HMDB0007999	PC(16:1(9Z)/14:1(9Z))	C38H72NO8P	M+H	702.5068	-0.3
	HMDB0112948	PE-NMe(16:1(9Z)/16:1(9Z))	C38H72NO8P	M+H	702.5068	-0.3
	HMDB0112947	PE-NMe(14:1(9Z)/18:1(11Z))	C38H72NO8P	M+H	702.5068	-0.3
	HMDB0112946	PE-NMe(14:1(9Z)/18:1(9Z))	C38H72NO8P	M+H	702.5068	-0.3
	HMDB0007903	PC(14:1(9Z)/16:1(9Z))	C38H72NO8P	M+H	702.5068	-0.3
702.5431	HMDB0008951	PE(16/P-18:1(11Z))	C39H76NO7P	M+H	702.5432	-0.2
	HMDB0011437	PE(P-18:1(9Z)/16)	C39H76NO7P	M+H	702.5432	-0.2
	HMDB0008952	PE(16/P-18:1(9Z))	C39H76NO7P	M+H	702.5432	-0.2
	HMDB0008983	PE(16:1(9Z)/P-18)	C39H76NO7P	M+H	702.5432	-0.2
	HMDB0009048	PE(18:1(11Z)/P-16)	C39H76NO7P	M+H	702.5432	-0.2
	HMDB0009081	PE(18:1(9Z)/P-16)	C39H76NO7P	M+H	702.5432	-0.2
	HMDB0011342	PE(P-16/18:1(9Z))	C39H76NO7P	M+H	702.5432	-0.2
	HMDB0011341	PEP-16/18:1(11Z))	C39H76NO7P	M+H	702.5432	-0.2
	HMDB0011372	PE(P-18/16:1(9Z))	C39H76NO7P	M+H	702.5432	-0.2
	HMDB0011404	PE(P-18:1(11Z)/16)	C39H76NO7P	M+H	702.5432	-0.2
703.5742	HMDB0013464	SM(d18/16:1(9Z))	C39H79N2O6P	M+H	703.5749	-0.9
	HMDB0010169	SM(d18:1/16)	C39H79N2O6P	M+H	703.5749	-0.9
	HMDB0061712	SM(d18:1/16)	C39H79N2O6P	M+H	703.5749	-0.9
704.5220	HMDB0115534	PA(:2(11Z,14Z)/15)	C38H71O8P	M+NH4	704.5225	-0.7
	HMDB0115508	PA(15/:2(11Z,14Z))	C38H71O8P	M+NH4	704.5225	-0.7
	HMDB0112951	PE-NMe(14/18:1(11Z))	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0113846	PE-NMe2(15/16:1(9Z))	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0112952	PE-NMe(14:1(9Z)/18)	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0113964	PE-NMe2(16:1(9Z)/15)	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0113137	PE-NMe(18:1(9Z)/14)	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0113110	PE-NMe(18:1(11Z)/14)	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0113064	PE-NMe(16:1(9Z)/16)	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0113085	PE-NMe(18/14:1(9Z))	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0007870	PC(14/16:1(9Z))	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0007902	PC(14:1(9Z)/16)	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0007966	PC(16/14:1(9Z))	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0007998	PC(16:1(9Z)/14)	C38H74NO8P	M+H	704.5225	-0.7

	HMDB0008893	PE(15/18:1(11Z))	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0008894	PE(15/18:1(9Z))	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0009021	PE(18:1(11Z)/15)	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0009054	PE(18:1(9Z)/15)	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0112949	PE-NMe(16/16:1(9Z))	C38H74NO8P	M+H	704.5225	-0.7
	HMDB0112950	PE-NMe(14/18:1(9Z))	C38H74NO8P	M+H	704.5225	-0.7
705.5905	HMDB0010168	SM(d18/16)	C39H81N2O6P	M+H	705.5905	0.0
	HMDB0062665	SM(d18/16)	C39H81N2O6P	M+H	705.5905	0.0
706.5378	HMDB0115093	PA(:1(11Z)/15)	C38H73O8P	M+NH4	706.5381	-0.5
	HMDB0010567	PE-NMe(16/16)	C38H76NO8P	M+H	706.5381	-0.5
	HMDB0008988	PE(18/15)	C38H76NO8P	M+H	706.5381	-0.5
	HMDB0008892	PE(15/18)	C38H76NO8P	M+H	706.5381	-0.5
	HMDB0007965	PC(16/14)	C38H76NO8P	M+H	706.5381	-0.5
	HMDB0007869	PC(14/16)	C38H76NO8P	M+H	706.5381	-0.5
	HMDB0113942	PE-NMe2(16/15)	C38H76NO8P	M+H	706.5381	-0.5
	HMDB0113084	PE-NMe(18/14)	C38H76NO8P	M+H	706.5381	-0.5
	HMDB0113865	PE-NMe2(15/16)	C38H76NO8P	M+H	706.5381	-0.5
	HMDB0112959	PE-NMe(14/18)	C38H76NO8P	M+H	706.5381	-0.5
	HMDB0007934	PC(15/15)	C38H76NO8P	M+H	706.5381	-0.5
707.5958	HMDB0183190	2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-yl (5Z,11Z,14Z)-8,9-dihydroxyicosa-5,11,14-trienoate	C47H78O4	M+H	707.5973	-2.1
	HMDB0186151	2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-yl (6Z,8E)-5-hydroxy-12-oxoicosa-6,8-dienoate	C47H78O4	M+H	707.5973	-2.1
709.5490	HMDB0113940	PE-NMe2(16/14)	C37H74NO8P	M+NH4	709.5490	0.0
	HMDB0113041	PE-NMe(16/15)	C37H74NO8P	M+NH4	709.5490	0.0
	HMDB0007868	PC(14/15)	C37H74NO8P	M+NH4	709.5490	0.0
	HMDB0007932	PC(15/14)	C37H74NO8P	M+NH4	709.5490	0.0
	HMDB0008826	PE(14/18)	C37H74NO8P	M+NH4	709.5490	0.0
	HMDB0008923	PE(16/16)	C37H74NO8P	M+NH4	709.5490	0.0
	HMDB0008986	PE(18/14)	C37H74NO8P	M+NH4	709.5490	0.0
	HMDB0029174	3-Sn-phosphatidylethanolamine	C37H74NO8P	M+NH4	709.5490	0.0
	HMDB0112964	PE-NMe(15/16)	C37H74NO8P	M+NH4	709.5490	0.0
	HMDB0113841	PE-NMe2(15/15)	C37H74NO8P	M+NH4	709.5490	0.0
	HMDB0113845	PE-NMe2(14/16)	C37H74NO8P	M+NH4	709.5490	0.0

714.5438	HMDB0011303	PC(P-18:1(9Z)/14:1(9Z))	C40H76NO7P	M+H	714.5432	0.8
	HMDB0011270	PC(P-18:1(11Z)/14:1(9Z))	C40H76NO7P	M+H	714.5432	0.8
	HMDB0007931	PC(14:1(9Z)/P-18:1(9Z))	C40H76NO7P	M+H	714.5432	0.8
	HMDB0007930	PC(14:1(9Z)/P-18:1(11Z))	C40H76NO7P	M+H	714.5432	0.8
714.6179	HMDB0006733	CE(22:6(4Z,7Z,Z,13Z,16Z,19Z))	C49H76O2	M+NH4	714.6184	-0.6
716.5222	HMDB0114978	PA(18:3(6Z,9Z,12Z)/18)	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0114805	PA(14:1(9Z)/22:2(13Z,16Z))	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0114840	PA(16/:3(5Z,8Z,11Z))	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0114878	PA(18/18:3(6Z,9Z,12Z))	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0114879	PA(18/18:3(9Z,12Z,15Z))	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0114902	PA(18:1(11Z)/18:2(9Z,12Z))	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0114927	PA(18:1(9Z)/18:2(9Z,12Z))	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0114953	PA(18:2(9Z,12Z)/18:1(9Z))	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0114952	PA(18:2(9Z,12Z)/18:1(11Z))	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0115005	PA(18:3(9Z,12Z,15Z)/18)	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0115536	PA(:2(11Z,14Z)/16:1(9Z))	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0115121	PA(:3(5Z,8Z,11Z)/16)	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0115297	PA(22:2(13Z,16Z)/14:1(9Z))	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0115512	PA(16:1(9Z)/:2(11Z,14Z))	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0115511	PA(16/:3(8Z,11Z,14Z))	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0115564	PA(:3(8Z,11Z,14Z)/16)	C39H71O8P	M+NH4	716.5225	-0.4
	HMDB0114039	PE-NMe2(18:1(9Z)/14:1(9Z))	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0114065	PE-NMe2(18:2(9Z,12Z)/14)	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0114012	PE-NMe2(18:1(11Z)/14:1(9Z))	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0113879	PE-NMe2(14/18:2(9Z,12Z))	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0113166	PE-NMe(18:2(9Z,12Z)/15)	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0113020	PE-NMe(15/18:2(9Z,12Z))	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0113849	PE-NMe2(16:1(9Z)/16:1(9Z))	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0009283	PE(:2(11Z,14Z)/14)	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0008867	PE(14:1(9Z)/:1(11Z))	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0008928	PE(16/18:2(9Z,12Z))	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0008959	PE(16:1(9Z)/18:1(11Z))	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0008960	PE(16:1(9Z)/18:1(9Z))	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0009023	PE(18:1(11Z)/16:1(9Z))	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0009056	PE(18:1(9Z)/16:1(9Z))	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0009088	PE(18:2(9Z,12Z)/16)	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0009251	PE(:1(11Z)/14:1(9Z))	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0113848	PE-NMe2(14:1(9Z)/18:1(11Z))	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0113847	PE-NMe2(14:1(9Z)/18:1(9Z))	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0008835	PE(14/:2(11Z,14Z))	C39H74NO8P	M+H	716.5225	-0.4
	HMDB0007897	PC(14/P-18:1(11Z))	C40H78NO7P	M+H	716.5589	-0.4

716.5586	HMDB0013411	PC(O-16:1(9Z)/16:1(9Z))	C40H78NO7P	M+H	716.5589	-0.4
	HMDB0007898	PC(14/P-18:1(9Z))	C40H78NO7P	M+H	716.5589	-0.4
	HMDB0007929	PC(14:1(9Z)/P-18)	C40H78NO7P	M+H	716.5589	-0.4
	HMDB0008027	PC(16:1(9Z)/P-16)	C40H78NO7P	M+H	716.5589	-0.4
	HMDB0011207	PC(P-16/16:1(9Z))	C40H78NO7P	M+H	716.5589	-0.4
	HMDB0011237	PC(P-18/14:1(9Z))	C40H78NO7P	M+H	716.5589	-0.4
	HMDB0011269	PC(P-18:1(11Z)/14)	C40H78NO7P	M+H	716.5589	-0.4
	HMDB0011302	PC(P-18:1(9Z)/14)	C40H78NO7P	M+H	716.5589	-0.4
716.6338	HMDB0010374	CE(22:5(4Z,7Z,Z,13Z,16Z))	C49H78O2	M+NH4	716.6340	-0.3
	HMDB0010375	LysoPC(15)	C49H78O2	M+NH4	716.6340	-0.3
	HMDB0062457	cholesteryl (7Z,Z,13Z,16Z,19Z)-docosapentaenoate	C49H78O2	M+NH4	716.6340	-0.3
717.5624	HMDB0032795	AS 1-2	C39H73NO9	M+NH4	717.5624	0.1
	HMDB0031983	Lucyobroside	C39H73NO9	M+NH4	717.5624	0.1
717.6365	HMDB0094108	DG(19/i-22)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094101	DG(19/22)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094203	DG(21)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094355	DG(21/)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094481	DG(22/19)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094107	DG(19/i-22)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0093705	DG(16/a-25)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0093703	DG(i-16/a-25)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094106	DG(i-19/i-22)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094104	DG(i-19/22)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0093879	DG(17/i-24)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0093875	DG(a-17/i-24)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0093877	DG(i-17/i-24)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094213	DG(/a-21)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094211	DG(/i-21)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094365	DG(21/i-)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094483	DG(i-22/19)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094485	DG(i-22/i-19)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094550	DG(i-24/17)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094552	DG(i-24/a-17)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094554	DG(i-24/i-17)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0093704	DG(16/a-25)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0093878	DG(17/i-24)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0093874	DG(a-17/i-24)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0093702	DG(i-16/a-25)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094363	DG(i-21/i-)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094357	DG(i-21/)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094209	DG(i-/i-21)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094487	DG(22/i-19)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094361	DG(a-21/)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094359	DG(a-21/i-)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094608	DG(a-25/16)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094606	DG(a-25/i-16)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094103	DG(i-19/22)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094105	DG(i-19/i-22)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094205	DG(i-/21)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094207	DG(i-/a-21)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0093876	DG(i-17/i-24)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094482	DG(22/19)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094488	DG(22/i-19)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094484	DG(i-22/19)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094486	DG(i-22/i-19)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094356	DG(21/)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094555	DG(i-24/i-17)	C44H86O5	M+Na	717.6367	-0.3

	HMDB0094607	DG(a-25/i-16)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094609	DG(a-25/16)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094553	DG(i-24/a-17)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094551	DG(i-24/17)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094360	DG(a-21/i-)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094366	DG(21/i-)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094214	DG(/a-21)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094210	DG(i-/i-21)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094206	DG(i-/21)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094102	DG(19/22)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094212	DG(i-/21)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094208	DG(i-/a-21)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094364	DG(i-21/i-)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094358	DG(i-21/)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094362	DG(a-21/)	C44H86O5	M+Na	717.6367	-0.3
	HMDB0094204	DG(/21)	C44H86O5	M+Na	717.6367	-0.3
718.5376	HMDB0115095	PA(:1(11Z)/16:1(9Z))	C39H73O8P	M+NH4	718.5381	-0.7
	HMDB0115535	PA(:2(11Z,14Z)/16)	C39H73O8P	M+NH4	718.5381	-0.7
	HMDB0115510	PA(16/:2(11Z,14Z))	C39H73O8P	M+NH4	718.5381	-0.7
	HMDB0115296	PA(22:2(13Z,16Z)/14)	C39H73O8P	M+NH4	718.5381	-0.7
	HMDB0115271	PA(22:1(13Z)/14:1(9Z))	C39H73O8P	M+NH4	718.5381	-0.7
	HMDB0114951	PA(18:2(9Z,12Z)/18)	C39H73O8P	M+NH4	718.5381	-0.7
	HMDB0114804	PA(14:1(9Z)/22:1(13Z))	C39H73O8P	M+NH4	718.5381	-0.7
	HMDB0116699	PA(14/22:2(13Z,16Z))	C39H73O8P	M+NH4	718.5381	-0.7
	HMDB0007864	PA(18:1(9Z)/18:1(11Z))	C39H73O8P	M+NH4	718.5381	-0.7
	HMDB0007863	PA(18:1(11Z)/18:1(9Z))	C39H73O8P	M+NH4	718.5381	-0.7
	HMDB0031129	9-Octadecenoic acid 1-[(phosphonoxy)methyl]-1,2-ethanediyl ester	C39H73O8P	M+NH4	718.5381	-0.7
	HMDB0007865	PA(18:1(9Z)/18:1(9Z))	C39H73O8P	M+NH4	718.5381	-0.7
	HMDB0007862	PA(18:1(11Z)/18:1(11Z))	C39H73O8P	M+NH4	718.5381	-0.7
	HMDB0007861	PA(18/18:2(9Z,12Z))	C39H73O8P	M+NH4	718.5381	-0.7
	HMDB0008834	PE(14/:1(11Z))	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0114038	PE-NMe2(18:1(9Z)/14)	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0114011	PE-NMe2(18:1(11Z)/14)	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0113986	PE-NMe2(18/14:1(9Z))	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0113112	PE-NMe(18:1(11Z)/15)	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0113139	PE-NMe(18:1(9Z)/15)	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0113965	PE-NMe2(16:1(9Z)/16)	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0009250	PE(:1(11Z)/14)	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0009218	PE(/14:1(9Z))	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0007936	PC(15/16:1(9Z))	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0008000	PC(16:1(9Z)/15)	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0008866	PE(14:1(9Z)/)	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0008926	PE(16/18:1(11Z))	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0008927	PE(16/18:1(9Z))	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0008958	PE(16:1(9Z)/18)	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0008990	PE(18/16:1(9Z))	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0009022	PE(18:1(11Z)/16)	C39H76NO8P	M+H	718.5381	-0.7

	HMDB0009055	PE(18:1(9Z)/16)	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0113851	PE-NMe2(14/18:1(9Z))	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0113852	PE-NMe2(14/18:1(11Z))	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0113853	PE-NMe2(14:1(9Z)/18)	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0113850	PE-NMe2(16/16:1(9Z))	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0112953	PE-NMe(15/18:1(9Z))	C39H76NO8P	M+H	718.5381	-0.7
	HMDB0112954	PE-NMe(15/18:1(11Z))	C39H76NO8P	M+H	718.5381	-0.7
718.5741	HMDB0007896	PC(14/P-18)	C40H80NO7P	M+H	718.5745	-0.6
	HMDB0013404	PC(O-16/16:1(9Z))	C40H80NO7P	M+H	718.5745	-0.6
	HMDB0007994	PC(16/P-16)	C40H80NO7P	M+H	718.5745	-0.6
	HMDB0011206	PC(P-16/16)	C40H80NO7P	M+H	718.5745	-0.6
	HMDB0011236	PC(P-18/14)	C40H80NO7P	M+H	718.5745	-0.6
718.6491	HMDB0006729	CE(22:4(7Z,Z,13Z,16Z))	C49H80O2	M+NH4	718.6497	-0.8
719.6528	HMDB0056120	DG(24/18:2n6)	C46H86O5	M+H	719.6548	-2.8
720.5549	HMDB0113985	PE-NMe2(18/14)	C39H78NO8P	M+H	720.5538	1.6
	HMDB0113086	PE-NMe(18/15)	C39H78NO8P	M+H	720.5538	1.6
	HMDB0113019	PE-NMe(15/18)	C39H78NO8P	M+H	720.5538	1.6
	HMDB0010566	PE-NMe2(16/16)	C39H78NO8P	M+H	720.5538	1.6
	HMDB0009217	PE(/14)	C39H78NO8P	M+H	720.5538	1.6
	HMDB0007935	PC(15/16)	C39H78NO8P	M+H	720.5538	1.6
	HMDB0007967	PC(16/15)	C39H78NO8P	M+H	720.5538	1.6
	HMDB0008833	PE(14/)	C39H78NO8P	M+H	720.5538	1.6
	HMDB0008925	PE(16/18)	C39H78NO8P	M+H	720.5538	1.6
	HMDB0008989	PE(18/16)	C39H78NO8P	M+H	720.5538	1.6
	HMDB0113860	PE-NMe2(14/18)	C39H78NO8P	M+H	720.5538	1.6
	HMDB0115270	PA(22:1(13Z)/14)	C39H75O8P	M+NH4	720.5538	1.6
	HMDB0114789	PA(14/22:1(13Z))	C39H75O8P	M+NH4	720.5538	1.6
	HMDB0114901	PA(18:1(11Z)/18)	C39H75O8P	M+NH4	720.5538	1.6
	HMDB0114926	PA(18:1(9Z)/18)	C39H75O8P	M+NH4	720.5538	1.6
	HMDB0115065	PA(/16:1(9Z))	C39H75O8P	M+NH4	720.5538	1.6
	HMDB0115094	PA(:1(11Z)/16)	C39H75O8P	M+NH4	720.5538	1.6
	HMDB0115241	PA(22/14:1(9Z))	C39H75O8P	M+NH4	720.5538	1.6
	HMDB0008985	PE(16:1(9Z)/P-18:1(9Z))	C39H74NO7P	M+Na	722.5095	2.9
	HMDB0009114	PE(18:2(9Z,12Z)/P-16)	C39H74NO7P	M+Na	722.5095	2.9
	HMDB0011343	PE(P-16/18:2(9Z,12Z))	C39H74NO7P	M+Na	722.5095	2.9
	HMDB0011405	PE(P-18:1(11Z)/16:1(9Z))	C39H74NO7P	M+Na	722.5095	2.9
	HMDB0011438	PE(P-18:1(9Z)/16:1(9Z))	C39H74NO7P	M+Na	722.5095	2.9

722.5116	HMDB0008984	PE(16:1(9Z)/P-18:1(11Z))	C39H74NO7P	M+Na	722.5095	2.9
	HMDB0011445	PE(P-18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO7P	M+H	722.5119	-0.4
	HMDB0011412	PE(P-18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO7P	M+H	722.5119	-0.4
	HMDB0011354	PE(P-16/:5(5Z,8Z,11Z,14Z,17Z))	C41H72NO7P	M+H	722.5119	-0.4
	HMDB0009477	PE(:5(5Z,8Z,11Z,14Z,17Z)/P-16)	C41H72NO7P	M+H	722.5119	-0.4
	HMDB0009216	PE(18:4(6Z,9Z,12Z,15Z)/P-18:1(9Z))	C41H72NO7P	M+H	722.5119	-0.4
	HMDB0009215	PE(18:4(6Z,9Z,12Z,15Z)/P-18:1(11Z))	C41H72NO7P	M+H	722.5119	-0.4
724.5271	HMDB0011437	PE(P-18:1(9Z)/16)	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0011404	PE(P-18:1(11Z)/16)	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0011372	PE(P-18/16:1(9Z))	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0011341	PEP-16/18:1(11Z))	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0011342	PE(P-16/18:1(9Z))	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0009081	PE(18:1(9Z)/P-16)	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0009048	PE(18:1(11Z)/P-16)	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0008983	PE(16:1(9Z)/P-18)	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0008951	PE(16/P-18:1(11Z))	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0008952	PE(16/P-18:1(9Z))	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0011437	PE(P-18:1(9Z)/16)	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0011404	PE(P-18:1(11Z)/16)	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0011372	PE(P-18/16:1(9Z))	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0011341	PEP-16/18:1(11Z))	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0011342	PE(P-16/18:1(9Z))	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0009081	PE(18:1(9Z)/P-16)	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0009048	PE(18:1(11Z)/P-16)	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0008983	PE(16:1(9Z)/P-18)	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0008951	PE(16/P-18:1(11Z))	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0008952	PE(16/P-18:1(9Z))	C39H76NO7P	M+Na	724.5252	2.7
	HMDB0011411	PE(P-18:1(11Z)/18:3(9Z,12Z,15Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0011443	PE(P-18:1(9Z)/18:3(6Z,9Z,12Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0011444	PE(P-18:1(9Z)/18:3(9Z,12Z,15Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0011410	PE(P-18:1(11Z)/18:3(6Z,9Z,12Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0011379	PE(P-18/18:4(6Z,9Z,12Z,15Z))	C41H74NO7P	M+H	724.5276	-0.6

	HMDB0009149	PE(18:3(6Z,9Z,12Z)/P-18:1(11Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0009150	PE(18:3(6Z,9Z,12Z)/P-18:1(9Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0009182	PE(18:3(9Z,12Z,15Z)/P-18:1(11Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0009183	PE(18:3(9Z,12Z,15Z)/P-18:1(9Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0009411	PE(:4(5Z,8Z,11Z,14Z)/P-16)	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0009444	PE(:4(8Z,11Z,14Z,17Z)/P-16)	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0009214	PE(18:4(6Z,9Z,12Z,15Z)/P-18)	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0011352	PE(P-16/:4(5Z,8Z,11Z,14Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0011353	PE(P-16/:4(8Z,11Z,14Z,17Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0011411	PE(P-18:1(11Z)/18:3(9Z,12Z,15Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0011443	PE(P-18:1(9Z)/18:3(6Z,9Z,12Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0011444	PE(P-18:1(9Z)/18:3(9Z,12Z,15Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0011410	PE(P-18:1(11Z)/18:3(6Z,9Z,12Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0011379	PE(P-18/18:4(6Z,9Z,12Z,15Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0009149	PE(18:3(6Z,9Z,12Z)/P-18:1(11Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0009150	PE(18:3(6Z,9Z,12Z)/P-18:1(9Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0009182	PE(18:3(9Z,12Z,15Z)/P-18:1(11Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0009183	PE(18:3(9Z,12Z,15Z)/P-18:1(9Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0009411	PE(:4(5Z,8Z,11Z,14Z)/P-16)	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0009444	PE(:4(8Z,11Z,14Z,17Z)/P-16)	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0009214	PE(18:4(6Z,9Z,12Z,15Z)/P-18)	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0011352	PE(P-16/:4(5Z,8Z,11Z,14Z))	C41H74NO7P	M+H	724.5276	-0.6
	HMDB0011353	PE(P-16/:4(8Z,11Z,14Z,17Z))	C41H74NO7P	M+H	724.5276	-0.6
726.5398	HMDB0007961	PC(15/P-16)	C39H78NO7P	M+Na	726.5408	-1.4
	HMDB0011371	PE(P-18/16)	C39H78NO7P	M+Na	726.5408	-1.4
	HMDB0011340	PE(P-16/18)	C39H78NO7P	M+Na	726.5408	-1.4
	HMDB0011205	PC(P-16/15)	C39H78NO7P	M+Na	726.5408	-1.4
	HMDB0011157	PE(O-16/18:1(9Z))	C39H78NO7P	M+Na	726.5408	-1.4
	HMDB0009015	PE(18/P-16)	C39H78NO7P	M+Na	726.5408	-1.4
	HMDB0008950	PE(16/P-18)	C39H78NO7P	M+Na	726.5408	-1.4
	HMDB0007961	PC(15/P-16)	C39H78NO7P	M+Na	726.5408	-1.4
	HMDB0011371	PE(P-18/16)	C39H78NO7P	M+Na	726.5408	-1.4

HMDB0011340	PE(P-16/18)	C39H78NO7P	M+Na	726.5408	-1.4
HMDB0011205	PC(P-16/15)	C39H78NO7P	M+Na	726.5408	-1.4
HMDB0011157	PE(O-16/18:1(9Z))	C39H78NO7P	M+Na	726.5408	-1.4
HMDB0009015	PE(18/P-16)	C39H78NO7P	M+Na	726.5408	-1.4
HMDB0008950	PE(16/P-18)	C39H78NO7P	M+Na	726.5408	-1.4
HMDB0007965	PC(16/14)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0007934	PC(15/15)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0008988	PE(18/15)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0007869	PC(14/16)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0010567	PE-NMe(16/16)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0112959	PE-NMe(14/18)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0113865	PE-NMe2(15/16)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0113084	PE-NMe(18/14)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0113942	PE-NMe2(16/15)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0008892	PE(15/18)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0007965	PC(16/14)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0007934	PC(15/15)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0008988	PE(18/15)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0007869	PC(14/16)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0010567	PE-NMe(16/16)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0112959	PE-NMe(14/18)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0113865	PE-NMe2(15/16)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0113084	PE-NMe(18/14)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0113942	PE-NMe2(16/15)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0008892	PE(15/18)	C38H76NO8P	M+Na	728.5201	2.4
HMDB0115325	PA(22:4(7Z,Z,13Z,16Z)/15)	C40H71O8P	M+NH4	728.5225	-0.9
HMDB0114827	PA(15/22:4(7Z,Z,13Z,16Z))	C40H71O8P	M+NH4	728.5225	-0.9
HMDB0113394	PE-NMe(:3(8Z,11Z,14Z)/14)	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113366	PE-NMe(:3(5Z,8Z,11Z)/14)	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113196	PE-NMe(18:3(6Z,9Z,12Z)/16)	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113168	PE-NMe(18:2(9Z,12Z)/16:1(9Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113065	PE-NMe(16:1(9Z)/18:2(9Z,12Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113224	PE-NMe(18:3(9Z,12Z,15Z)/16)	C40H74NO8P	M+H	728.5225	-0.9

728.5218

HMDB0113043	PE-NMe(16/18:3(6Z,9Z,12Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113044	PE-NMe(16/18:3(9Z,12Z,15Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0112986	PE-NMe(14/3(8Z,11Z,14Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0112985	PE-NMe(14/3(5Z,8Z,11Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113922	PE-NMe2(15/18:3(9Z,12Z,15Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113921	PE-NMe2(15/18:3(6Z,9Z,12Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0114096	PE-NMe2(18:3(6Z,9Z,12Z)/15)	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113338	PE-NMe(:2(11Z,14Z)/14:1(9Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113004	PE-NMe(14:1(9Z)/:2(11Z,14Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0114125	PE-NMe2(18:3(9Z,12Z,15Z)/15)	C40H74NO8P	M+H	728.5225	-0.9
HMDB0008196	PC(18:3(9Z,12Z,15Z)/14)	C40H74NO8P	M+H	728.5225	-0.9
HMDB0009351	PE(:3(8Z,11Z,14Z)/15)	C40H74NO8P	M+H	728.5225	-0.9
HMDB0009318	PE(:3(5Z,8Z,11Z)/15)	C40H74NO8P	M+H	728.5225	-0.9
HMDB0007876	PC(14/18:3(9Z,12Z,15Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0007907	PC(14:1(9Z)/18:2(9Z,12Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0008163	PC(18:3(6Z,9Z,12Z)/14)	C40H74NO8P	M+H	728.5225	-0.9
HMDB0007875	PC(14/18:3(6Z,9Z,12Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0008902	PE(15/:3(5Z,8Z,11Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0008903	PE(15/:3(8Z,11Z,14Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0008131	PC(18:2(9Z,12Z)/14:1(9Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0115325	PA(22:4(7Z,Z,13Z,16Z)/15)	C40H71O8P	M+NH4	728.5225	-0.9
HMDB0114827	PA(15/22:4(7Z,Z,13Z,16Z))	C40H71O8P	M+NH4	728.5225	-0.9
HMDB0113394	PE-NMe(:3(8Z,11Z,14Z)/14)	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113366	PE-NMe(:3(5Z,8Z,11Z)/14)	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113196	PE-NMe(18:3(6Z,9Z,12Z)/16)	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113168	PE-NMe(18:2(9Z,12Z)/16:1(9Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113065	PE-NMe(16:1(9Z)/18:2(9Z,12Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113224	PE-NMe(18:3(9Z,12Z,15Z)/16)	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113043	PE-NMe(16/18:3(6Z,9Z,12Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113044	PE-NMe(16/18:3(9Z,12Z,15Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0112986	PE-NMe(14/3(8Z,11Z,14Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0112985	PE-NMe(14/3(5Z,8Z,11Z))	C40H74NO8P	M+H	728.5225	-0.9
HMDB0113922	PE-NMe2(15/18:3(9Z,12Z,15Z))	C40H74NO8P	M+H	728.5225	-0.9

	HMDB0113921	PE-NMe2(15/18:3(6Z,9Z,12Z))	C40H74NO8P	M+H	728.5225	-0.9
	HMDB0114096	PE-NMe2(18:3(6Z,9Z,12Z)/15)	C40H74NO8P	M+H	728.5225	-0.9
	HMDB0113338	PE-NMe(:2(11Z,14Z)/14:1(9Z))	C40H74NO8P	M+H	728.5225	-0.9
	HMDB0113004	PE-NMe(14:1(9Z):2(11Z,14Z))	C40H74NO8P	M+H	728.5225	-0.9
	HMDB0114125	PE-NMe2(18:3(9Z,12Z,15Z)/15)	C40H74NO8P	M+H	728.5225	-0.9
	HMDB0008196	PC(18:3(9Z,12Z,15Z)/14)	C40H74NO8P	M+H	728.5225	-0.9
	HMDB0009351	PE(:3(8Z,11Z,14Z)/15)	C40H74NO8P	M+H	728.5225	-0.9
	HMDB0009318	PE(:3(5Z,8Z,11Z)/15)	C40H74NO8P	M+H	728.5225	-0.9
	HMDB0007876	PC(14/18:3(9Z,12Z,15Z))	C40H74NO8P	M+H	728.5225	-0.9
	HMDB0007907	PC(14:1(9Z)/18:2(9Z,12Z))	C40H74NO8P	M+H	728.5225	-0.9
	HMDB0008163	PC(18:3(6Z,9Z,12Z)/14)	C40H74NO8P	M+H	728.5225	-0.9
	HMDB0007875	PC(14/18:3(6Z,9Z,12Z))	C40H74NO8P	M+H	728.5225	-0.9
	HMDB0008902	PE(15/:3(5Z,8Z,11Z))	C40H74NO8P	M+H	728.5225	-0.9
	HMDB0008903	PE(15/:3(8Z,11Z,14Z))	C40H74NO8P	M+H	728.5225	-0.9
	HMDB0008131	PC(18:2(9Z,12Z)/14:1(9Z))	C40H74NO8P	M+H	728.5225	-0.9
728.5585	HMDB0009050	PE(18:1(11Z)/P-18:1(11Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0009051	PE(18:1(11Z)/P-18:1(9Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0009083	PE(18:1(9Z)/P-18:1(11Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0009084	PE(18:1(9Z)/P-18:1(9Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0009115	PE(18:2(9Z,12Z)/P-18)	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0009312	PE(:2(11Z,14Z)/P-16)	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0011349	PE(P-16/:2(11Z,14Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0011376	PE(P-18/18:2(9Z,12Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0011408	PE(P-18:1(11Z)/18:1(9Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0011407	PE(P-18:1(11Z)/18:1(11Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0011440	PE(P-18:1(9Z)/18:1(11Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0011441	PE(P-18:1(9Z)/18:1(9Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0009050	PE(18:1(11Z)/P-18:1(11Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0009051	PE(18:1(11Z)/P-18:1(9Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0009083	PE(18:1(9Z)/P-18:1(11Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0009084	PE(18:1(9Z)/P-18:1(9Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0009115	PE(18:2(9Z,12Z)/P-18)	C41H78NO7P	M+H	728.5589	-0.5

	HMDB0009312	PE(:2(11Z,14Z)/P-16)	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0011349	PE(P-16/:2(11Z,14Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0011376	PE(P-18/18:2(9Z,12Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0011408	PE(P-18:1(11Z)/18:1(9Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0011407	PE(P-18:1(11Z)/18:1(11Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0011440	PE(P-18:1(9Z)/18:1(11Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0011441	PE(P-18:1(9Z)/18:1(9Z))	C41H78NO7P	M+H	728.5589	-0.5
	HMDB0061332	1-alkyl-2-acylglycerol 3 phosphate(18/:4)	C41H75O7P	M+NH4	728.5589	-0.5
	HMDB0061332	1-alkyl-2-acylglycerol 3 phosphate(18/:4)	C41H75O7P	M+NH4	728.5589	-0.5
	HMDB0116370	(2S)-1- {[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+H	729.5664	-1.9
729.5650	HMDB0116432	(2S)-1- {[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116426	(2S)-1- {[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116421	(2S)-3-hydroxy-2- {[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116416	(2S)-3-hydroxy-2- {[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116411	(2S)-2- {[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116399	(2S)-1-hydroxy-3- {[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propan-2-yl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116392	(2S)-1-hydroxy-3- {[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116385	(2S)-2- {[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropyl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116378	(2S)-1- {[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116445	(2S)-1-hydroxy-3- {[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116370	(2S)-1- {[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116432	(2S)-1- {[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116426	(2S)-1- {[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116421	(2S)-3-hydroxy-2- {[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116416	(2S)-3-hydroxy-2- {[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+H	729.5664	-1.9

	HMDB0116411	(2S)-2-([9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy)-3-hydroxypropyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116399	(2S)-1-hydroxy-3-([11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propan-2-yl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116392	(2S)-1-hydroxy-3-([11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy)propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116385	(2S)-2-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-3-hydroxypropyl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116378	(2S)-1-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate	C45H76O7	M+H	729.5664	-1.9
	HMDB0116445	(2S)-1-hydroxy-3-([9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy)propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+H	729.5664	-1.9
730.5376	HMDB0112957	PE-NMe(16:1(9Z)/18:1(11Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0113337	PE-NMe(:2(11Z,14Z)/14)	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0112984	PE-NMe(14:2(11Z,14Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0114067	PE-NMe2(18:2(9Z,12Z)/15)	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0113920	PE-NMe2(15/18:2(9Z,12Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0113309	PE-NMe(:1(11Z)/14:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0113167	PE-NMe(18:2(9Z,12Z)/16)	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0113141	PE-NMe(18:1(9Z)/16:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0113114	PE-NMe(18:1(11Z)/16:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0113042	PE-NMe(16/18:2(9Z,12Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0112956	PE-NMe(16:1(9Z)/18:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0112955	PE-NMe(14:1(9Z)/:1(11Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0009285	PE(:2(11Z,14Z)/15)	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0008901	PE(15/:2(11Z,14Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0008130	PC(18:2(9Z,12Z)/14)	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0008098	PC(18:1(9Z)/14:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0008065	PC(18:1(11Z)/14:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0008002	PC(16:1(9Z)/16:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0007906	PC(14:1(9Z)/18:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0007905	PC(14:1(9Z)/18:1(11Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0007874	PC(14/18:2(9Z,12Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0112957	PE-NMe(16:1(9Z)/18:1(11Z))	C40H76NO8P	M+H	730.5381	-0.7
	HMDB0113337	PE-NMe(:2(11Z,14Z)/14)	C40H76NO8P	M+H	730.5381	-0.7

HMDB0112984	PE-NMe(14:2(11Z,14Z))	C40H76NO8P	M+H	730.5381	-0.7
HMDB0114067	PE-NMe2(18:2(9Z,12Z)/15)	C40H76NO8P	M+H	730.5381	-0.7
HMDB0113920	PE-NMe2(15/18:2(9Z,12Z))	C40H76NO8P	M+H	730.5381	-0.7
HMDB0113309	PE-NMe(:1(11Z)/14:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
HMDB0113167	PE-NMe(18:2(9Z,12Z)/16)	C40H76NO8P	M+H	730.5381	-0.7
HMDB0113141	PE-NMe(18:1(9Z)/16:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
HMDB0113114	PE-NMe(18:1(11Z)/16:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
HMDB0113042	PE-NMe(16/18:2(9Z,12Z))	C40H76NO8P	M+H	730.5381	-0.7
HMDB0112956	PE-NMe(16:1(9Z)/18:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
HMDB0112955	PE-NMe(14:1(9Z)/:1(11Z))	C40H76NO8P	M+H	730.5381	-0.7
HMDB0009285	PE(:2(11Z,14Z)/15)	C40H76NO8P	M+H	730.5381	-0.7
HMDB0008901	PE(15/:2(11Z,14Z))	C40H76NO8P	M+H	730.5381	-0.7
HMDB0008130	PC(18:2(9Z,12Z)/14)	C40H76NO8P	M+H	730.5381	-0.7
HMDB0008098	PC(18:1(9Z)/14:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
HMDB0008065	PC(18:1(11Z)/14:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
HMDB0008002	PC(16:1(9Z)/16:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
HMDB0007906	PC(14:1(9Z)/18:1(9Z))	C40H76NO8P	M+H	730.5381	-0.7
HMDB0007905	PC(14:1(9Z)/18:1(11Z))	C40H76NO8P	M+H	730.5381	-0.7
HMDB0007874	PC(14/18:2(9Z,12Z))	C40H76NO8P	M+H	730.5381	-0.7
HMDB0114826	PA(15/22:2(13Z,16Z))	C40H75O8P	M+NH4	732.5538	-0.8
HMDB0115298	PA(22:2(13Z,16Z)/15)	C40H75O8P	M+NH4	732.5538	-0.8
HMDB0113855	PE-NMe2(15/18:1(11Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0113854	PE-NMe2(15/18:1(9Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0112962	PE-NMe(16:1(9Z)/18)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0112958	PE-NMe(14/:1(11Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0112960	PE-NMe(14:1(9Z)/)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0112961	PE-NMe(16/18:1(11Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0114013	PE-NMe2(18:1(11Z)/15)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0114040	PE-NMe2(18:1(9Z)/15)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0113308	PE-NMe(:1(11Z)/14)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0113280	PE-NMe(/14:1(9Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0113140	PE-NMe(18:1(9Z)/16)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0113088	PE-NMe(18/16:1(9Z))	C40H78NO8P	M+H	732.5538	-0.8

732.5532

HMDB0113113	PE-NMe(18:1(11Z)/16)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0007873	PC(14/18:1(9Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0010569	PE-NMe(16/18:1(9Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0007872	PC(14/18:1(11Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0007904	PC(14:1(9Z)/18)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0007969	PC(16/16:1(9Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0008001	PC(16:1(9Z)/16)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0008032	PC(18/14:1(9Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0008064	PC(18:1(11Z)/14)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0008097	PC(18:1(9Z)/14)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0008900	PE(15:1(11Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0009252	PE(:1(11Z)/15)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0114826	PA(15/22:2(13Z,16Z))	C40H75O8P	M+NH4	732.5538	-0.8
HMDB0115298	PA(22:2(13Z,16Z)/15)	C40H75O8P	M+NH4	732.5538	-0.8
HMDB0113855	PE-NMe2(15/18:1(11Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0113854	PE-NMe2(15/18:1(9Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0112962	PE-NMe(16:1(9Z)/18)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0112958	PE-NMe(14:1(11Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0112960	PE-NMe(14:1(9Z)/)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0112961	PE-NMe(16/18:1(11Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0114013	PE-NMe2(18:1(11Z)/15)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0114040	PE-NMe2(18:1(9Z)/15)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0113308	PE-NMe(:1(11Z)/14)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0113280	PE-NMe(/14:1(9Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0113140	PE-NMe(18:1(9Z)/16)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0113088	PE-NMe(18/16:1(9Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0113113	PE-NMe(18:1(11Z)/16)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0007873	PC(14/18:1(9Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0010569	PE-NMe(16/18:1(9Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0007872	PC(14/18:1(11Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0007904	PC(14:1(9Z)/18)	C40H78NO8P	M+H	732.5538	-0.8
HMDB0007969	PC(16/16:1(9Z))	C40H78NO8P	M+H	732.5538	-0.8
HMDB0008001	PC(16:1(9Z)/16)	C40H78NO8P	M+H	732.5538	-0.8

	HMDB0008032	PC(18/14:1(9Z))	C40H78NO8P	M+H	732.5538	-0.8
	HMDB0008064	PC(18:1(11Z)/14)	C40H78NO8P	M+H	732.5538	-0.8
	HMDB0008097	PC(18:1(9Z)/14)	C40H78NO8P	M+H	732.5538	-0.8
	HMDB0008900	PE(15/:1(11Z))	C40H78NO8P	M+H	732.5538	-0.8
	HMDB0009252	PE(:1(11Z)/15)	C40H78NO8P	M+H	732.5538	-0.8
734.5691	HMDB0114825	PA(15/22:1(13Z))	C40H77O8P	M+NH4	734.5694	-0.4
	HMDB0115272	PA(22:1(13Z)/15)	C40H77O8P	M+NH4	734.5694	-0.4
	HMDB0000564	PC(16/16)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0007871	PC(14/18)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0008031	PC(18/14)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0008899	PE(15/)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0009219	PE(/15)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0112965	PE-NMe(16/18)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0112983	PE-NMe(14/)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0113279	PE-NMe(/14)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0113919	PE-NMe2(15/18)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0113987	PE-NMe2(18/15)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0113087	PE-NMe(18/16)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0114825	PA(15/22:1(13Z))	C40H77O8P	M+NH4	734.5694	-0.4
	HMDB0115272	PA(22:1(13Z)/15)	C40H77O8P	M+NH4	734.5694	-0.4
	HMDB0000564	PC(16/16)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0007871	PC(14/18)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0008031	PC(18/14)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0008899	PE(15/)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0009219	PE(/15)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0112965	PE-NMe(16/18)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0112983	PE-NMe(14/)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0113279	PE-NMe(/14)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0113919	PE-NMe2(15/18)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0113987	PE-NMe2(18/15)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0113087	PE-NMe(18/16)	C40H80NO8P	M+H	734.5694	-0.5
	HMDB0007935	PC(15/16)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0113985	PE-NMe2(18/14)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0113086	PE-NMe(18/15)	C39H78NO8P	M+NH4	737.5803	-2.9

737.5782	HMDB0007967	PC(16/15)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0008833	PE(14/)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0008925	PE(16/18)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0008989	PE(18/16)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0009217	PE(/14)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0010566	PE-NMe2(16/16)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0113860	PE-NMe2(14/18)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0113019	PE-NMe(15/18)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0007935	PC(15/16)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0113985	PE-NMe2(18/14)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0113086	PE-NMe(18/15)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0007967	PC(16/15)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0008833	PE(14/)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0008925	PE(16/18)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0008989	PE(18/16)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0009217	PE(/14)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0010566	PE-NMe2(16/16)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0113860	PE-NMe2(14/18)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0113019	PE-NMe(15/18)	C39H78NO8P	M+NH4	737.5803	-2.9
	HMDB0114039	PE-NMe2(18:1(9Z)/14:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
	HMDB0113879	PE-NMe2(14/18:2(9Z,12Z))	C39H74NO8P	M+Na	738.5044	2.3
	HMDB0114012	PE-NMe2(18:1(11Z)/14:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
	HMDB0113166	PE-NMe(18:2(9Z,12Z)/15)	C39H74NO8P	M+Na	738.5044	2.3
	HMDB0113020	PE-NMe(15/18:2(9Z,12Z))	C39H74NO8P	M+Na	738.5044	2.3
	HMDB0114065	PE-NMe2(18:2(9Z,12Z)/14)	C39H74NO8P	M+Na	738.5044	2.3
	HMDB0009283	PE(:2(11Z,14Z)/14)	C39H74NO8P	M+Na	738.5044	2.3
	HMDB0008867	PE(14:1(9Z)/:1(11Z))	C39H74NO8P	M+Na	738.5044	2.3
	HMDB0008959	PE(16:1(9Z)/18:1(11Z))	C39H74NO8P	M+Na	738.5044	2.3
	HMDB0008960	PE(16:1(9Z)/18:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
	HMDB0009251	PE(:1(11Z)/14:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
	HMDB0009056	PE(18:1(9Z)/16:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
	HMDB0009088	PE(18:2(9Z,12Z)/16)	C39H74NO8P	M+Na	738.5044	2.3

HMDB0009023	PE(18:1(11Z)/16:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0008928	PE(16/18:2(9Z,12Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0008835	PE(14/:2(11Z,14Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0113849	PE-NMe2(16:1(9Z)/16:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0113848	PE-NMe2(14:1(9Z)/18:1(11Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0113847	PE-NMe2(14:1(9Z)/18:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0114039	PE-NMe2(18:1(9Z)/14:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0113879	PE-NMe2(14/18:2(9Z,12Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0114012	PE-NMe2(18:1(11Z)/14:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0113166	PE-NMe(18:2(9Z,12Z)/15)	C39H74NO8P	M+Na	738.5044	2.3
HMDB0113020	PE-NMe(15/18:2(9Z,12Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0114065	PE-NMe2(18:2(9Z,12Z)/14)	C39H74NO8P	M+Na	738.5044	2.3
HMDB0009283	PE(:2(11Z,14Z)/14)	C39H74NO8P	M+Na	738.5044	2.3
HMDB0008867	PE(14:1(9Z)/:1(11Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0008959	PE(16:1(9Z)/18:1(11Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0008960	PE(16:1(9Z)/18:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0009251	PE(:1(11Z)/14:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0009056	PE(18:1(9Z)/16:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0009088	PE(18:2(9Z,12Z)/16)	C39H74NO8P	M+Na	738.5044	2.3
HMDB0009023	PE(18:1(11Z)/16:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0008928	PE(16/18:2(9Z,12Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0008835	PE(14/:2(11Z,14Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0113849	PE-NMe2(16:1(9Z)/16:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0113848	PE-NMe2(14:1(9Z)/18:1(11Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0113847	PE-NMe2(14:1(9Z)/18:1(9Z))	C39H74NO8P	M+Na	738.5044	2.3
HMDB0114987	PA(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115152	PA(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115127	PA(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115014	PA(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114962	PA(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114961	PA(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114936	PA(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114911	PA(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114868	PA(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114869	PA(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114849	PA(16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115179	PA(:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115203	PA(:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115128	PA(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115570	PA(:3(8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C41H69O8P	M+NH4	738.5068	-1.0

738.5061

HMDB0115569	PA(:3(8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115542	PA(:2(11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115525	PA(18:3(9Z,12Z,15Z)/:3(8Z,11Z,14Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115526	PA(18:4(6Z,9Z,12Z,15Z)/:2(11Z,14Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115523	PA(18:3(6Z,9Z,12Z)/:3(8Z,11Z,14Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115404	PA(22:6(4Z,7Z,Z,13Z,16Z,19Z)/16)	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115379	PA(22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115353	PA(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115204	PA(:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114381	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/14)	C41H72NO8P	M+H	738.5068	-1.0
HMDB0114353	PE-NMe2(:4(8Z,11Z,14Z,17Z)/14:1(9Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0114325	PE-NMe2(:4(5Z,8Z,11Z,14Z)/14:1(9Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0114156	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/16:1(9Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0113969	PE-NMe2(16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0113907	PE-NMe2(14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0113908	PE-NMe2(14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0113889	PE-NMe2(14/:5(5Z,8Z,11Z,14Z,17Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0113481	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/15)	C41H72NO8P	M+H	738.5068	-1.0
HMDB0113030	PE-NMe(15/:5(5Z,8Z,11Z,14Z,17Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009386	PE(:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009451	PE(:5(5Z,8Z,11Z,14Z,17Z)/16)	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009581	PE(22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009613	PE(22:5(4Z,7Z,Z,13Z,16Z)/14)	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009646	PE(22:5(7Z,Z,13Z,16Z,19Z)/14)	C41H72NO8P	M+H	738.5068	-1.0
HMDB0008939	PE(16/:5(5Z,8Z,11Z,14Z,17Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009419	PE(:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0008970	PE(16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0008971	PE(16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009190	PE(18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009191	PE(18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009159	PE(18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009126	PE(18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009095	PE(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009094	PE(18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009063	PE(18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009030	PE(18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0008845	PE(14/22:5(4Z,7Z,Z,13Z,16Z))	C41H72NO8P	M+H	738.5068	-1.0

HMDB0008877	PE(14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0008846	PE(14/22:5(7Z,Z,13Z,16Z,19Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0114987	PA(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115152	PA(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115127	PA(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115014	PA(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114962	PA(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114961	PA(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114936	PA(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114911	PA(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114868	PA(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114869	PA(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114849	PA(16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115179	PA(:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115203	PA(:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115128	PA(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115570	PA(:3(8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115569	PA(:3(8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115542	PA(:2(11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115525	PA(18:3(9Z,12Z,15Z)/:3(8Z,11Z,14Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115526	PA(18:4(6Z,9Z,12Z,15Z)/:2(11Z,14Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115523	PA(18:3(6Z,9Z,12Z)/:3(8Z,11Z,14Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115404	PA(22:6(4Z,7Z,Z,13Z,16Z,19Z)/16)	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115379	PA(22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115353	PA(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0115204	PA(:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C41H69O8P	M+NH4	738.5068	-1.0
HMDB0114381	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/14)	C41H72NO8P	M+H	738.5068	-1.0
HMDB0114353	PE-NMe2(:4(8Z,11Z,14Z,17Z)/14:1(9Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0114325	PE-NMe2(:4(5Z,8Z,11Z,14Z)/14:1(9Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0114156	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/16:1(9Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0113969	PE-NMe2(16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0113907	PE-NMe2(14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0113908	PE-NMe2(14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0113889	PE-NMe2(14/:5(5Z,8Z,11Z,14Z,17Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0113481	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/15)	C41H72NO8P	M+H	738.5068	-1.0
HMDB0113030	PE-NMe(15/:5(5Z,8Z,11Z,14Z,17Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009386	PE(:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009451	PE(:5(5Z,8Z,11Z,14Z,17Z)/16)	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009581	PE(22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009613	PE(22:5(4Z,7Z,Z,13Z,16Z)/14)	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009646	PE(22:5(7Z,Z,13Z,16Z,19Z)/14)	C41H72NO8P	M+H	738.5068	-1.0
HMDB0008939	PE(16/:5(5Z,8Z,11Z,14Z,17Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0009419	PE(:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C41H72NO8P	M+H	738.5068	-1.0
HMDB0008970	PE(16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C41H72NO8P	M+H	738.5068	-1.0

	HMDB0008971	PE(16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C41H72NO8P	M+H	738.5068	-1.0
	HMDB0009190	PE(18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C41H72NO8P	M+H	738.5068	-1.0
	HMDB0009191	PE(18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C41H72NO8P	M+H	738.5068	-1.0
	HMDB0009159	PE(18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C41H72NO8P	M+H	738.5068	-1.0
	HMDB0009126	PE(18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C41H72NO8P	M+H	738.5068	-1.0
	HMDB0009095	PE(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C41H72NO8P	M+H	738.5068	-1.0
	HMDB0009094	PE(18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C41H72NO8P	M+H	738.5068	-1.0
	HMDB0009063	PE(18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO8P	M+H	738.5068	-1.0
	HMDB0009030	PE(18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO8P	M+H	738.5068	-1.0
	HMDB0008845	PE(14/22:5(4Z,7Z,Z,13Z,16Z))	C41H72NO8P	M+H	738.5068	-1.0
	HMDB0008877	PE(14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C41H72NO8P	M+H	738.5068	-1.0
	HMDB0008846	PE(14/22:5(7Z,Z,13Z,16Z,19Z))	C41H72NO8P	M+H	738.5068	-1.0
738.5440	HMDB0008258	PC(18:4(6Z,9Z,12Z,15Z)/P-16)	C42H76NO7P	M+H	738.5432	1.1
	HMDB0011214	PC(P-16/18:4(6Z,9Z,12Z,15Z))	C42H76NO7P	M+H	738.5432	1.1
	HMDB0008258	PC(18:4(6Z,9Z,12Z,15Z)/P-16)	C42H76NO7P	M+H	738.5432	1.1
	HMDB0011214	PC(P-16/18:4(6Z,9Z,12Z,15Z))	C42H76NO7P	M+H	738.5432	1.1
	HMDB0113112	PE-NMe(18:1(11Z)/15)	C39H76NO8P	M+Na	740.5201	2.7
	HMDB0113853	PE-NMe2(14:1(9Z)/18)	C39H76NO8P	M+Na	740.5201	2.7
	HMDB0113139	PE-NMe(18:1(9Z)/15)	C39H76NO8P	M+Na	740.5201	2.7
	HMDB0113965	PE-NMe2(16:1(9Z)/16)	C39H76NO8P	M+Na	740.5201	2.7
	HMDB0114038	PE-NMe2(18:1(9Z)/14)	C39H76NO8P	M+Na	740.5201	2.7
	HMDB0114011	PE-NMe2(18:1(11Z)/14)	C39H76NO8P	M+Na	740.5201	2.7
	HMDB0113986	PE-NMe2(18/14:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
	HMDB0008000	PC(16:1(9Z)/15)	C39H76NO8P	M+Na	740.5201	2.7
	HMDB0007936	PC(15/16:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
	HMDB0008834	PE(14/:1(11Z))	C39H76NO8P	M+Na	740.5201	2.7
	HMDB0008866	PE(14:1(9Z)/)	C39H76NO8P	M+Na	740.5201	2.7
	HMDB0008926	PE(16/18:1(11Z))	C39H76NO8P	M+Na	740.5201	2.7
	HMDB0008927	PE(16/18:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
	HMDB0008958	PE(16:1(9Z)/18)	C39H76NO8P	M+Na	740.5201	2.7
	HMDB0008990	PE(18/16:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
	HMDB0009022	PE(18:1(11Z)/16)	C39H76NO8P	M+Na	740.5201	2.7

HMDB0009055	PE(18:1(9Z)/16)	C39H76NO8P	M+Na	740.5201	2.7
HMDB0009218	PE(/14:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0009250	PE(:1(11Z)/14)	C39H76NO8P	M+Na	740.5201	2.7
HMDB0112954	PE-NMe(15/18:1(11Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0113850	PE-NMe2(16/16:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0113851	PE-NMe2(14/18:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0112953	PE-NMe(15/18:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0113852	PE-NMe2(14/18:1(11Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0113112	PE-NMe(18:1(11Z)/15)	C39H76NO8P	M+Na	740.5201	2.7
HMDB0113853	PE-NMe2(14:1(9Z)/18)	C39H76NO8P	M+Na	740.5201	2.7
HMDB0113139	PE-NMe(18:1(9Z)/15)	C39H76NO8P	M+Na	740.5201	2.7
HMDB0113965	PE-NMe2(16:1(9Z)/16)	C39H76NO8P	M+Na	740.5201	2.7
HMDB0114038	PE-NMe2(18:1(9Z)/14)	C39H76NO8P	M+Na	740.5201	2.7
HMDB0114011	PE-NMe2(18:1(11Z)/14)	C39H76NO8P	M+Na	740.5201	2.7
HMDB0113986	PE-NMe2(18/14:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0008000	PC(16:1(9Z)/15)	C39H76NO8P	M+Na	740.5201	2.7
HMDB0007936	PC(15/16:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0008834	PE(14/:1(11Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0008866	PE(14:1(9Z)/)	C39H76NO8P	M+Na	740.5201	2.7
HMDB0008926	PE(16/18:1(11Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0008927	PE(16/18:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0008958	PE(16:1(9Z)/18)	C39H76NO8P	M+Na	740.5201	2.7
HMDB0008990	PE(18/16:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0009022	PE(18:1(11Z)/16)	C39H76NO8P	M+Na	740.5201	2.7
HMDB0009055	PE(18:1(9Z)/16)	C39H76NO8P	M+Na	740.5201	2.7
HMDB0009218	PE(/14:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0009250	PE(:1(11Z)/14)	C39H76NO8P	M+Na	740.5201	2.7
HMDB0112954	PE-NMe(15/18:1(11Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0113850	PE-NMe2(16/16:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0113851	PE-NMe2(14/18:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0112953	PE-NMe(15/18:1(9Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0113852	PE-NMe2(14/18:1(11Z))	C39H76NO8P	M+Na	740.5201	2.7
HMDB0115521	PA(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C41H71O8P	M+NH4	740.5225	-0.5

HMDB0115178	PA(:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0116704	PA(:5(5Z,8Z,11Z,14Z,17Z)/18)	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115177	PA(:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114848	PA(16/22:5(7Z,Z,13Z,16Z,19Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115524	PA(18:3(9Z,12Z,15Z)/:2(11Z,14Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115327	PA(22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115352	PA(22:5(4Z,7Z,Z,13Z,16Z)/16)	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115540	PA(:2(11Z,14Z)/18:3(6Z,9Z,12Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115378	PA(22:5(7Z,Z,13Z,16Z,19Z)/16)	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115541	PA(:2(11Z,14Z)/18:3(9Z,12Z,15Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115522	PA(18:3(6Z,9Z,12Z)/:2(11Z,14Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115495	PA(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115151	PA(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115150	PA(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114847	PA(16/22:5(4Z,7Z,Z,13Z,16Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114867	PA(16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114886	PA(18/:5(5Z,8Z,11Z,14Z,17Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115102	PA(:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114909	PA(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114910	PA(18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114934	PA(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114935	PA(18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114960	PA(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115126	PA(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115040	PA(18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114269	PE-NMe2(:3(5Z,8Z,11Z)/14:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0114297	PE-NMe2(:3(8Z,11Z,14Z)/14:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0114324	PE-NMe2(:4(5Z,8Z,11Z,14Z)/14)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0114352	PE-NMe2(:4(8Z,11Z,14Z,17Z)/14)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0114155	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/16)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0114127	PE-NMe2(18:3(9Z,12Z,15Z)/16:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113028	PE-NMe(15/:4(5Z,8Z,11Z,14Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113029	PE-NMe(15/:4(8Z,11Z,14Z,17Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113424	PE-NMe(:4(5Z,8Z,11Z,14Z)/15)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113452	PE-NMe(:4(8Z,11Z,14Z,17Z)/15)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113887	PE-NMe2(14/:4(5Z,8Z,11Z,14Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113888	PE-NMe2(14/:4(8Z,11Z,14Z,17Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113906	PE-NMe2(14:1(9Z)/:3(8Z,11Z,14Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113905	PE-NMe2(14:1(9Z)/:3(5Z,8Z,11Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113968	PE-NMe2(16:1(9Z)/18:3(9Z,12Z,15Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113967	PE-NMe2(16:1(9Z)/18:3(6Z,9Z,12Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0114098	PE-NMe2(18:3(6Z,9Z,12Z)/16:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009157	PE(18:3(9Z,12Z,15Z)/18:1(11Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009093	PE(18:2(9Z,12Z)/18:2(9Z,12Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009124	PE(18:3(6Z,9Z,12Z)/18:1(11Z))	C41H74NO8P	M+H	740.5225	-0.5

HMDB0009125	PE(18:3(6Z,9Z,12Z)/18:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009158	PE(18:3(9Z,12Z,15Z)/18:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113946	PE-NMe2(16/18:4(6Z,9Z,12Z,15Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009189	PE(18:4(6Z,9Z,12Z,15Z)/18)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009320	PE(:3(5Z,8Z,11Z)/16:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009353	PE(:3(8Z,11Z,14Z)/16:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009385	PE(:4(5Z,8Z,11Z,14Z)/16)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009061	PE(18:1(9Z)/18:3(6Z,9Z,12Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009062	PE(18:1(9Z)/18:3(9Z,12Z,15Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0007943	PC(15/18:4(6Z,9Z,12Z,15Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0008231	PC(18:4(6Z,9Z,12Z,15Z)/15)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0008844	PE(14/22:4(7Z,Z,13Z,16Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0008937	PE(16/:4(5Z,8Z,11Z,14Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0008938	PE(16/:4(8Z,11Z,14Z,17Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0008968	PE(16:1(9Z)/:3(5Z,8Z,11Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0008997	PE(18/18:4(6Z,9Z,12Z,15Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009028	PE(18:1(11Z)/18:3(6Z,9Z,12Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009029	PE(18:1(11Z)/18:3(9Z,12Z,15Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009418	PE(:4(8Z,11Z,14Z,17Z)/16)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009580	PE(22:4(7Z,Z,13Z,16Z)/14)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0115521	PA(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115178	PA(:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0116704	PA(:5(5Z,8Z,11Z,14Z,17Z)/18)	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115177	PA(:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114848	PA(16/22:5(7Z,Z,13Z,16Z,19Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115524	PA(18:3(9Z,12Z,15Z)/:2(11Z,14Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115327	PA(22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115352	PA(22:5(4Z,7Z,Z,13Z,16Z)/16)	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115540	PA(:2(11Z,14Z)/18:3(6Z,9Z,12Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115378	PA(22:5(7Z,Z,13Z,16Z,19Z)/16)	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115541	PA(:2(11Z,14Z)/18:3(9Z,12Z,15Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115522	PA(18:3(6Z,9Z,12Z)/:2(11Z,14Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115495	PA(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115151	PA(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115150	PA(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114847	PA(16/22:5(4Z,7Z,Z,13Z,16Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114867	PA(16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114886	PA(18/:5(5Z,8Z,11Z,14Z,17Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115102	PA(:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114909	PA(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114910	PA(18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114934	PA(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114935	PA(18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114960	PA(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0115126	PA(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C41H71O8P	M+NH4	740.5225	-0.5

HMDB0115040	PA(18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C41H71O8P	M+NH4	740.5225	-0.5
HMDB0114269	PE-NMe2(:3(5Z,8Z,11Z)/14:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0114297	PE-NMe2(:3(8Z,11Z,14Z)/14:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0114324	PE-NMe2(:4(5Z,8Z,11Z,14Z)/14)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0114352	PE-NMe2(:4(8Z,11Z,14Z,17Z)/14)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0114155	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/16)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0114127	PE-NMe2(18:3(9Z,12Z,15Z)/16:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113028	PE-NMe(15/:4(5Z,8Z,11Z,14Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113029	PE-NMe(15/:4(8Z,11Z,14Z,17Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113424	PE-NMe(:4(5Z,8Z,11Z,14Z)/15)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113452	PE-NMe(:4(8Z,11Z,14Z,17Z)/15)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113887	PE-NMe2(14/:4(5Z,8Z,11Z,14Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113888	PE-NMe2(14/:4(8Z,11Z,14Z,17Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113906	PE-NMe2(14:1(9Z)/:3(8Z,11Z,14Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113905	PE-NMe2(14:1(9Z)/:3(5Z,8Z,11Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113968	PE-NMe2(16:1(9Z)/18:3(9Z,12Z,15Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113967	PE-NMe2(16:1(9Z)/18:3(6Z,9Z,12Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0114098	PE-NMe2(18:3(6Z,9Z,12Z)/16:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009157	PE(18:3(9Z,12Z,15Z)/18:1(11Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009093	PE(18:2(9Z,12Z)/18:2(9Z,12Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009124	PE(18:3(6Z,9Z,12Z)/18:1(11Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009125	PE(18:3(6Z,9Z,12Z)/18:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009158	PE(18:3(9Z,12Z,15Z)/18:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0113946	PE-NMe2(16/18:4(6Z,9Z,12Z,15Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009189	PE(18:4(6Z,9Z,12Z,15Z)/18)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009320	PE(:3(5Z,8Z,11Z)/16:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009353	PE(:3(8Z,11Z,14Z)/16:1(9Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009385	PE(:4(5Z,8Z,11Z,14Z)/16)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009061	PE(18:1(9Z)/18:3(6Z,9Z,12Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0009062	PE(18:1(9Z)/18:3(9Z,12Z,15Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0007943	PC(15/18:4(6Z,9Z,12Z,15Z))	C41H74NO8P	M+H	740.5225	-0.5
HMDB0008231	PC(18:4(6Z,9Z,12Z,15Z)/15)	C41H74NO8P	M+H	740.5225	-0.5
HMDB0008844	PE(14/22:4(7Z,Z,13Z,16Z))	C41H74NO8P	M+H	740.5225	-0.5

	HMDB0008937	PE(16/:4(5Z,8Z,11Z,14Z))	C41H74NO8P	M+H	740.5225	-0.5
	HMDB0008938	PE(16/:4(8Z,11Z,14Z,17Z))	C41H74NO8P	M+H	740.5225	-0.5
	HMDB0008968	PE(16:1(9Z)/:3(5Z,8Z,11Z))	C41H74NO8P	M+H	740.5225	-0.5
	HMDB0008997	PE(18/18:4(6Z,9Z,12Z,15Z))	C41H74NO8P	M+H	740.5225	-0.5
	HMDB0009028	PE(18:1(11Z)/18:3(6Z,9Z,12Z))	C41H74NO8P	M+H	740.5225	-0.5
	HMDB0009029	PE(18:1(11Z)/18:3(9Z,12Z,15Z))	C41H74NO8P	M+H	740.5225	-0.5
	HMDB0009418	PE(:4(8Z,11Z,14Z,17Z)/16)	C41H74NO8P	M+H	740.5225	-0.5
	HMDB0009580	PE(22:4(7Z,Z,13Z,16Z)/14)	C41H74NO8P	M+H	740.5225	-0.5
740.5577	HMDB0011212	PC(P-16/18:3(6Z,9Z,12Z))	C42H78NO7P	M+H	740.5589	-1.6
	HMDB0011213	PC(P-16/18:3(9Z,12Z,15Z))	C42H78NO7P	M+H	740.5589	-1.6
	HMDB0008225	PC(18:3(9Z,12Z,15Z)/P-16)	C42H78NO7P	M+H	740.5589	-1.6
	HMDB0008192	PC(18:3(6Z,9Z,12Z)/P-16)	C42H78NO7P	M+H	740.5589	-1.6
	HMDB0007994	PC(16/P-16)	C40H80NO7P	M+Na	740.5565	1.7
	HMDB0011206	PC(P-16/16)	C40H80NO7P	M+Na	740.5565	1.7
	HMDB0011236	PC(P-18/14)	C40H80NO7P	M+Na	740.5565	1.7
	HMDB0013404	PC(O-16/16:1(9Z))	C40H80NO7P	M+Na	740.5565	1.7
	HMDB0007896	PC(14/P-18)	C40H80NO7P	M+Na	740.5565	1.7
	HMDB0011212	PC(P-16/18:3(6Z,9Z,12Z))	C42H78NO7P	M+H	740.5589	-1.6
	HMDB0011213	PC(P-16/18:3(9Z,12Z,15Z))	C42H78NO7P	M+H	740.5589	-1.6
	HMDB0008225	PC(18:3(9Z,12Z,15Z)/P-16)	C42H78NO7P	M+H	740.5589	-1.6
	HMDB0008192	PC(18:3(6Z,9Z,12Z)/P-16)	C42H78NO7P	M+H	740.5589	-1.6
	HMDB0007994	PC(16/P-16)	C40H80NO7P	M+Na	740.5565	1.7
	HMDB0011206	PC(P-16/16)	C40H80NO7P	M+Na	740.5565	1.7
	HMDB0011236	PC(P-18/14)	C40H80NO7P	M+Na	740.5565	1.7
	HMDB0013404	PC(O-16/16:1(9Z))	C40H80NO7P	M+Na	740.5565	1.7
	HMDB0007896	PC(14/P-18)	C40H80NO7P	M+Na	740.5565	1.7
	HMDB0007967	PC(16/15)	C39H78NO8P	M+Na	742.5357	2.7
	HMDB0113086	PE-NMe(18/15)	C39H78NO8P	M+Na	742.5357	2.7
	HMDB0113985	PE-NMe2(18/14)	C39H78NO8P	M+Na	742.5357	2.7
	HMDB0010566	PE-NMe2(16/16)	C39H78NO8P	M+Na	742.5357	2.7
	HMDB0113019	PE-NMe(15/18)	C39H78NO8P	M+Na	742.5357	2.7
	HMDB0009217	PE(/14)	C39H78NO8P	M+Na	742.5357	2.7

HMDB0113860	PE-NMe2(14/18)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0008989	PE(18/16)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0008925	PE(16/18)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0008833	PE(14/)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0007935	PC(15/16)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0007967	PC(16/15)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0113086	PE-NMe(18/15)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0113985	PE-NMe2(18/14)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0010566	PE-NMe2(16/16)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0113019	PE-NMe(15/18)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0009217	PE(/14)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0113860	PE-NMe2(14/18)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0008989	PE(18/16)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0008925	PE(16/18)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0008833	PE(14/)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0007935	PC(15/16)	C39H78NO8P	M+Na	742.5357	2.7
HMDB0114846	PA(16/22:4(7Z,Z,13Z,16Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115149	PA(:4(5Z,8Z,11Z,14Z)/18)	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115124	PA(:3(5Z,8Z,11Z)/18:1(11Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115125	PA(:3(5Z,8Z,11Z)/18:1(9Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115101	PA(:1(11Z)/18:3(9Z,12Z,15Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115100	PA(:1(11Z)/18:3(6Z,9Z,12Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115073	PA(/18:4(6Z,9Z,12Z,15Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115039	PA(18:4(6Z,9Z,12Z,15Z)/)	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115013	PA(18:3(9Z,12Z,15Z)/:1(11Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0114986	PA(18:3(6Z,9Z,12Z)/:1(11Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0114933	PA(18:1(9Z)/:3(5Z,8Z,11Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0114908	PA(18:1(11Z)/:3(5Z,8Z,11Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0114884	PA(18/:4(5Z,8Z,11Z,14Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0114885	PA(18/:4(8Z,11Z,14Z,17Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115176	PA(:4(8Z,11Z,14Z,17Z)/18)	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115568	PA(:3(8Z,11Z,14Z)/18:1(9Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115326	PA(22:4(7Z,Z,13Z,16Z)/16)	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115567	PA(:3(8Z,11Z,14Z)/18:1(11Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115520	PA(18:2(9Z,12Z)/:2(11Z,14Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115519	PA(18:1(9Z)/:3(8Z,11Z,14Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115517	PA(18:1(11Z)/:3(8Z,11Z,14Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115493	PA(:2(11Z,14Z)/18:2(9Z,12Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0113368	PE-NMe(:3(5Z,8Z,11Z)/15)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113026	PE-NMe(15/:3(5Z,8Z,11Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113027	PE-NMe(15/:3(8Z,11Z,14Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113396	PE-NMe(:3(8Z,11Z,14Z)/15)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113886	PE-NMe2(14/:3(8Z,11Z,14Z))	C41H76NO8P	M+H	742.5381	-0.6

742.5377

HMDB0113885	PE-NMe2(14/:3(5Z,8Z,11Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0114240	PE-NMe2(:2(11Z,14Z)/14:1(9Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113904	PE-NMe2(14:1(9Z)/:2(11Z,14Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0114296	PE-NMe2(:3(8Z,11Z,14Z)/14)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0114268	PE-NMe2(:3(5Z,8Z,11Z)/14)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0114126	PE-NMe2(18:3(9Z,12Z,15Z)/16)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0114097	PE-NMe2(18:3(6Z,9Z,12Z)/16)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0114069	PE-NMe2(18:2(9Z,12Z)/16:1(9Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113966	PE-NMe2(16:1(9Z)/18:2(9Z,12Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113945	PE-NMe2(16/18:3(9Z,12Z,15Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113944	PE-NMe2(16/18:3(6Z,9Z,12Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009123	PE(18:3(6Z,9Z,12Z)/18)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009156	PE(18:3(9Z,12Z,15Z)/18)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009287	PE(:2(11Z,14Z)/16:1(9Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009319	PE(:3(5Z,8Z,11Z)/16)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009352	PE(:3(8Z,11Z,14Z)/16)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009548	PE(22:2(13Z,16Z)/14:1(9Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0008995	PE(18/18:3(6Z,9Z,12Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009092	PE(18:2(9Z,12Z)/18:1(9Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009091	PE(18:2(9Z,12Z)/18:1(11Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0007942	PC(15/18:3(9Z,12Z,15Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0007941	PC(15/18:3(6Z,9Z,12Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0008165	PC(18:3(6Z,9Z,12Z)/15)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0008198	PC(18:3(9Z,12Z,15Z)/15)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0008876	PE(14:1(9Z)/22:2(13Z,16Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0008935	PE(16/:3(5Z,8Z,11Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0008936	PE(16/:3(8Z,11Z,14Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0008967	PE(16:1(9Z)/:2(11Z,14Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0008996	PE(18/18:3(9Z,12Z,15Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009027	PE(18:1(11Z)/18:2(9Z,12Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009060	PE(18:1(9Z)/18:2(9Z,12Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0114846	PA(16/22:4(7Z,Z,13Z,16Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115149	PA(:4(5Z,8Z,11Z,14Z)/18)	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115124	PA(:3(5Z,8Z,11Z)/18:1(11Z))	C41H73O8P	M+NH4	742.5381	-0.6

HMDB0115125	PA(:3(5Z,8Z,11Z)/18:1(9Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115101	PA(:1(11Z)/18:3(9Z,12Z,15Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115100	PA(:1(11Z)/18:3(6Z,9Z,12Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115073	PA(/18:4(6Z,9Z,12Z,15Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115039	PA(18:4(6Z,9Z,12Z,15Z)/)	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115013	PA(18:3(9Z,12Z,15Z)/:1(11Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0114986	PA(18:3(6Z,9Z,12Z)/:1(11Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0114933	PA(18:1(9Z)/:3(5Z,8Z,11Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0114908	PA(18:1(11Z)/:3(5Z,8Z,11Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0114884	PA(18/:4(5Z,8Z,11Z,14Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0114885	PA(18/:4(8Z,11Z,14Z,17Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115176	PA(:4(8Z,11Z,14Z,17Z)/18)	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115568	PA(:3(8Z,11Z,14Z)/18:1(9Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115326	PA(22:4(7Z,Z,13Z,16Z)/16)	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115567	PA(:3(8Z,11Z,14Z)/18:1(11Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115520	PA(18:2(9Z,12Z)/:2(11Z,14Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115519	PA(18:1(9Z)/:3(8Z,11Z,14Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115517	PA(18:1(11Z)/:3(8Z,11Z,14Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0115493	PA(:2(11Z,14Z)/18:2(9Z,12Z))	C41H73O8P	M+NH4	742.5381	-0.6
HMDB0113368	PE-NMe(:3(5Z,8Z,11Z)/15)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113026	PE-NMe(15/:3(5Z,8Z,11Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113027	PE-NMe(15/:3(8Z,11Z,14Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113396	PE-NMe(:3(8Z,11Z,14Z)/15)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113886	PE-NMe2(14/:3(8Z,11Z,14Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113885	PE-NMe2(14/:3(5Z,8Z,11Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0114240	PE-NMe2(:2(11Z,14Z)/14:1(9Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113904	PE-NMe2(14:1(9Z)/:2(11Z,14Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0114296	PE-NMe2(:3(8Z,11Z,14Z)/14)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0114268	PE-NMe2(:3(5Z,8Z,11Z)/14)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0114126	PE-NMe2(18:3(9Z,12Z,15Z)/16)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0114097	PE-NMe2(18:3(6Z,9Z,12Z)/16)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0114069	PE-NMe2(18:2(9Z,12Z)/16:1(9Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113966	PE-NMe2(16:1(9Z)/18:2(9Z,12Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113945	PE-NMe2(16/18:3(9Z,12Z,15Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0113944	PE-NMe2(16/18:3(6Z,9Z,12Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009123	PE(18:3(6Z,9Z,12Z)/18)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009156	PE(18:3(9Z,12Z,15Z)/18)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009287	PE(:2(11Z,14Z)/16:1(9Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009319	PE(:3(5Z,8Z,11Z)/16)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009352	PE(:3(8Z,11Z,14Z)/16)	C41H76NO8P	M+H	742.5381	-0.6
HMDB0009548	PE(22:2(13Z,16Z)/14:1(9Z))	C41H76NO8P	M+H	742.5381	-0.6
HMDB0008995	PE(18/18:3(6Z,9Z,12Z))	C41H76NO8P	M+H	742.5381	-0.6

	HMDB0009092	PE(18:2(9Z,12Z)/18:1(9Z))	C41H76NO8P	M+H	742.5381	-0.6
	HMDB0009091	PE(18:2(9Z,12Z)/18:1(11Z))	C41H76NO8P	M+H	742.5381	-0.6
	HMDB0007942	PC(15/18:3(9Z,12Z,15Z))	C41H76NO8P	M+H	742.5381	-0.6
	HMDB0007941	PC(15/18:3(6Z,9Z,12Z))	C41H76NO8P	M+H	742.5381	-0.6
	HMDB0008165	PC(18:3(6Z,9Z,12Z)/15)	C41H76NO8P	M+H	742.5381	-0.6
	HMDB0008198	PC(18:3(9Z,12Z,15Z)/15)	C41H76NO8P	M+H	742.5381	-0.6
	HMDB0008876	PE(14:1(9Z)/22:2(13Z,16Z))	C41H76NO8P	M+H	742.5381	-0.6
	HMDB0008935	PE(16/:3(5Z,8Z,11Z))	C41H76NO8P	M+H	742.5381	-0.6
	HMDB0008936	PE(16/:3(8Z,11Z,14Z))	C41H76NO8P	M+H	742.5381	-0.6
	HMDB0008967	PE(16:1(9Z)/:2(11Z,14Z))	C41H76NO8P	M+H	742.5381	-0.6
	HMDB0008996	PE(18/18:3(9Z,12Z,15Z))	C41H76NO8P	M+H	742.5381	-0.6
	HMDB0009027	PE(18:1(11Z)/18:2(9Z,12Z))	C41H76NO8P	M+H	742.5381	-0.6
	HMDB0009060	PE(18:1(9Z)/18:2(9Z,12Z))	C41H76NO8P	M+H	742.5381	-0.6
742.5743	HMDB0008030	PC(16:1(9Z)/P-18:1(9Z))	C42H80NO7P	M+H	742.5745	-0.3
	HMDB0013413	PC(O-16:1(9Z)/18:2(9Z,12Z))	C42H80NO7P	M+H	742.5745	-0.3
	HMDB0008029	PC(16:1(9Z)/P-18:1(11Z))	C42H80NO7P	M+H	742.5745	-0.3
	HMDB0008159	PC(18:2(9Z,12Z)/P-16)	C42H80NO7P	M+H	742.5745	-0.3
	HMDB0011211	PC(P-16/18:2(9Z,12Z))	C42H80NO7P	M+H	742.5745	-0.3
	HMDB0011273	PC(P-18:1(11Z)/16:1(9Z))	C42H80NO7P	M+H	742.5745	-0.3
	HMDB0011306	PC(P-18:1(9Z)/16:1(9Z))	C42H80NO7P	M+H	742.5745	-0.3
	HMDB0008030	PC(16:1(9Z)/P-18:1(9Z))	C42H80NO7P	M+H	742.5745	-0.3
	HMDB0013413	PC(O-16:1(9Z)/18:2(9Z,12Z))	C42H80NO7P	M+H	742.5745	-0.3
	HMDB0008029	PC(16:1(9Z)/P-18:1(11Z))	C42H80NO7P	M+H	742.5745	-0.3
	HMDB0008159	PC(18:2(9Z,12Z)/P-16)	C42H80NO7P	M+H	742.5745	-0.3
	HMDB0011211	PC(P-16/18:2(9Z,12Z))	C42H80NO7P	M+H	742.5745	-0.3
	HMDB0011273	PC(P-18:1(11Z)/16:1(9Z))	C42H80NO7P	M+H	742.5745	-0.3
	HMDB0011306	PC(P-18:1(9Z)/16:1(9Z))	C42H80NO7P	M+H	742.5745	-0.3
	HMDB0009216	PE(18:4(6Z,9Z,12Z,15Z)/P-18:1(9Z))	C41H72NO7P	M+Na	744.4939	1.9
	HMDB0009477	PE(:5(5Z,8Z,11Z,14Z,17Z)/P-16)	C41H72NO7P	M+Na	744.4939	1.9
	HMDB0011354	PE(P-16/:5(5Z,8Z,11Z,14Z,17Z))	C41H72NO7P	M+Na	744.4939	1.9
	HMDB0011412	PE(P-18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO7P	M+Na	744.4939	1.9
	HMDB0011445	PE(P-18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO7P	M+Na	744.4939	1.9

744.4953	HMDB0009215	PE(18:4(6Z,9Z,12Z,15Z)/P-18:1(11Z))	C41H72NO7P	M+Na	744.4939	1.9
	HMDB0009216	PE(18:4(6Z,9Z,12Z,15Z)/P-18:1(9Z))	C41H72NO7P	M+Na	744.4939	1.9
	HMDB0009477	PE(:5(5Z,8Z,11Z,14Z,17Z)/P-16)	C41H72NO7P	M+Na	744.4939	1.9
	HMDB0011354	PE(P-16/:5(5Z,8Z,11Z,14Z,17Z))	C41H72NO7P	M+Na	744.4939	1.9
	HMDB0011412	PE(P-18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO7P	M+Na	744.4939	1.9
	HMDB0011445	PE(P-18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO7P	M+Na	744.4939	1.9
	HMDB0009215	PE(18:4(6Z,9Z,12Z,15Z)/P-18:1(11Z))	C41H72NO7P	M+Na	744.4939	1.9
	HMDB0115123	PA(:3(5Z,8Z,11Z)/18)	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0115072	PA(/18:3(9Z,12Z,15Z))	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0115071	PA(/18:3(6Z,9Z,12Z))	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0115012	PA(18:3(9Z,12Z,15Z)/)	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0114985	PA(18:3(6Z,9Z,12Z)/)	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0114959	PA(18:2(9Z,12Z)/:1(11Z))	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0114883	PA(18/:3(5Z,8Z,11Z))	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0114866	PA(16:1(9Z)/22:2(13Z,16Z))	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0115099	PA(:1(11Z)/18:2(9Z,12Z))	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0115300	PA(22:2(13Z,16Z)/16:1(9Z))	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0115515	PA(18/:3(8Z,11Z,14Z))	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0115518	PA(18:1(9Z)/:2(11Z,14Z))	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0115566	PA(:3(8Z,11Z,14Z)/18)	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0115539	PA(:2(11Z,14Z)/18:1(9Z))	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0115538	PA(:2(11Z,14Z)/18:1(11Z))	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0115516	PA(18:1(11Z)/:2(11Z,14Z))	C41H75O8P	M+NH4	744.5538	-0.8
	HMDB0113858	PE-NMe2(16:1(9Z)/18:1(11Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0113856	PE-NMe2(14:1(9Z)/:1(11Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0113857	PE-NMe2(16:1(9Z)/18:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0114211	PE-NMe2(:1(11Z)/14:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0114239	PE-NMe2(:2(11Z,14Z)/14)	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0113884	PE-NMe2(14/:2(11Z,14Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0113339	PE-NMe(:2(11Z,14Z)/15)	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0113025	PE-NMe(15/:2(11Z,14Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0114068	PE-NMe2(18:2(9Z,12Z)/16)	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0114042	PE-NMe2(18:1(9Z)/16:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0114015	PE-NMe2(18:1(11Z)/16:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0113943	PE-NMe2(16/18:2(9Z,12Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0007940	PC(15/18:2(9Z,12Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0009547	PE(22:2(13Z,16Z)/14)	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0009515	PE(22:1(13Z)/14:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0009286	PE(:2(11Z,14Z)/16)	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0009254	PE(:1(11Z)/16:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8

744.5532

HMDB0008132	PC(18:2(9Z,12Z)/15)	C41H78NO8P	M+H	744.5538	-0.8
HMDB0008843	PE(14/22:2(13Z,16Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0008875	PE(14:1(9Z)/22:1(13Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0008934	PE(16/:2(11Z,14Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0008966	PE(16:1(9Z)/:1(11Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0008994	PE(18/18:2(9Z,12Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0009025	PE(18:1(11Z)/18:1(11Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0009026	PE(18:1(11Z)/18:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0009058	PE(18:1(9Z)/18:1(11Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0009059	PE(18:1(9Z)/18:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0009090	PE(18:2(9Z,12Z)/18)	C41H78NO8P	M+H	744.5538	-0.8
HMDB0115123	PA(:3(5Z,8Z,11Z)/18)	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0115072	PA(/18:3(9Z,12Z,15Z))	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0115071	PA(/18:3(6Z,9Z,12Z))	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0115012	PA(18:3(9Z,12Z,15Z)/)	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0114985	PA(18:3(6Z,9Z,12Z)/)	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0114959	PA(18:2(9Z,12Z)/:1(11Z))	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0114883	PA(18/:3(5Z,8Z,11Z))	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0114866	PA(16:1(9Z)/22:2(13Z,16Z))	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0115099	PA(:1(11Z)/18:2(9Z,12Z))	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0115300	PA(22:2(13Z,16Z)/16:1(9Z))	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0115515	PA(18/:3(8Z,11Z,14Z))	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0115518	PA(18:1(9Z)/:2(11Z,14Z))	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0115566	PA(:3(8Z,11Z,14Z)/18)	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0115539	PA(:2(11Z,14Z)/18:1(9Z))	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0115538	PA(:2(11Z,14Z)/18:1(11Z))	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0115516	PA(18:1(11Z)/:2(11Z,14Z))	C41H75O8P	M+NH4	744.5538	-0.8
HMDB0113858	PE-NMe2(16:1(9Z)/18:1(11Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0113856	PE-NMe2(14:1(9Z)/:1(11Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0113857	PE-NMe2(16:1(9Z)/18:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0114211	PE-NMe2(:1(11Z)/14:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0114239	PE-NMe2(:2(11Z,14Z)/14)	C41H78NO8P	M+H	744.5538	-0.8
HMDB0113884	PE-NMe2(14/:2(11Z,14Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0113339	PE-NMe(:2(11Z,14Z)/15)	C41H78NO8P	M+H	744.5538	-0.8
HMDB0113025	PE-NMe(15/:2(11Z,14Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0114068	PE-NMe2(18:2(9Z,12Z)/16)	C41H78NO8P	M+H	744.5538	-0.8
HMDB0114042	PE-NMe2(18:1(9Z)/16:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0114015	PE-NMe2(18:1(11Z)/16:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0113943	PE-NMe2(16/18:2(9Z,12Z))	C41H78NO8P	M+H	744.5538	-0.8
HMDB0007940	PC(15/18:2(9Z,12Z))	C41H78NO8P	M+H	744.5538	-0.8

	HMDB0009547	PE(22:2(13Z,16Z)/14)	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0009515	PE(22:1(13Z)/14:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0009286	PE(:2(11Z,14Z)/16)	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0009254	PE(:1(11Z)/16:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0008132	PC(18:2(9Z,12Z)/15)	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0008843	PE(14/22:2(13Z,16Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0008875	PE(14:1(9Z)/22:1(13Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0008934	PE(16/:2(11Z,14Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0008966	PE(16:1(9Z)/:1(11Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0008994	PE(18/18:2(9Z,12Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0009025	PE(18:1(11Z)/18:1(11Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0009026	PE(18:1(11Z)/18:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0009058	PE(18:1(9Z)/18:1(11Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0009059	PE(18:1(9Z)/18:1(9Z))	C41H78NO8P	M+H	744.5538	-0.8
	HMDB0009090	PE(18:2(9Z,12Z)/18)	C41H78NO8P	M+H	744.5538	-0.8
744.5898	HMDB0007996	PC(16/P-18:1(11Z))	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0007997	PC(16/P-18:1(9Z))	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0008028	PC(16:1(9Z)/P-18)	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0008093	PC(18:1(11Z)/P-16)	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0008126	PC(18:1(9Z)/P-16)	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0011151	Pc(o-16/18:2(9z,12z))	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0011209	PC(P-16/18:1(11Z))	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0011210	PC(P-16/18:1(9Z))	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0011240	PC(P-18/16:1(9Z))	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0011305	PC(P-18:1(9Z)/16)	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0011272	PC(P-18:1(11Z)/16)	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0007996	PC(16/P-18:1(11Z))	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0007997	PC(16/P-18:1(9Z))	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0008028	PC(16:1(9Z)/P-18)	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0008093	PC(18:1(11Z)/P-16)	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0008126	PC(18:1(9Z)/P-16)	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0011151	Pc(o-16/18:2(9z,12z))	C42H82NO7P	M+H	744.5902	-0.5

	HMDB0011209	PC(P-16/18:1(11Z))	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0011210	PC(P-16/18:1(9Z))	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0011240	PC(P-18/16:1(9Z))	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0011305	PC(P-18:1(9Z)/16)	C42H82NO7P	M+H	744.5902	-0.5
	HMDB0011272	PC(P-18:1(11Z)/16)	C42H82NO7P	M+H	744.5902	-0.5
745.5932	HMDB0035990	Cerebroside B	C41H77NO9	M+NH4	745.5937	-0.6
	HMDB0035990	Cerebroside B	C41H77NO9	M+NH4	745.5937	-0.6
	HMDB0114811	PA(14:1(9Z)/24:1(15Z))	C41H77O8P	M+NH4	746.5694	-0.4
	HMDB0115537	PA(:2(11Z,14Z)/18)	C41H77O8P	M+NH4	746.5694	-0.4
	HMDB0114845	PA(16/22:2(13Z,16Z))	C41H77O8P	M+NH4	746.5694	-0.4
	HMDB0114865	PA(16:1(9Z)/22:1(13Z))	C41H77O8P	M+NH4	746.5694	-0.4
	HMDB0114907	PA(18:1(11Z)/:1(11Z))	C41H77O8P	M+NH4	746.5694	-0.4
	HMDB0114932	PA(18:1(9Z)/:1(11Z))	C41H77O8P	M+NH4	746.5694	-0.4
	HMDB0114958	PA(18:2(9Z,12Z)/)	C41H77O8P	M+NH4	746.5694	-0.4
	HMDB0115070	PA(/18:2(9Z,12Z))	C41H77O8P	M+NH4	746.5694	-0.4
	HMDB0115097	PA(:1(11Z)/18:1(11Z))	C41H77O8P	M+NH4	746.5694	-0.4
	HMDB0115514	PA(18/:2(11Z,14Z))	C41H77O8P	M+NH4	746.5694	-0.4
	HMDB0115456	PA(24:1(15Z)/14:1(9Z))	C41H77O8P	M+NH4	746.5694	-0.4
	HMDB0115299	PA(22:2(13Z,16Z)/16)	C41H77O8P	M+NH4	746.5694	-0.4
	HMDB0115274	PA(22:1(13Z)/16:1(9Z))	C41H77O8P	M+NH4	746.5694	-0.4
	HMDB0115098	PA(:1(11Z)/18:1(9Z))	C41H77O8P	M+NH4	746.5694	-0.4
	HMDB0009514	PE(22:1(13Z)/14)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0008874	PE(14:1(9Z)/22)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0007939	PC(15/18:1(9Z))	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0008066	PC(18:1(11Z)/15)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0008099	PC(18:1(9Z)/15)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0008842	PE(14/22:1(13Z))	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0008933	PE(16/:1(11Z))	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0008965	PE(16:1(9Z)/)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0008992	PE(18/18:1(11Z))	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0009024	PE(18:1(11Z)/18)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0010568	PE-NMe2(16/18:1(9Z))	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0009221	PE(/16:1(9Z))	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0009253	PE(:1(11Z)/16)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0009482	PE(22/14:1(9Z))	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0007938	PC(15/18:1(11Z))	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0114210	PE-NMe2(:1(11Z)/14)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0113310	PE-NMe(:1(11Z)/15)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0114014	PE-NMe2(18:1(11Z)/16)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0114041	PE-NMe2(18:1(9Z)/16)	C41H80NO8P	M+H	746.5694	-0.4

746.5691

HMDB0113989	PE-NMe2(18/16:1(9Z))	C41H80NO8P	M+H	746.5694	-0.4
HMDB0009057	PE(18:1(9Z)/18)	C41H80NO8P	M+H	746.5694	-0.4
HMDB0008993	PE(18/18:1(9Z))	C41H80NO8P	M+H	746.5694	-0.4
HMDB0114182	PE-NMe2(/14:1(9Z))	C41H80NO8P	M+H	746.5694	-0.4
HMDB0113863	PE-NMe2(16:1(9Z)/18)	C41H80NO8P	M+H	746.5694	-0.4
HMDB0113862	PE-NMe2(16/18:1(11Z))	C41H80NO8P	M+H	746.5694	-0.4
HMDB0113859	PE-NMe2(14/:1(11Z))	C41H80NO8P	M+H	746.5694	-0.4
HMDB0113861	PE-NMe2(14:1(9Z)/)	C41H80NO8P	M+H	746.5694	-0.4
HMDB0112963	PE-NMe(15/:1(11Z))	C41H80NO8P	M+H	746.5694	-0.4
HMDB0114811	PA(14:1(9Z)/24:1(15Z))	C41H77O8P	M+NH4	746.5694	-0.4
HMDB0115537	PA(:2(11Z,14Z)/18)	C41H77O8P	M+NH4	746.5694	-0.4
HMDB0114845	PA(16/22:2(13Z,16Z))	C41H77O8P	M+NH4	746.5694	-0.4
HMDB0114865	PA(16:1(9Z)/22:1(13Z))	C41H77O8P	M+NH4	746.5694	-0.4
HMDB0114907	PA(18:1(11Z)/:1(11Z))	C41H77O8P	M+NH4	746.5694	-0.4
HMDB0114932	PA(18:1(9Z)/:1(11Z))	C41H77O8P	M+NH4	746.5694	-0.4
HMDB0114958	PA(18:2(9Z,12Z)/)	C41H77O8P	M+NH4	746.5694	-0.4
HMDB0115070	PA(/18:2(9Z,12Z))	C41H77O8P	M+NH4	746.5694	-0.4
HMDB0115097	PA(:1(11Z)/18:1(11Z))	C41H77O8P	M+NH4	746.5694	-0.4
HMDB0115514	PA(18/:2(11Z,14Z))	C41H77O8P	M+NH4	746.5694	-0.4
HMDB0115456	PA(24:1(15Z)/14:1(9Z))	C41H77O8P	M+NH4	746.5694	-0.4
HMDB0115299	PA(22:2(13Z,16Z)/16)	C41H77O8P	M+NH4	746.5694	-0.4
HMDB0115274	PA(22:1(13Z)/16:1(9Z))	C41H77O8P	M+NH4	746.5694	-0.4
HMDB0115098	PA(:1(11Z)/18:1(9Z))	C41H77O8P	M+NH4	746.5694	-0.4
HMDB0009514	PE(22:1(13Z)/14)	C41H80NO8P	M+H	746.5694	-0.4
HMDB0008874	PE(14:1(9Z)/22)	C41H80NO8P	M+H	746.5694	-0.4
HMDB0007939	PC(15/18:1(9Z))	C41H80NO8P	M+H	746.5694	-0.4
HMDB0008066	PC(18:1(11Z)/15)	C41H80NO8P	M+H	746.5694	-0.4
HMDB0008099	PC(18:1(9Z)/15)	C41H80NO8P	M+H	746.5694	-0.4
HMDB0008842	PE(14/22:1(13Z))	C41H80NO8P	M+H	746.5694	-0.4
HMDB0008933	PE(16/:1(11Z))	C41H80NO8P	M+H	746.5694	-0.4
HMDB0008965	PE(16:1(9Z)/)	C41H80NO8P	M+H	746.5694	-0.4
HMDB0008992	PE(18/18:1(11Z))	C41H80NO8P	M+H	746.5694	-0.4
HMDB0009024	PE(18:1(11Z)/18)	C41H80NO8P	M+H	746.5694	-0.4
HMDB0010568	PE-NMe2(16/18:1(9Z))	C41H80NO8P	M+H	746.5694	-0.4
HMDB0009221	PE(/16:1(9Z))	C41H80NO8P	M+H	746.5694	-0.4
HMDB0009253	PE(:1(11Z)/16)	C41H80NO8P	M+H	746.5694	-0.4
HMDB0009482	PE(22/14:1(9Z))	C41H80NO8P	M+H	746.5694	-0.4
HMDB0007938	PC(15/18:1(11Z))	C41H80NO8P	M+H	746.5694	-0.4
HMDB0114210	PE-NMe2(:1(11Z)/14)	C41H80NO8P	M+H	746.5694	-0.4

	HMDB0113310	PE-NMe(:1(11Z)/15)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0114014	PE-NMe2(18:1(11Z)/16)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0114041	PE-NMe2(18:1(9Z)/16)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0113989	PE-NMe2(18/16:1(9Z))	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0009057	PE(18:1(9Z)/18)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0008993	PE(18/18:1(9Z))	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0114182	PE-NMe2(/14:1(9Z))	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0113863	PE-NMe2(16:1(9Z)/18)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0113862	PE-NMe2(16/18:1(11Z))	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0113859	PE-NMe2(14/:1(11Z))	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0113861	PE-NMe2(14:1(9Z)/)	C41H80NO8P	M+H	746.5694	-0.4
	HMDB0112963	PE-NMe(15/:1(11Z))	C41H80NO8P	M+H	746.5694	-0.4
746.6054	HMDB0007995	PC(16/P-18)	C42H84NO7P	M+H	746.6058	-0.6
	HMDB0013426	PC(O-18:1(9Z)/16)	C42H84NO7P	M+H	746.6058	-0.6
	HMDB0013424	PC(O-18:1(11Z)/16)	C42H84NO7P	M+H	746.6058	-0.6
	HMDB0013412	PC(O-16:1(9Z)/18)	C42H84NO7P	M+H	746.6058	-0.6
	HMDB0008060	PC(18/P-16)	C42H84NO7P	M+H	746.6058	-0.6
	HMDB0011208	PC(P-16/18)	C42H84NO7P	M+H	746.6058	-0.6
	HMDB0011239	PC(P-18/16)	C42H84NO7P	M+H	746.6058	-0.6
	HMDB0007995	PC(16/P-18)	C42H84NO7P	M+H	746.6058	-0.6
	HMDB0013426	PC(O-18:1(9Z)/16)	C42H84NO7P	M+H	746.6058	-0.6
	HMDB0013424	PC(O-18:1(11Z)/16)	C42H84NO7P	M+H	746.6058	-0.6
	HMDB0013412	PC(O-16:1(9Z)/18)	C42H84NO7P	M+H	746.6058	-0.6
	HMDB0008060	PC(18/P-16)	C42H84NO7P	M+H	746.6058	-0.6
	HMDB0011208	PC(P-16/18)	C42H84NO7P	M+H	746.6058	-0.6
	HMDB0011239	PC(P-18/16)	C42H84NO7P	M+H	746.6058	-0.6
748.5270	HMDB0011453	PE(P-18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H74NO7P	M+H	748.5276	0.4
	HMDB0011420	PE(P-18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H74NO7P	M+H	748.5276	0.4
	HMDB0009708	PE(22:6(4Z,7Z,Z,13Z,16Z,19Z)/P-16)	C43H74NO7P	M+H	748.5276	0.4
	HMDB0009479	PE(:5(5Z,8Z,11Z,14Z,17Z)/P-18:1(11Z))	C43H74NO7P	M+H	748.5276	0.4
	HMDB0009480	PE(:5(5Z,8Z,11Z,14Z,17Z)/P-18:1(9Z))	C43H74NO7P	M+H	748.5276	0.4
	HMDB0005780	PE(P-16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H74NO7P	M+H	748.5276	0.4

748.5217	HMDB0011453	PE(P-18:1(9Z):5(5Z,8Z,11Z,14Z,17Z))	C43H74NO7P	M+H	748.5276	0.4
	HMDB0011420	PE(P-18:1(11Z):5(5Z,8Z,11Z,14Z,17Z))	C43H74NO7P	M+H	748.5276	0.4
	HMDB0009708	PE(22:6(4Z,7Z,Z,13Z,16Z,19Z)/P-16)	C43H74NO7P	M+H	748.5276	0.4
	HMDB0009479	PE(:5(5Z,8Z,11Z,14Z,17Z)/P-18:1(11Z))	C43H74NO7P	M+H	748.5276	0.4
	HMDB0009480	PE(:5(5Z,8Z,11Z,14Z,17Z)/P-18:1(9Z))	C43H74NO7P	M+H	748.5276	0.4
	HMDB0005780	PE(P-16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H74NO7P	M+H	748.5276	0.4
749.5312	HMDB0010573	PG(16/18:1(11Z))	C40H77O10P	M+H	749.5327	-2.0
	HMDB0010630	PG(18:1(9Z)/16)	C40H77O10P	M+H	749.5327	-2.0
	HMDB0010615	PG(18:1(11Z)/16)	C40H77O10P	M+H	749.5327	-2.0
	HMDB0010601	PG(18/16:1(9Z))	C40H77O10P	M+H	749.5327	-2.0
	HMDB0010587	PG(16:1(9Z)/18)	C40H77O10P	M+H	749.5327	-2.0
	HMDB0010574	PG(16/18:1(9Z))	C40H77O10P	M+H	749.5327	-2.0
	HMDB0010573	PG(16/18:1(11Z))	C40H77O10P	M+H	749.5327	-2.0
	HMDB0010630	PG(18:1(9Z)/16)	C40H77O10P	M+H	749.5327	-2.0
	HMDB0010615	PG(18:1(11Z)/16)	C40H77O10P	M+H	749.5327	-2.0
	HMDB0010601	PG(18/16:1(9Z))	C40H77O10P	M+H	749.5327	-2.0
	HMDB0010587	PG(16:1(9Z)/18)	C40H77O10P	M+H	749.5327	-2.0
	HMDB0010574	PG(16/18:1(9Z))	C40H77O10P	M+H	749.5327	-2.0
749.5900	HMDB0033621	Araliacerebroside	C40H77NO10	M+NH4	749.5886	1.9
	HMDB0033621	Araliacerebroside	C40H77NO10	M+NH4	749.5886	1.9
	HMDB0009050	PE(18:1(11Z)/P-18:1(11Z))	C41H78NO7P	M+Na	750.5408	2.8
	HMDB0011407	PE(P-18:1(11Z)/18:1(11Z))	C41H78NO7P	M+Na	750.5408	2.8
	HMDB0011408	PE(P-18:1(11Z)/18:1(9Z))	C41H78NO7P	M+Na	750.5408	2.8
	HMDB0011376	PE(P-18/18:2(9Z,12Z))	C41H78NO7P	M+Na	750.5408	2.8
	HMDB0011349	PE(P-16/:2(11Z,14Z))	C41H78NO7P	M+Na	750.5408	2.8
	HMDB0009312	PE(:2(11Z,14Z)/P-16)	C41H78NO7P	M+Na	750.5408	2.8
	HMDB0009115	PE(18:2(9Z,12Z)/P-18)	C41H78NO7P	M+Na	750.5408	2.8
	HMDB0009084	PE(18:1(9Z)/P-18:1(9Z))	C41H78NO7P	M+Na	750.5408	2.8
	HMDB0009083	PE(18:1(9Z)/P-18:1(11Z))	C41H78NO7P	M+Na	750.5408	2.8
	HMDB0011440	PE(P-18:1(9Z)/18:1(11Z))	C41H78NO7P	M+Na	750.5408	2.8
	HMDB0011441	PE(P-18:1(9Z)/18:1(9Z))	C41H78NO7P	M+Na	750.5408	2.8
	HMDB0009051	PE(18:1(11Z)/P-18:1(9Z))	C41H78NO7P	M+Na	750.5408	2.8

750.5429

HMDB0009050	PE(18:1(11Z)/P-18:1(11Z))	C41H78NO7P	M+Na	750.5408	2.8
HMDB0011407	PE(P-18:1(11Z)/18:1(11Z))	C41H78NO7P	M+Na	750.5408	2.8
HMDB0011408	PE(P-18:1(11Z)/18:1(9Z))	C41H78NO7P	M+Na	750.5408	2.8
HMDB0011376	PE(P-18/18:2(9Z,12Z))	C41H78NO7P	M+Na	750.5408	2.8
HMDB0011349	PE(P-16/:2(11Z,14Z))	C41H78NO7P	M+Na	750.5408	2.8
HMDB0009312	PE(:2(11Z,14Z)/P-16)	C41H78NO7P	M+Na	750.5408	2.8
HMDB0009115	PE(18:2(9Z,12Z)/P-18)	C41H78NO7P	M+Na	750.5408	2.8
HMDB0009084	PE(18:1(9Z)/P-18:1(9Z))	C41H78NO7P	M+Na	750.5408	2.8
HMDB0009083	PE(18:1(9Z)/P-18:1(11Z))	C41H78NO7P	M+Na	750.5408	2.8
HMDB0011440	PE(P-18:1(9Z)/18:1(11Z))	C41H78NO7P	M+Na	750.5408	2.8
HMDB0011441	PE(P-18:1(9Z)/18:1(9Z))	C41H78NO7P	M+Na	750.5408	2.8
HMDB0009051	PE(18:1(11Z)/P-18:1(9Z))	C41H78NO7P	M+Na	750.5408	2.8
HMDB0011451	PE(P-18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0011452	PE(P-18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0011419	PE(P-18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0011387	PE(P-18/:5(5Z,8Z,11Z,14Z,17Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0009413	PE(:4(5Z,8Z,11Z,14Z)/P-18:1(11Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0009414	PE(:4(5Z,8Z,11Z,14Z)/P-18:1(9Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0009446	PE(:4(8Z,11Z,14Z,17Z)/P-18:1(11Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0009447	PE(:4(8Z,11Z,14Z,17Z)/P-18:1(9Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0009478	PE(:5(5Z,8Z,11Z,14Z,17Z)/P-18)	C43H76NO7P	M+H	750.5432	-0.4
HMDB0009642	PE(22:5(4Z,7Z,Z,13Z,16Z)/P-16)	C43H76NO7P	M+H	750.5432	-0.4
HMDB0009675	PE(22:5(7Z,Z,13Z,16Z,19Z)/P-16)	C43H76NO7P	M+H	750.5432	-0.4
HMDB0011418	PE(P-18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0011360	PE(P-16/22:5(7Z,Z,13Z,16Z,19Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0011359	PE(P-16/22:5(4Z,7Z,Z,13Z,16Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0011451	PE(P-18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0011452	PE(P-18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0011419	PE(P-18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0011387	PE(P-18/:5(5Z,8Z,11Z,14Z,17Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0009413	PE(:4(5Z,8Z,11Z,14Z)/P-18:1(11Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0009414	PE(:4(5Z,8Z,11Z,14Z)/P-18:1(9Z))	C43H76NO7P	M+H	750.5432	-0.4

HMDB0009446	PE(:4(8Z,11Z,14Z,17Z)/P-18:1(11Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0009447	PE(:4(8Z,11Z,14Z,17Z)/P-18:1(9Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0009478	PE(:5(5Z,8Z,11Z,14Z,17Z)/P-18)	C43H76NO7P	M+H	750.5432	-0.4
HMDB0009642	PE(22:5(4Z,7Z,Z,13Z,16Z)/P-16)	C43H76NO7P	M+H	750.5432	-0.4
HMDB0009675	PE(22:5(7Z,Z,13Z,16Z,19Z)/P-16)	C43H76NO7P	M+H	750.5432	-0.4
HMDB0011418	PE(P-18:1(11Z):4(5Z,8Z,11Z,14Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0011360	PE(P-16/22:5(7Z,Z,13Z,16Z,19Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0011359	PE(P-16/22:5(4Z,7Z,Z,13Z,16Z))	C43H76NO7P	M+H	750.5432	-0.4
HMDB0116445	(2S)-1-hydroxy-3- {[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116370	(2S)-1- {[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy} -3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116378	(2S)-1- {[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy} -3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116385	(2S)-2- {[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy} -3-hydroxypropyl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116392	(2S)-1-hydroxy-3- {[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116399	(2S)-1-hydroxy-3- {[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propan-2-yl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116411	(2S)-2- {[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy} -3-hydroxypropyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116416	(2S)-3-hydroxy-2- {[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116421	(2S)-3-hydroxy-2- {[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116426	(2S)-1- {[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy} -3-hydroxypropan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116432	(2S)-1- {[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy} -3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0010572	PG(16/18)	C40H79O10P	M+H	751.5484	-2.6
HMDB0010600	PG(18/16)	C40H79O10P	M+H	751.5484	-2.6
HMDB0116670	PG(i-12/i-22)	C40H79O10P	M+H	751.5484	-2.6
HMDB0116640	PG(a-13/a-21)	C40H79O10P	M+H	751.5484	-2.6
HMDB0116651	PG(a-13/i-21)	C40H79O10P	M+H	751.5484	-2.6
HMDB0116687	PG(i-13/i-21)	C40H79O10P	M+H	751.5484	-2.6
HMDB0116676	PG(i-13/a-21)	C40H79O10P	M+H	751.5484	-2.6

HMDB0116445	(2S)-1-hydroxy-3-{{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116370	(2S)-1-{{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116378	(2S)-1-{{[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116385	(2S)-2-{{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropyl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116392	(2S)-1-hydroxy-3-{{[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116399	(2S)-1-hydroxy-3-{{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propan-2-yl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116411	(2S)-2-{{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116416	(2S)-3-hydroxy-2-{{[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116421	(2S)-3-hydroxy-2-{{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116426	(2S)-1-{{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0116432	(2S)-1-{{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+Na	751.5483	-2.6
HMDB0010572	PG(16/18)	C40H79O10P	M+H	751.5484	-2.6
HMDB0010600	PG(18/16)	C40H79O10P	M+H	751.5484	-2.6
HMDB0116670	PG(i-12/i-22)	C40H79O10P	M+H	751.5484	-2.6
HMDB0116640	PG(a-13/a-21)	C40H79O10P	M+H	751.5484	-2.6
HMDB0116651	PG(a-13/i-21)	C40H79O10P	M+H	751.5484	-2.6
HMDB0116687	PG(i-13/i-21)	C40H79O10P	M+H	751.5484	-2.6
HMDB0116676	PG(i-13/a-21)	C40H79O10P	M+H	751.5484	-2.6
HMDB0011348	PE(P-16/:1(11Z))	C41H80NO7P	M+Na	752.5565	3.0
HMDB0007964	PC(15/P-18:1(9Z))	C41H80NO7P	M+Na	752.5565	3.0
HMDB0011439	PE(P-18:1(9Z)/18)	C41H80NO7P	M+Na	752.5565	3.0
HMDB0011271	PC(P-18:1(11Z)/15)	C41H80NO7P	M+Na	752.5565	3.0
HMDB0011406	PE(P-18:1(11Z)/18)	C41H80NO7P	M+Na	752.5565	3.0
HMDB0011304	PC(P-18:1(9Z)/15)	C41H80NO7P	M+Na	752.5565	3.0
HMDB0011375	PE(P-18/18:1(9Z))	C41H80NO7P	M+Na	752.5565	3.0
HMDB0009279	PE(:1(11Z)/P-16)	C41H80NO7P	M+Na	752.5565	3.0
HMDB0007963	PC(15/P-18:1(11Z))	C41H80NO7P	M+Na	752.5565	3.0

752.5587

HMDB0009017	PE(18/P-18:1(11Z))	C41H80NO7P	M+Na	752.5565	3.0
HMDB0009018	PE(18/P-18:1(9Z))	C41H80NO7P	M+Na	752.5565	3.0
HMDB0009049	PE(18:1(11Z)/P-18)	C41H80NO7P	M+Na	752.5565	3.0
HMDB0009082	PE(18:1(9Z)/P-18)	C41H80NO7P	M+Na	752.5565	3.0
HMDB0011374	PE(P-18/18:1(11Z))	C41H80NO7P	M+Na	752.5565	3.0
HMDB0011348	PE(P-16/:1(11Z))	C41H80NO7P	M+Na	752.5565	3.0
HMDB0007964	PC(15/P-18:1(9Z))	C41H80NO7P	M+Na	752.5565	3.0
HMDB0011439	PE(P-18:1(9Z)/18)	C41H80NO7P	M+Na	752.5565	3.0
HMDB0011271	PC(P-18:1(11Z)/15)	C41H80NO7P	M+Na	752.5565	3.0
HMDB0011406	PE(P-18:1(11Z)/18)	C41H80NO7P	M+Na	752.5565	3.0
HMDB0011304	PC(P-18:1(9Z)/15)	C41H80NO7P	M+Na	752.5565	3.0
HMDB0011375	PE(P-18/18:1(9Z))	C41H80NO7P	M+Na	752.5565	3.0
HMDB0009279	PE(:1(11Z)/P-16)	C41H80NO7P	M+Na	752.5565	3.0
HMDB0007963	PC(15/P-18:1(11Z))	C41H80NO7P	M+Na	752.5565	3.0
HMDB0009017	PE(18/P-18:1(11Z))	C41H80NO7P	M+Na	752.5565	3.0
HMDB0009018	PE(18/P-18:1(9Z))	C41H80NO7P	M+Na	752.5565	3.0
HMDB0009049	PE(18:1(11Z)/P-18)	C41H80NO7P	M+Na	752.5565	3.0
HMDB0009082	PE(18:1(9Z)/P-18)	C41H80NO7P	M+Na	752.5565	3.0
HMDB0011374	PE(P-18/18:1(11Z))	C41H80NO7P	M+Na	752.5565	3.0
HMDB0011386	PE(P-18/:4(8Z,11Z,14Z,17Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0011416	PE(P-18:1(11Z)/:3(5Z,8Z,11Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0011417	PE(P-18:1(11Z)/:3(8Z,11Z,14Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0011449	PE(P-18:1(9Z)/:3(5Z,8Z,11Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0011358	PE(P-16/22:4(7Z,Z,13Z,16Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0009380	PE(:3(8Z,11Z,14Z)/P-18:1(11Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0009347	PE(:3(5Z,8Z,11Z)/P-18:1(11Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0009348	PE(:3(5Z,8Z,11Z)/P-18:1(9Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0009381	PE(:3(8Z,11Z,14Z)/P-18:1(9Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0009412	PE(:4(5Z,8Z,11Z,14Z)/P-18)	C43H78NO7P	M+H	752.5589	-0.2
HMDB0009445	PE(:4(8Z,11Z,14Z,17Z)/P-18)	C43H78NO7P	M+H	752.5589	-0.2
HMDB0009609	PE(22:4(7Z,Z,13Z,16Z)/P-16)	C43H78NO7P	M+H	752.5589	-0.2
HMDB0005779	PE(P-18/:4(5Z,8Z,11Z,14Z))	C43H78NO7P	M+H	752.5589	-0.2

HMDB0061335	PE(P-18/:4(5Z,8Z,11Z,14Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0011386	PE(P-18/:4(8Z,11Z,14Z,17Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0011416	PE(P-18:1(11Z)/:3(5Z,8Z,11Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0011417	PE(P-18:1(11Z)/:3(8Z,11Z,14Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0011449	PE(P-18:1(9Z)/:3(5Z,8Z,11Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0011358	PE(P-16/22:4(7Z,Z,13Z,16Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0009380	PE(:3(8Z,11Z,14Z)/P-18:1(11Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0009347	PE(:3(5Z,8Z,11Z)/P-18:1(11Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0009348	PE(:3(5Z,8Z,11Z)/P-18:1(9Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0009381	PE(:3(8Z,11Z,14Z)/P-18:1(9Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0009412	PE(:4(5Z,8Z,11Z,14Z)/P-18)	C43H78NO7P	M+H	752.5589	-0.2
HMDB0009445	PE(:4(8Z,11Z,14Z,17Z)/P-18)	C43H78NO7P	M+H	752.5589	-0.2
HMDB0009609	PE(22:4(7Z,Z,13Z,16Z)/P-16)	C43H78NO7P	M+H	752.5589	-0.2
HMDB0005779	PE(P-18/:4(5Z,8Z,11Z,14Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0061335	PE(P-18/:4(5Z,8Z,11Z,14Z))	C43H78NO7P	M+H	752.5589	-0.2
HMDB0113145	PE-NMe(18:1(9Z)/18:3(9Z,12Z,15Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113144	PE-NMe(18:1(9Z)/18:3(6Z,9Z,12Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113118	PE-NMe(18:1(11Z)/18:3(9Z,12Z,15Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113117	PE-NMe(18:1(11Z)/18:3(6Z,9Z,12Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113092	PE-NMe(18/18:4(6Z,9Z,12Z,15Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113070	PE-NMe(16:1(9Z)/:3(5Z,8Z,11Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113071	PE-NMe(16:1(9Z)/:3(8Z,11Z,14Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113050	PE-NMe(16/:4(5Z,8Z,11Z,14Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0116725	PE-NMe(16/:4(8Z,11Z,14Z,17Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0112993	PE-NMe(14/22:4(7Z,Z,13Z,16Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113172	PE-NMe(18:2(9Z,12Z)/18:2(9Z,12Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113199	PE-NMe(18:3(6Z,9Z,12Z)/18:1(11Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113200	PE-NMe(18:3(6Z,9Z,12Z)/18:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0114354	PE-NMe2(:4(8Z,11Z,14Z,17Z)/15)	C42H76NO8P	M+H	754.5381	0.2
HMDB0114326	PE-NMe2(:4(5Z,8Z,11Z,14Z)/15)	C42H76NO8P	M+H	754.5381	0.2
HMDB0113929	PE-NMe2(15/:4(8Z,11Z,14Z,17Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113928	PE-NMe2(15/:4(5Z,8Z,11Z,14Z))	C42H76NO8P	M+H	754.5381	0.2

754.5383

HMDB0113592	PE-NMe(22:4(7Z,Z,13Z,16Z)/14)	C42H76NO8P	M+H	754.5381	0.2
HMDB0113453	PE-NMe(:4(8Z,11Z,14Z,17Z)/16)	C42H76NO8P	M+H	754.5381	0.2
HMDB0113425	PE-NMe(:4(5Z,8Z,11Z,14Z)/16)	C42H76NO8P	M+H	754.5381	0.2
HMDB0113398	PE-NMe(:3(8Z,11Z,14Z)/16:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113370	PE-NMe(:3(5Z,8Z,11Z)/16:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113255	PE-NMe(18:4(6Z,9Z,12Z,15Z)/18)	C42H76NO8P	M+H	754.5381	0.2
HMDB0113227	PE-NMe(18:3(9Z,12Z,15Z)/18:1(11Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113228	PE-NMe(18:3(9Z,12Z,15Z)/18:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0009582	PE(22:4(7Z,Z,13Z,16Z)/15)	C42H76NO8P	M+H	754.5381	0.2
HMDB0008910	PE(15/22:4(7Z,Z,13Z,16Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0008459	PC(:4(8Z,11Z,14Z,17Z)/14)	C42H76NO8P	M+H	754.5381	0.2
HMDB0008426	PC(:4(5Z,8Z,11Z,14Z)/14)	C42H76NO8P	M+H	754.5381	0.2
HMDB0008395	PC(:3(8Z,11Z,14Z)/14:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0008362	PC(:3(5Z,8Z,11Z)/14:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0008232	PC(18:4(6Z,9Z,12Z,15Z)/16)	C42H76NO8P	M+H	754.5381	0.2
HMDB0008200	PC(18:3(9Z,12Z,15Z)/16:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0008167	PC(18:3(6Z,9Z,12Z)/16:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0008008	PC(16:1(9Z)/18:3(9Z,12Z,15Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0008007	PC(16:1(9Z)/18:3(6Z,9Z,12Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0007976	PC(16/18:4(6Z,9Z,12Z,15Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0007915	PC(14:1(9Z)/:3(8Z,11Z,14Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0007914	PC(14:1(9Z)/:3(5Z,8Z,11Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0007884	PC(14/:4(8Z,11Z,14Z,17Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0007883	PC(14/:4(5Z,8Z,11Z,14Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113145	PE-NMe(18:1(9Z)/18:3(9Z,12Z,15Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113144	PE-NMe(18:1(9Z)/18:3(6Z,9Z,12Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113118	PE-NMe(18:1(11Z)/18:3(9Z,12Z,15Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113117	PE-NMe(18:1(11Z)/18:3(6Z,9Z,12Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113092	PE-NMe(18/18:4(6Z,9Z,12Z,15Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113070	PE-NMe(16:1(9Z)/:3(5Z,8Z,11Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113071	PE-NMe(16:1(9Z)/:3(8Z,11Z,14Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113050	PE-NMe(16/:4(5Z,8Z,11Z,14Z))	C42H76NO8P	M+H	754.5381	0.2

HMDB0116725	PE-NMe(16:4(8Z,11Z,14Z,17Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0112993	PE-NMe(14:22:4(7Z,Z,13Z,16Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113172	PE-NMe(18:2(9Z,12Z)/18:2(9Z,12Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113199	PE-NMe(18:3(6Z,9Z,12Z)/18:1(11Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113200	PE-NMe(18:3(6Z,9Z,12Z)/18:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0114354	PE-NMe2(:4(8Z,11Z,14Z,17Z)/15)	C42H76NO8P	M+H	754.5381	0.2
HMDB0114326	PE-NMe2(:4(5Z,8Z,11Z,14Z)/15)	C42H76NO8P	M+H	754.5381	0.2
HMDB0113929	PE-NMe2(15/:4(8Z,11Z,14Z,17Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113928	PE-NMe2(15/:4(5Z,8Z,11Z,14Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113592	PE-NMe(22:4(7Z,Z,13Z,16Z)/14)	C42H76NO8P	M+H	754.5381	0.2
HMDB0113453	PE-NMe(:4(8Z,11Z,14Z,17Z)/16)	C42H76NO8P	M+H	754.5381	0.2
HMDB0113425	PE-NMe(:4(5Z,8Z,11Z,14Z)/16)	C42H76NO8P	M+H	754.5381	0.2
HMDB0113398	PE-NMe(:3(8Z,11Z,14Z)/16:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113370	PE-NMe(:3(5Z,8Z,11Z)/16:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113255	PE-NMe(18:4(6Z,9Z,12Z,15Z)/18)	C42H76NO8P	M+H	754.5381	0.2
HMDB0113227	PE-NMe(18:3(9Z,12Z,15Z)/18:1(11Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0113228	PE-NMe(18:3(9Z,12Z,15Z)/18:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0009582	PE(22:4(7Z,Z,13Z,16Z)/15)	C42H76NO8P	M+H	754.5381	0.2
HMDB0008910	PE(15:22:4(7Z,Z,13Z,16Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0008459	PC(:4(8Z,11Z,14Z,17Z)/14)	C42H76NO8P	M+H	754.5381	0.2
HMDB0008426	PC(:4(5Z,8Z,11Z,14Z)/14)	C42H76NO8P	M+H	754.5381	0.2
HMDB0008395	PC(:3(8Z,11Z,14Z)/14:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0008362	PC(:3(5Z,8Z,11Z)/14:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0008232	PC(18:4(6Z,9Z,12Z,15Z)/16)	C42H76NO8P	M+H	754.5381	0.2
HMDB0008200	PC(18:3(9Z,12Z,15Z)/16:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0008167	PC(18:3(6Z,9Z,12Z)/16:1(9Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0008008	PC(16:1(9Z)/18:3(9Z,12Z,15Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0008007	PC(16:1(9Z)/18:3(6Z,9Z,12Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0007976	PC(16/18:4(6Z,9Z,12Z,15Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0007915	PC(14:1(9Z)/:3(8Z,11Z,14Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0007914	PC(14:1(9Z)/:3(5Z,8Z,11Z))	C42H76NO8P	M+H	754.5381	0.2
HMDB0007884	PC(14/:4(8Z,11Z,14Z,17Z))	C42H76NO8P	M+H	754.5381	0.2

	HMDB0007883	PC(14/:4(5Z,8Z,11Z,14Z))	C42H76NO8P	M+H	754.5381	0.2
755.5404	HMDB0040991	Ternatin	C37H67N7O8	M+NH4	755.5389	1.9
	HMDB0040991	Ternatin	C37H67N7O8	M+NH4	755.5389	1.9
	HMDB0113087	PE-NMe(18/16)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0112965	PE-NMe(16/18)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0112983	PE-NMe(14/)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0113279	PE-NMe(/14)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0113919	PE-NMe2(15/18)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0113987	PE-NMe2(18/15)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0009219	PE(/15)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0008899	PE(15/)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0000564	PC(16/16)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0008031	PC(18/14)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0007871	PC(14/18)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0113087	PE-NMe(18/16)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0112965	PE-NMe(16/18)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0112983	PE-NMe(14/)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0113279	PE-NMe(/14)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0113919	PE-NMe2(15/18)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0113987	PE-NMe2(18/15)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0009219	PE(/15)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0008899	PE(15/)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0000564	PC(16/16)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0008031	PC(18/14)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0007871	PC(14/18)	C40H80NO8P	M+Na	756.5514	2.7
	HMDB0113170	PE-NMe(18:2(9Z,12Z)/18:1(11Z))	C42H78NO8P	M+H	756.5538	-0.5
	HMDB0113143	PE-NMe(18:1(9Z)/18:2(9Z,12Z))	C42H78NO8P	M+H	756.5538	-0.5
	HMDB0113116	PE-NMe(18:1(11Z)/18:2(9Z,12Z))	C42H78NO8P	M+H	756.5538	-0.5
	HMDB0113090	PE-NMe(18/18:3(6Z,9Z,12Z))	C42H78NO8P	M+H	756.5538	-0.5
	HMDB0113091	PE-NMe(18/18:3(9Z,12Z,15Z))	C42H78NO8P	M+H	756.5538	-0.5
	HMDB0113049	PE-NMe(16/:3(8Z,11Z,14Z))	C42H78NO8P	M+H	756.5538	-0.5
	HMDB0113048	PE-NMe(16/:3(5Z,8Z,11Z))	C42H78NO8P	M+H	756.5538	-0.5

756.5534

HMDB0113011	PE-NMe(14:1(9Z)/22:2(13Z,16Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113171	PE-NMe(18:2(9Z,12Z)/18:1(9Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113198	PE-NMe(18:3(6Z,9Z,12Z)/18)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113226	PE-NMe(18:3(9Z,12Z,15Z)/18)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113341	PE-NMe(:2(11Z,14Z)/16:1(9Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113069	PE-NMe(16:1(9Z)/:2(11Z,14Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0114298	PE-NMe2(:3(8Z,11Z,14Z)/15)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0114270	PE-NMe2(:3(5Z,8Z,11Z)/15)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113927	PE-NMe2(15/:3(8Z,11Z,14Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113926	PE-NMe2(15/:3(5Z,8Z,11Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113564	PE-NMe(22:2(13Z,16Z)/14:1(9Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113397	PE-NMe(:3(8Z,11Z,14Z)/16)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113369	PE-NMe(:3(5Z,8Z,11Z)/16)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0008394	PC(:3(8Z,11Z,14Z)/14)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0008361	PC(:3(5Z,8Z,11Z)/14)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0008329	PC(:2(11Z,14Z)/14:1(9Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0008199	PC(18:3(9Z,12Z,15Z)/16)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0008166	PC(18:3(6Z,9Z,12Z)/16)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0008134	PC(18:2(9Z,12Z)/16:1(9Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0008006	PC(16:1(9Z)/18:2(9Z,12Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0007974	PC(16/18:3(6Z,9Z,12Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0007975	PC(16/18:3(9Z,12Z,15Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0007913	PC(14:1(9Z)/:2(11Z,14Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0007881	PC(14/:3(5Z,8Z,11Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0007882	PC(14/:3(8Z,11Z,14Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113170	PE-NMe(18:2(9Z,12Z)/18:1(11Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113143	PE-NMe(18:1(9Z)/18:2(9Z,12Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113116	PE-NMe(18:1(11Z)/18:2(9Z,12Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113090	PE-NMe(18/18:3(6Z,9Z,12Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113091	PE-NMe(18/18:3(9Z,12Z,15Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113049	PE-NMe(16/:3(8Z,11Z,14Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113048	PE-NMe(16/:3(5Z,8Z,11Z))	C42H78NO8P	M+H	756.5538	-0.5

HMDB0113011	PE-NMe(14:1(9Z)/22:2(13Z,16Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113171	PE-NMe(18:2(9Z,12Z)/18:1(9Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113198	PE-NMe(18:3(6Z,9Z,12Z)/18)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113226	PE-NMe(18:3(9Z,12Z,15Z)/18)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113341	PE-NMe(:2(11Z,14Z)/16:1(9Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113069	PE-NMe(16:1(9Z)/:2(11Z,14Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0114298	PE-NMe2(:3(8Z,11Z,14Z)/15)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0114270	PE-NMe2(:3(5Z,8Z,11Z)/15)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113927	PE-NMe2(15/:3(8Z,11Z,14Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113926	PE-NMe2(15/:3(5Z,8Z,11Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113564	PE-NMe(22:2(13Z,16Z)/14:1(9Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113397	PE-NMe(:3(8Z,11Z,14Z)/16)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0113369	PE-NMe(:3(5Z,8Z,11Z)/16)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0008394	PC(:3(8Z,11Z,14Z)/14)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0008361	PC(:3(5Z,8Z,11Z)/14)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0008329	PC(:2(11Z,14Z)/14:1(9Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0008199	PC(18:3(9Z,12Z,15Z)/16)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0008166	PC(18:3(6Z,9Z,12Z)/16)	C42H78NO8P	M+H	756.5538	-0.5
HMDB0008134	PC(18:2(9Z,12Z)/16:1(9Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0008006	PC(16:1(9Z)/18:2(9Z,12Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0007974	PC(16/18:3(6Z,9Z,12Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0007975	PC(16/18:3(9Z,12Z,15Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0007913	PC(14:1(9Z)/:2(11Z,14Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0007881	PC(14/:3(5Z,8Z,11Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0007882	PC(14/:3(8Z,11Z,14Z))	C42H78NO8P	M+H	756.5538	-0.5
HMDB0010565	PE-NMe(18:1(9Z)/18:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0009549	PE(22:2(13Z,16Z)/15)	C42H80NO8P	M+H	758.5694	-1.0
HMDB0007880	PC(14/:2(11Z,14Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0007912	PC(14:1(9Z)/:1(11Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0007973	PC(16/18:2(9Z,12Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0008005	PC(16:1(9Z)/18:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0008004	PC(16:1(9Z)/18:1(11Z))	C42H80NO8P	M+H	758.5694	-1.0

758.5687

HMDB0008068	PC(18:1(11Z)/16:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0008909	PE(15/22:2(13Z,16Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0008328	PC(:2(11Z,14Z)/14)	C42H80NO8P	M+H	758.5694	-1.0
HMDB0008296	PC(:1(11Z)/14:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0008133	PC(18:2(9Z,12Z)/16)	C42H80NO8P	M+H	758.5694	-1.0
HMDB0008101	PC(18:1(9Z)/16:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0112992	PE-NMe(14/22:2(13Z,16Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0112967	PE-NMe(18:1(9Z)/18:1(11Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113010	PE-NMe(14:1(9Z)/22:1(13Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113089	PE-NMe(18/18:2(9Z,12Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113169	PE-NMe(18:2(9Z,12Z)/18)	C42H80NO8P	M+H	758.5694	-1.0
HMDB0114241	PE-NMe2(:2(11Z,14Z)/15)	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113925	PE-NMe2(15/:2(11Z,14Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113340	PE-NMe(:2(11Z,14Z)/16)	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113047	PE-NMe(16/:2(11Z,14Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113563	PE-NMe(22:2(13Z,16Z)/14)	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113536	PE-NMe(22:1(13Z)/14:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113312	PE-NMe(:1(11Z)/16:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0112968	PE-NMe(18:1(11Z)/18:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0112969	PE-NMe(18:1(11Z)/18:1(11Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0112966	PE-NMe(16:1(9Z)/:1(11Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0010565	PE-NMe(18:1(9Z)/18:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0009549	PE(22:2(13Z,16Z)/15)	C42H80NO8P	M+H	758.5694	-1.0
HMDB0007880	PC(14/:2(11Z,14Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0007912	PC(14:1(9Z)/:1(11Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0007973	PC(16/18:2(9Z,12Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0008005	PC(16:1(9Z)/18:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0008004	PC(16:1(9Z)/18:1(11Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0008068	PC(18:1(11Z)/16:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0008909	PE(15/22:2(13Z,16Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0008328	PC(:2(11Z,14Z)/14)	C42H80NO8P	M+H	758.5694	-1.0
HMDB0008296	PC(:1(11Z)/14:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0

HMDB0008133	PC(18:2(9Z,12Z)/16)	C42H80NO8P	M+H	758.5694	-1.0
HMDB0008101	PC(18:1(9Z)/16:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0112992	PE-NMe(14/22:2(13Z,16Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0112967	PE-NMe(18:1(9Z)/18:1(11Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113010	PE-NMe(14:1(9Z)/22:1(13Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113089	PE-NMe(18/18:2(9Z,12Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113169	PE-NMe(18:2(9Z,12Z)/18)	C42H80NO8P	M+H	758.5694	-1.0
HMDB0114241	PE-NMe2(:2(11Z,14Z)/15)	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113925	PE-NMe2(15/:2(11Z,14Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113340	PE-NMe(:2(11Z,14Z)/16)	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113047	PE-NMe(16/:2(11Z,14Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113563	PE-NMe(22:2(13Z,16Z)/14)	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113536	PE-NMe(22:1(13Z)/14:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0113312	PE-NMe(:1(11Z)/16:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0112968	PE-NMe(18:1(11Z)/18:1(9Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0112969	PE-NMe(18:1(11Z)/18:1(11Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0112966	PE-NMe(16:1(9Z)/:1(11Z))	C42H80NO8P	M+H	758.5694	-1.0
HMDB0138304	6-{2-[6-(2,4-dihydroxybenzoyl)-5-{4-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-2,6-dihydroxyphenyl}-3-methylcyclohex-3-en-1-yl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H38O15	M+H	759.2283	0.9
HMDB0138301	6-{4-[6-(2,4-dihydroxyphenyl)-2-{4-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-2,6-dihydroxyphenyl}-4-methylcyclohex-3-ene-1-carbonyl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H38O15	M+H	759.2283	0.9
HMDB0138303	6-{4-[6-(2,4-dihydroxybenzoyl)-5-{4-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-2,6-dihydroxyphenyl}-3-methylcyclohex-3-en-1-yl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H38O15	M+H	759.2283	0.9
HMDB0138300	6-{2-[(E)-2-{4-[6-(2,4-dihydroxybenzoyl)-5-(2,4-dihydroxyphenyl)-3-methylcyclohex-2-en-1-yl]-3,5-dihydroxyphenyl}ethenyl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H38O15	M+H	759.2283	0.9
HMDB0138302	6-{2-[6-(2,4-dihydroxyphenyl)-2-{4-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-2,6-dihydroxyphenyl}-4-methylcyclohex-3-ene-1-carbonyl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H38O15	M+H	759.2283	0.9
HMDB0138298	6-{2-[6-(2,4-dihydroxybenzoyl)-5-(2,4-dihydroxyphenyl)-3-methylcyclohex-2-en-1-yl]-5-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H38O15	M+H	759.2283	0.9
HMDB0138299	6-{4-[(E)-2-{4-[6-(2,4-dihydroxybenzoyl)-5-(2,4-dihydroxyphenyl)-3-methylcyclohex-2-en-1-yl]-3,5-dihydroxyphenyl}ethenyl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H38O15	M+H	759.2283	0.9

	HMDB0138304	6-{2-[6-(2,4-dihydroxybenzoyl)-5-{4-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-2,6-dihydroxyphenyl}-3-methylcyclohex-3-en-1-yl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H38O15	M+H	759.2283	0.9
	HMDB0138301	6-{4-[6-(2,4-dihydroxyphenyl)-2-{4-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-2,6-dihydroxyphenyl}-4-methylcyclohex-3-ene-1-carbonyl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H38O15	M+H	759.2283	0.9
	HMDB0138303	6-{4-[6-(2,4-dihydroxybenzoyl)-5-{4-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-2,6-dihydroxyphenyl}-3-methylcyclohex-3-en-1-yl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H38O15	M+H	759.2283	0.9
	HMDB0138300	6-{2-[(E)-2-{4-[6-(2,4-dihydroxybenzoyl)-5-(2,4-dihydroxyphenyl)-3-methylcyclohex-2-en-1-yl]-3,5-dihydroxyphenyl}ethenyl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H38O15	M+H	759.2283	0.9
	HMDB0138302	6-{2-[6-(2,4-dihydroxyphenyl)-2-{4-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-2,6-dihydroxyphenyl}-4-methylcyclohex-3-ene-1-carbonyl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H38O15	M+H	759.2283	0.9
	HMDB0138298	6-{2-[6-(2,4-dihydroxybenzoyl)-5-(2,4-dihydroxyphenyl)-3-methylcyclohex-2-en-1-yl]-5-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H38O15	M+H	759.2283	0.9
	HMDB0138299	6-{4-[(E)-2-{4-[6-(2,4-dihydroxybenzoyl)-5-(2,4-dihydroxyphenyl)-3-methylcyclohex-2-en-1-yl]-3,5-dihydroxyphenyl}ethenyl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H38O15	M+H	759.2283	0.9
759.3883	HMDB0031227	Marshdimerin	C48H54O8	M+H	759.3891	-1.1
	HMDB0031227	Marshdimerin	C48H54O8	M+H	759.3891	-1.1
	HMDB0007879	PC(14:1(11Z))	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0007911	PC(14:1(9Z)/)	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0007971	PC(16/18:1(11Z))	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0007972	PC(16/18:1(9Z))	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0008003	PC(16:1(9Z)/18)	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0008035	PC(18/16:1(9Z))	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0008067	PC(18:1(11Z)/16)	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0008100	PC(18:1(9Z)/16)	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0008263	PC(/14:1(9Z))	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0008295	PC(:1(11Z)/14)	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0008908	PE(15/22:1(13Z))	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0009516	PE(22:1(13Z)/15)	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0113864	PE-NMe2(15/:1(11Z))	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0112974	PE-NMe(16:1(9Z)/)	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0114212	PE-NMe2(:1(11Z)/15)	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0113535	PE-NMe(22:1(13Z)/14)	C42H82NO8P	M+H	760.5851	-1.3

760.5841

HMDB0113509	PE-NMe(22/14:1(9Z))	C42H82NO8P	M+H	760.5851	-1.3
HMDB0113311	PE-NMe(:1(11Z)/16)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0113283	PE-NMe(/16:1(9Z))	C42H82NO8P	M+H	760.5851	-1.3
HMDB0113142	PE-NMe(18:1(9Z)/18)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0113115	PE-NMe(18:1(11Z)/18)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0112991	PE-NMe(14/22:1(13Z))	C42H82NO8P	M+H	760.5851	-1.3
HMDB0112972	PE-NMe(14:1(9Z)/22)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0112973	PE-NMe(16/:1(11Z))	C42H82NO8P	M+H	760.5851	-1.3
HMDB0112971	PE-NMe(18/18:1(11Z))	C42H82NO8P	M+H	760.5851	-1.3
HMDB0112970	PE-NMe(18/18:1(9Z))	C42H82NO8P	M+H	760.5851	-1.3
HMDB0007879	PC(14/:1(11Z))	C42H82NO8P	M+H	760.5851	-1.3
HMDB0007911	PC(14:1(9Z)/)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0007971	PC(16/18:1(11Z))	C42H82NO8P	M+H	760.5851	-1.3
HMDB0007972	PC(16/18:1(9Z))	C42H82NO8P	M+H	760.5851	-1.3
HMDB0008003	PC(16:1(9Z)/18)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0008035	PC(18/16:1(9Z))	C42H82NO8P	M+H	760.5851	-1.3
HMDB0008067	PC(18:1(11Z)/16)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0008100	PC(18:1(9Z)/16)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0008263	PC(/14:1(9Z))	C42H82NO8P	M+H	760.5851	-1.3
HMDB0008295	PC(:1(11Z)/14)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0008908	PE(15/22:1(13Z))	C42H82NO8P	M+H	760.5851	-1.3
HMDB0009516	PE(22:1(13Z)/15)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0113864	PE-NMe2(15/:1(11Z))	C42H82NO8P	M+H	760.5851	-1.3
HMDB0112974	PE-NMe(16:1(9Z)/)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0114212	PE-NMe2(:1(11Z)/15)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0113535	PE-NMe(22:1(13Z)/14)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0113509	PE-NMe(22/14:1(9Z))	C42H82NO8P	M+H	760.5851	-1.3
HMDB0113311	PE-NMe(:1(11Z)/16)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0113283	PE-NMe(/16:1(9Z))	C42H82NO8P	M+H	760.5851	-1.3
HMDB0113142	PE-NMe(18:1(9Z)/18)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0113115	PE-NMe(18:1(11Z)/18)	C42H82NO8P	M+H	760.5851	-1.3
HMDB0112991	PE-NMe(14/22:1(13Z))	C42H82NO8P	M+H	760.5851	-1.3

	HMDB0112972	PE-NMe(14:1(9Z)/22)	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0112973	PE-NMe(16:1(11Z))	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0112971	PE-NMe(18/18:1(11Z))	C42H82NO8P	M+H	760.5851	-1.3
	HMDB0112970	PE-NMe(18/18:1(9Z))	C42H82NO8P	M+H	760.5851	-1.3
761.1826	HMDB0170489	6-({14-chloro-5-hydroxy-2,9,26-trimethyl-4,,22,29-tetraoxo-3,19,23,28-tetraoxaocetacyclo[16.9.1.1?,,??,nonacos-11-en-15-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H39ClO16	M+Na	761.1819	0.9
	HMDB0170490	6-({14-chloro-15-hydroxy-2,9,26-trimethyl-4,,22,29-tetraoxo-3,19,23,28-tetraoxaocetacyclo[16.9.1.1?,,??,nonacos-11-en-5-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H39ClO16	M+Na	761.1819	0.9
	HMDB0170489	6-({14-chloro-5-hydroxy-2,9,26-trimethyl-4,,22,29-tetraoxo-3,19,23,28-tetraoxaocetacyclo[16.9.1.1?,,??,nonacos-11-en-15-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H39ClO16	M+Na	761.1819	0.9
	HMDB0170490	6-({14-chloro-15-hydroxy-2,9,26-trimethyl-4,,22,29-tetraoxo-3,19,23,28-tetraoxaocetacyclo[16.9.1.1?,,??,nonacos-11-en-5-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H39ClO16	M+Na	761.1819	0.9
762.3747	HMDB0176206	4,6a,6b,11,11,14b-hexamethyl-2-(sulfooxy)-3-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricene-4,8a-dicarboxylic acid	C36H56O14S	M+NH4	762.3729	2.4
	HMDB0177771	11-hydroxy-2-(methoxycarbonyl)-2,6a,6b,9,12a-pentamethyl-9-[(sulfooxy)methyl]--[(3,4,5-trihydroxyoxan-2-yl)oxy]-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C36H56O14S	M+NH4	762.3729	2.4
	HMDB0177772	-{[4,5-dihydroxy-3-(sulfooxy)oxan-2-yl]oxy}-11-hydroxy-9-(hydroxymethyl)-2-(methoxycarbonyl)-2,6a,6b,9,12a-pentamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C36H56O14S	M+NH4	762.3729	2.4
	HMDB0177775	9-(hydroxymethyl)-2-(methoxycarbonyl)-2,6a,6b,9,12a-pentamethyl-11-(sulfooxy)--[(3,4,5-trihydroxyoxan-2-yl)oxy]-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C36H56O14S	M+NH4	762.3729	2.4
	HMDB0177773	-{[3,5-dihydroxy-4-(sulfooxy)oxan-2-yl]oxy}-11-hydroxy-9-(hydroxymethyl)-2-(methoxycarbonyl)-2,6a,6b,9,12a-pentamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C36H56O14S	M+NH4	762.3729	2.4
	HMDB0177774	-{[3,4-dihydroxy-5-(sulfooxy)oxan-2-yl]oxy}-11-hydroxy-9-(hydroxymethyl)-2-(methoxycarbonyl)-2,6a,6b,9,12a-pentamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C36H56O14S	M+NH4	762.3729	2.4
	HMDB0010576	PG(16/18:3(6Z,9Z,12Z))	C40H73O10P	M+NH4	762.5280	-0.3
	HMDB0010577	PG(16/18:3(9Z,12Z,15Z))	C40H73O10P	M+NH4	762.5280	-0.3
	HMDB0010590	PG(16:1(9Z)/18:2(9Z,12Z))	C40H73O10P	M+NH4	762.5280	-0.3
	HMDB0010646	PG(18:2(9Z,12Z)/16:1(9Z))	C40H73O10P	M+NH4	762.5280	-0.3
	HMDB0010660	PG(18:3(6Z,9Z,12Z)/16)	C40H73O10P	M+NH4	762.5280	-0.3
	HMDB0010675	Pg(18:3(9z,12z,15z)/16)	C40H73O10P	M+NH4	762.5280	-0.3

762.5277	HMDB0112274	PS(14:1(11Z))	C40H76NO10P	M+H	762.5280	-0.3
	HMDB0112277	PS(14:1(9Z)/)	C40H76NO10P	M+H	762.5280	-0.3
	HMDB0112512	PS(/14:1(9Z))	C40H76NO10P	M+H	762.5280	-0.3
	HMDB0112540	PS(:1(11Z)/14)	C40H76NO10P	M+H	762.5280	-0.3
	HMDB0012377	PS(18/16:1(9Z))	C40H76NO10P	M+H	762.5280	-0.3
	HMDB0012387	PS(18:1(9Z)/16)	C40H76NO10P	M+H	762.5280	-0.3
	HMDB0012357	PS(16/18:1(9Z))	C40H76NO10P	M+H	762.5280	-0.3
	HMDB0112267	PS(16/18:1(11Z))	C40H76NO10P	M+H	762.5280	-0.3
	HMDB0112270	PS(18:1(11Z)/16)	C40H76NO10P	M+H	762.5280	-0.3
	HMDB0012367	PS(16:1(9Z)/18)	C40H76NO10P	M+H	762.5280	-0.3
	HMDB0162324	3,4,5-trihydroxy-6-[(7-hydroxy--{5-hydroxy-8,-dimethoxy-2-methyl-4-oxo-4H-benzo[h]chromen-6-yl}-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-5-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
	HMDB0162326	3,4,5-trihydroxy-6-[(9-hydroxy-6-{5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl}-8,-dimethoxy-2-methyl-4-oxo-4H-benzo[h]chromen-5-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
	HMDB0162327	6-[-{5,9-dihydroxy-8,-dimethoxy-2-methyl-4-oxo-4H-benzo[h]chromen-6-yl}-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-5-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
	HMDB0162340	3,4,5-trihydroxy-6-[(6-{5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl}-2-(hydroxymethyl)-8,-dimethoxy-4-oxo-4H-benzo[h]chromen-5-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
	HMDB0162341	3,4,5-trihydroxy-6-(-{5-hydroxy-2-(hydroxymethyl)-8,-dimethoxy-4-oxo-4H-benzo[h]chromen-6-yl}-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-5-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
	HMDB0162344	3,4,5-trihydroxy-6-[-(5-hydroxy-8,-dimethoxy-2-methyl-4-oxo-4H-benzo[h]chromen-6-yl)-2-(hydroxymethyl)-6,8-dimethoxy-4-oxo-4H-benzo[g]chromen-5-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
	HMDB0162343	3,4,5-trihydroxy-6-({6-[5-hydroxy-2-(hydroxymethyl)-6,8-dimethoxy-4-oxo-4H-benzo[g]chromen--yl]-8,-dimethoxy-2-methyl-4-oxo-4H-benzo[h]chromen-5-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
	HMDB0168101	3,4,5-trihydroxy-6-[(5-hydroxy--{5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-7-yl}-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-7-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
	HMDB0168103	3,4,5-trihydroxy-6-[(7-hydroxy--{5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-7-yl}-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-5-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
	HMDB0168102	6-[(7-{5,7-dihydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl}-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-5-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
	HMDB0168113	3,4,5-trihydroxy-6-[(7-{5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl}-2-(hydroxymethyl)-6,8-dimethoxy-4-oxo-4H-benzo[g]chromen-5-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3

763.1879

HMDB0168114	3,4,5-trihydroxy-6-((-[5-hydroxy-2-(hydroxymethyl)-6,8-dimethoxy-4-oxo-4H-benzo[g]chromen-7-yl]-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-5-yl)oxy)oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
HMDB0168117	3,4,5-trihydroxy-6-((-[5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-7-yl]-2-(hydroxymethyl)-6,8-dimethoxy-4-oxo-4H-benzo[g]chromen-5-yl)oxy)oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
HMDB0162325	3,4,5-trihydroxy-6-[(5-hydroxy-6-{5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl})-8,-dimethoxy-2-methyl-4-oxo-4H-benzo[h]chromen-9-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
HMDB0162323	6-[(6-{5,7-dihydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl})-8,-dimethoxy-2-methyl-4-oxo-4H-benzo[h]chromen-5-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
HMDB0162210	3,4,5-trihydroxy-6-[(6-hydroxy--{6-hydroxy-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-7-yl})-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-7-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
HMDB0162211	6-[(7-{6,7-dihydroxy-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl})-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-6-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
HMDB0162212	3,4,5-trihydroxy-6-[(7-hydroxy--{6-hydroxy-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-7-yl})-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-6-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
HMDB0162225	3,4,5-trihydroxy-6-[(7-{6-hydroxy-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl})-2-(hydroxymethyl)-5,8-dimethoxy-4-oxo-4H-benzo[g]chromen-6-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
HMDB0162226	3,4,5-trihydroxy-6-((-[6-hydroxy-2-(hydroxymethyl)-5,8-dimethoxy-4-oxo-4H-benzo[g]chromen-7-yl]-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-6-yl)oxy)oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
HMDB0162228	3,4,5-trihydroxy-6-((7-[6-hydroxy-2-(hydroxymethyl)-5,8-dimethoxy-4-oxo-4H-benzo[g]chromen--yl]-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-6-yl)oxy)oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
HMDB0162229	3,4,5-trihydroxy-6-((-[6-hydroxy-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-7-yl]-2-(hydroxymethyl)-5,8-dimethoxy-4-oxo-4H-benzo[g]chromen-6-yl)oxy)oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
HMDB0162269	3,4,5-trihydroxy-6-[(7-hydroxy--{5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl})-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-5-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
HMDB0162268	6-[(5-{5,7-dihydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl})-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-5-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
HMDB0162267	3,4,5-trihydroxy-6-[(5-hydroxy--{5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl})-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-7-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
HMDB0162277	3,4,5-trihydroxy-6-((-[5-hydroxy-2-(hydroxymethyl)-6,8-dimethoxy-4-oxo-4H-benzo[g]chromen--yl]-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-5-yl)oxy)oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
HMDB0162276	3,4,5-trihydroxy-6-((-[5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl]-2-(hydroxymethyl)-6,8-dimethoxy-4-oxo-4H-benzo[g]chromen-5-yl)oxy)oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3

	HMDB0162322	3,4,5-trihydroxy-6-[(5-hydroxy--{5-hydroxy-8,-dimethoxy-2-methyl-4-oxo-4H-benzo[h]chromen-6-yl}-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-7-yl)oxy]oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
	HMDB0168116	3,4,5-trihydroxy-6-({7-[5-hydroxy-2-(hydroxymethyl)-6,8-dimethoxy-4-oxo-4H-benzo[g]chromen--yl]-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-5-yl}oxy)oxane-2-carboxylic acid	C38H34O17	M+H	763.1869	1.3
763.4331	HMDB0115051	PA(18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H65O8P	M+Na	763.4309	2.9
	HMDB0115214	PA(:5(5Z,8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H65O8P	M+Na	763.4309	2.9
	HMDB0115412	PA(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C43H65O8P	M+Na	763.4309	2.9
763.5942	HMDB0007938	PC(15/18:1(11Z))	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0007939	PC(15/18:1(9Z))	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0008066	PC(18:1(11Z)/15)	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0008099	PC(18:1(9Z)/15)	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0008842	PE(14/22:1(13Z))	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0008874	PE(14:1(9Z)/22)	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0008933	PE(16/:1(11Z))	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0008965	PE(16:1(9Z)/)	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0008992	PE(18/18:1(11Z))	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0010568	PE-NMe2(16/18:1(9Z))	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0009514	PE(22:1(13Z)/14)	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0009482	PE(22/14:1(9Z))	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0009253	PE(:1(11Z)/16)	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0009221	PE(/16:1(9Z))	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0009024	PE(18:1(11Z)/18)	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0113863	PE-NMe2(16:1(9Z)/18)	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0113862	PE-NMe2(16/18:1(11Z))	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0113861	PE-NMe2(14:1(9Z)/)	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0113310	PE-NMe(:1(11Z)/15)	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0114210	PE-NMe2(:1(11Z)/14)	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0114182	PE-NMe2(/14:1(9Z))	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0114041	PE-NMe2(18:1(9Z)/16)	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0114014	PE-NMe2(18:1(11Z)/16)	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0113989	PE-NMe2(18/16:1(9Z))	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0113859	PE-NMe2(14/:1(11Z))	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0009057	PE(18:1(9Z)/18)	C41H80NO8P	M+NH4	763.5960	-2.3

	HMDB0112963	PE-NMe(15/1(11Z))	C41H80NO8P	M+NH4	763.5960	-2.3
	HMDB0008993	PE(18/18:1(9Z))	C41H80NO8P	M+NH4	763.5960	-2.3
764.0940	HMDB0187603	3,4,5-trihydroxy-6-([4-hydroxy-5-([hydroxy([hydroxy([3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})phosphoryl]oxy})phosphoryl]oxy)methyl)-2-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-3-yl]oxy}oxane-2-carboxylic acid	C21H33N3O2 2P2	M+Na	764.0923	2.2
	HMDB0187606	6-{[2-([([3,4-dihydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy)(hydroxy)phosphoryl]oxy}-3,5-dihydroxy-6-(hydroxymethyl)oxan-4-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H33N3O2 2P2	M+Na	764.0923	2.2
	HMDB0187604	3,4,5-trihydroxy-6-([4-hydroxy-2-([hydroxy([hydroxy([3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})phosphoryl]oxy})phosphoryl]oxy)methyl)-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-3-yl]oxy}oxane-2-carboxylic acid	C21H33N3O2 2P2	M+Na	764.0923	2.2
	HMDB0187605	6-{[2-([([3,4-dihydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy)(hydroxy)phosphoryl]oxy}-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H33N3O2 2P2	M+Na	764.0923	2.2
	HMDB0187607	6-{[6-([([3,4-dihydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy)(hydroxy)phosphoryl]oxy}-4,5-dihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H33N3O2 2P2	M+Na	764.0923	2.2
	HMDB0187608	6-{[6-([([3,4-dihydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy)(hydroxy)phosphoryl]oxy}-3,4,5-trihydroxyoxan-2-yl]methoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H33N3O2 2P2	M+Na	764.0923	2.2
	HMDB0187609	6-([1-[3,4-dihydroxy-5-([hydroxy([hydroxy([3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})phosphoryl]oxy})phosphoryl]oxy)methyl)oxolan-2-yl]-2-hydroxy-1,4-dihydropyrimidin-4-ylidene)amino)-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H33N3O2 2P2	M+Na	764.0923	2.2
764.2349	HMDB0126283	({4-[2,4-dihydroxy-3-(3-methylbut-2-en-1-yl)benzoyl]-5-(2,4-dihydroxyphenyl)-3-{4-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-2,6-dihydroxyphenyl}cyclohex-1-en-1-yl]methoxy)sulfonic acid	C39H38O13S	M+NH4	764.2371	-2.9
	HMDB0126291	{5-[2,4-dihydroxy-3-(3-methylbut-2-en-1-yl)benzoyl]-6-(2,4-dihydroxyphenyl)-4-{4-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-2,6-dihydroxyphenyl}-2-methylcyclohex-2-en-1-yl}oxidanesulfonic acid	C39H38O13S	M+NH4	764.2371	-2.9
	HMDB0126299	[(4-{3-[6-(2,4-dihydroxyphenyl)-2-{4-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-2,6-dihydroxyphenyl}-4-methylcyclohex-3-ene-1-carbonyl]-2,6-dihydroxyphenyl}-2-methylbut-2-en-1-yl)oxy]sulfonic acid	C39H38O13S	M+NH4	764.2371	-2.9
	HMDB0126306	{[(2E)-4-{3-[6-(2,4-dihydroxyphenyl)-2-{4-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-2,6-dihydroxyphenyl}-4-methylcyclohex-3-ene-1-carbonyl]-2,6-dihydroxyphenyl}-2-methylbut-2-en-1-yl]oxy}sulfonic acid	C39H38O13S	M+NH4	764.2371	-2.9

764.3864	HMDB0175672	[,11-dihydroxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-4a-({[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}carbonyl)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-1-yl]oxidanesulfonic acid	C36H58O14S	M+NH4	764.3886	-2.8
	HMDB0175671	{[2,3,12-trihydroxy-4,6a,6b,11,11,14b-hexamethyl-8a-({[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}carbonyl)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-4-yl]methoxy}sulfonic acid	C36H58O14S	M+NH4	764.3886	-2.8
	HMDB0175674	[3,12-dihydroxy-4-(hydroxymethyl)-4,6a,6b,11,11,14b-hexamethyl-8a-({[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}carbonyl)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-2-yl]oxidanesulfonic acid	C36H58O14S	M+NH4	764.3886	-2.8
	HMDB0175673	[2,12-dihydroxy-4-(hydroxymethyl)-4,6a,6b,11,11,14b-hexamethyl-8a-({[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}carbonyl)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-3-yl]oxidanesulfonic acid	C36H58O14S	M+NH4	764.3886	-2.8
	HMDB0114918	PA(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0114943	PA(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0114969	PA(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0114994	PA(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115021	PA(18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115133	PA(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115408	PA(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115407	PA(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115501	PA(:4(8Z,11Z,14Z,17Z)/:3(8Z,11Z,14Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115575	PA(:3(8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115499	PA(:4(5Z,8Z,11Z,14Z)/:3(8Z,11Z,14Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115550	PA(:2(11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0114968	PA(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115576	PA(:3(8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115587	PA(:5(5Z,8Z,11Z,14Z,17Z)/:2(11Z,14Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115332	PA(22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115383	PA(22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115158	PA(:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115357	PA(22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115185	PA(:4(8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0116707	PA(22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0115134	PA(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C43H71O8P	M+NH4	764.5225	-2.1
	HMDB0009359	PE(:3(8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C43H74NO8P	M+H	764.5225	-2.1
	HMDB0009650	PE(22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C43H74NO8P	M+H	764.5225	-2.1
	HMDB0009358	PE(:3(8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C43H74NO8P	M+H	764.5225	-2.1
	HMDB0009390	PE(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C43H74NO8P	M+H	764.5225	-2.1
	HMDB0009423	PE(:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C43H74NO8P	M+H	764.5225	-2.1
	HMDB0009455	PE(:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C43H74NO8P	M+H	764.5225	-2.1
	HMDB0009454	PE(:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C43H74NO8P	M+H	764.5225	-2.1
	HMDB0009617	PE(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C43H74NO8P	M+H	764.5225	-2.1
	HMDB0113675	PE-NMe(22:6(4Z,7Z,Z,13Z,16Z,19Z)/15)	C43H74NO8P	M+H	764.5225	-2.1
	HMDB0009326	PE(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C43H74NO8P	M+H	764.5225	-2.1
	HMDB0009325	PE(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C43H74NO8P	M+H	764.5225	-2.1

764.5209

HMDB0008946	PE(16:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0008978	PE(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0008977	PE(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0009038	PE(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0009071	PE(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0009102	PE(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0009103	PE(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0009133	PE(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0009134	PE(18:3(6Z,9Z,12Z)/:3(8Z,11Z,14Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0009167	PE(18:3(9Z,12Z,15Z)/:3(8Z,11Z,14Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0009198	PE(18:4(6Z,9Z,12Z,15Z)/:2(11Z,14Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0009294	PE(:2(11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0009166	PE(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0114076	PE-NMe2(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0114104	PE-NMe2(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0114103	PE-NMe2(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0114133	PE-NMe2(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0114132	PE-NMe2(18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0114160	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0114385	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/16:1(9Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0114524	PE-NMe2(22:5(4Z,7Z,Z,13Z,16Z)/14:1(9Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0114550	PE-NMe2(22:5(7Z,Z,13Z,16Z,19Z)/14:1(9Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0114576	PE-NMe2(22:6(4Z,7Z,Z,13Z,16Z,19Z)/14)	C43H74NO8P	M+H	764.5225	-2.1
HMDB0113975	PE-NMe2(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0113914	PE-NMe2(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0113913	PE-NMe2(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0009682	PE(22:6(4Z,7Z,Z,13Z,16Z,19Z)/16)	C43H74NO8P	M+H	764.5225	-2.1
HMDB0113036	PE-NMe(15:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0113896	PE-NMe2(14:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H74NO8P	M+H	764.5225	-2.1
HMDB0113966	PE-NMe2(16:1(9Z)/18:2(9Z,12Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0114069	PE-NMe2(18:2(9Z,12Z)/16:1(9Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0114097	PE-NMe2(18:3(6Z,9Z,12Z)/16)	C41H76NO8P	M+Na	764.5201	1.1

HMDB0114126	PE-NMe2(18:3(9Z,12Z,15Z)/16)	C41H76NO8P	M+Na	764.5201	1.1
HMDB0114268	PE-NMe2(:3(5Z,8Z,11Z)/14)	C41H76NO8P	M+Na	764.5201	1.1
HMDB0114296	PE-NMe2(:3(8Z,11Z,14Z)/14)	C41H76NO8P	M+Na	764.5201	1.1
HMDB0113904	PE-NMe2(14:1(9Z):2(11Z,14Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0114240	PE-NMe2(:2(11Z,14Z)/14:1(9Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0113945	PE-NMe2(16/18:3(9Z,12Z,15Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0113944	PE-NMe2(16/18:3(6Z,9Z,12Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0113886	PE-NMe2(14/:3(8Z,11Z,14Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0113027	PE-NMe(15/:3(8Z,11Z,14Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0113026	PE-NMe(15/:3(5Z,8Z,11Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0113368	PE-NMe(:3(5Z,8Z,11Z)/15)	C41H76NO8P	M+Na	764.5201	1.1
HMDB0113396	PE-NMe(:3(8Z,11Z,14Z)/15)	C41H76NO8P	M+Na	764.5201	1.1
HMDB0113885	PE-NMe2(14/:3(5Z,8Z,11Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0009123	PE(18:3(6Z,9Z,12Z)/18)	C41H76NO8P	M+Na	764.5201	1.1
HMDB0009548	PE(22:2(13Z,16Z)/14:1(9Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0009092	PE(18:2(9Z,12Z)/18:1(9Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0009091	PE(18:2(9Z,12Z)/18:1(11Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0009060	PE(18:1(9Z)/18:2(9Z,12Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0009027	PE(18:1(11Z)/18:2(9Z,12Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0008995	PE(18/18:3(6Z,9Z,12Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0008996	PE(18/18:3(9Z,12Z,15Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0008967	PE(16:1(9Z):2(11Z,14Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0009156	PE(18:3(9Z,12Z,15Z)/18)	C41H76NO8P	M+Na	764.5201	1.1
HMDB0008935	PE(16/:3(5Z,8Z,11Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0007942	PC(15/18:3(9Z,12Z,15Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0007941	PC(15/18:3(6Z,9Z,12Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0008165	PC(18:3(6Z,9Z,12Z)/15)	C41H76NO8P	M+Na	764.5201	1.1
HMDB0008198	PC(18:3(9Z,12Z,15Z)/15)	C41H76NO8P	M+Na	764.5201	1.1
HMDB0008876	PE(14:1(9Z)/22:2(13Z,16Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0009319	PE(:3(5Z,8Z,11Z)/16)	C41H76NO8P	M+Na	764.5201	1.1
HMDB0008936	PE(16/:3(8Z,11Z,14Z))	C41H76NO8P	M+Na	764.5201	1.1
HMDB0009352	PE(:3(8Z,11Z,14Z)/16)	C41H76NO8P	M+Na	764.5201	1.1

	HMDB0009287	PE(:2(11Z,14Z)/16:1(9Z))	C41H76NO8P	M+Na	764.5201	1.1
764.5595	HMDB0011313	PC(P-18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C44H78NO7P	M+H	764.5589	0.8
	HMDB0011280	PC(P-18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C44H78NO7P	M+H	764.5589	0.8
	HMDB0011222	PC(P-16/:5(5Z,8Z,11Z,14Z,17Z))	C44H78NO7P	M+H	764.5589	0.8
	HMDB0008521	PC(:5(5Z,8Z,11Z,14Z,17Z)/P-16)	C44H78NO7P	M+H	764.5589	0.8
	HMDB0008261	PC(18:4(6Z,9Z,12Z,15Z)/P-18:1(9Z))	C44H78NO7P	M+H	764.5589	0.8
	HMDB0008260	PC(18:4(6Z,9Z,12Z,15Z)/P-18:1(11Z))	C44H78NO7P	M+H	764.5589	0.8
765.5630	HMDB0116381	(2S)-1- {[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate	C46H78O7	M+Na	765.5640	-1.3
	HMDB0116374	(2S)-1- {[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C46H78O7	M+Na	765.5640	-1.3
	HMDB0116397	(2S)-1-hydroxy-3- {[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C46H78O7	M+Na	765.5640	-1.3
	HMDB0116407	(2S)-3-hydroxy-2- {[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C46H78O7	M+Na	765.5640	-1.3
	HMDB0116413	(2S)-3-hydroxy-2- {[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C46H78O7	M+Na	765.5640	-1.3
	HMDB0116414	(2S)-2- {[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C46H78O7	M+Na	765.5640	-1.3
	HMDB0116436	(2S)-1- {[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C46H78O7	M+Na	765.5640	-1.3
	HMDB0116444	(2S)-1-hydroxy-3- {[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C46H78O7	M+Na	765.5640	-1.3
	HMDB0116391	(2S)-1-hydroxy-3- {[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C46H78O7	M+Na	765.5640	-1.3
	HMDB0116688	PG(i-13/i-22)	C41H81O10P	M+H	765.5640	-1.3
	HMDB0116652	PG(a-13/i-22)	C41H81O10P	M+H	765.5640	-1.3
	HMDB0114068	PE-NMe2(18:2(9Z,12Z)/16)	C41H78NO8P	M+Na	766.5357	2.8
	HMDB0113858	PE-NMe2(16:1(9Z)/18:1(11Z))	C41H78NO8P	M+Na	766.5357	2.8
	HMDB0113339	PE-NMe(:2(11Z,14Z)/15)	C41H78NO8P	M+Na	766.5357	2.8
	HMDB0113884	PE-NMe2(14/:2(11Z,14Z))	C41H78NO8P	M+Na	766.5357	2.8
	HMDB0114239	PE-NMe2(:2(11Z,14Z)/14)	C41H78NO8P	M+Na	766.5357	2.8
	HMDB0113856	PE-NMe2(14:1(9Z)/:1(11Z))	C41H78NO8P	M+Na	766.5357	2.8
	HMDB0114211	PE-NMe2(:1(11Z)/14:1(9Z))	C41H78NO8P	M+Na	766.5357	2.8
	HMDB0114042	PE-NMe2(18:1(9Z)/16:1(9Z))	C41H78NO8P	M+Na	766.5357	2.8
	HMDB0114015	PE-NMe2(18:1(11Z)/16:1(9Z))	C41H78NO8P	M+Na	766.5357	2.8
	HMDB0113943	PE-NMe2(16/18:2(9Z,12Z))	C41H78NO8P	M+Na	766.5357	2.8

HMDB0113025	PE-NMe(15/:2(11Z,14Z))	C41H78NO8P	M+Na	766.5357	2.8
HMDB0007940	PC(15/18:2(9Z,12Z))	C41H78NO8P	M+Na	766.5357	2.8
HMDB0009547	PE(22:2(13Z,16Z)/14)	C41H78NO8P	M+Na	766.5357	2.8
HMDB0009515	PE(22:1(13Z)/14:1(9Z))	C41H78NO8P	M+Na	766.5357	2.8
HMDB0008132	PC(18:2(9Z,12Z)/15)	C41H78NO8P	M+Na	766.5357	2.8
HMDB0008843	PE(14/22:2(13Z,16Z))	C41H78NO8P	M+Na	766.5357	2.8
HMDB0008875	PE(14:1(9Z)/22:1(13Z))	C41H78NO8P	M+Na	766.5357	2.8
HMDB0008934	PE(16/:2(11Z,14Z))	C41H78NO8P	M+Na	766.5357	2.8
HMDB0008966	PE(16:1(9Z)/:1(11Z))	C41H78NO8P	M+Na	766.5357	2.8
HMDB0008994	PE(18/18:2(9Z,12Z))	C41H78NO8P	M+Na	766.5357	2.8
HMDB0009025	PE(18:1(11Z)/18:1(11Z))	C41H78NO8P	M+Na	766.5357	2.8
HMDB0009026	PE(18:1(11Z)/18:1(9Z))	C41H78NO8P	M+Na	766.5357	2.8
HMDB0009058	PE(18:1(9Z)/18:1(11Z))	C41H78NO8P	M+Na	766.5357	2.8
HMDB0009059	PE(18:1(9Z)/18:1(9Z))	C41H78NO8P	M+Na	766.5357	2.8
HMDB0009090	PE(18:2(9Z,12Z)/18)	C41H78NO8P	M+Na	766.5357	2.8
HMDB0009254	PE(:1(11Z)/16:1(9Z))	C41H78NO8P	M+Na	766.5357	2.8
HMDB0113857	PE-NMe2(16:1(9Z)/18:1(9Z))	C41H78NO8P	M+Na	766.5357	2.8
HMDB0009286	PE(:2(11Z,14Z)/16)	C41H78NO8P	M+Na	766.5357	2.8
HMDB0114942	PA(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115496	PA(:3(8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0114916	PA(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0114893	PA(18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115497	PA(:3(8Z,11Z,14Z)/:3(8Z,11Z,14Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115498	PA(:4(5Z,8Z,11Z,14Z)/:2(11Z,14Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115381	PA(22:5(7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115500	PA(:4(8Z,11Z,14Z,17Z)/:2(11Z,14Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0114941	PA(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115406	PA(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18)	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115382	PA(22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115356	PA(22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0114967	PA(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115047	PA(18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115108	PA(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115132	PA(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115210	PA(:5(5Z,8Z,11Z,14Z,17Z)/:1(11Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115307	PA(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115331	PA(22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115355	PA(22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0114917	PA(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115494	PA(:3(5Z,8Z,11Z)/:3(8Z,11Z,14Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115548	PA(:2(11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0115549	PA(:2(11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C43H73O8P	M+NH4	766.5381	-0.3
HMDB0009100	PE(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0114075	PE-NMe2(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C43H76NO8P	M+H	766.5381	-0.3

766.5379

HMDB0113894	PE-NMe2(14/22:5(4Z,7Z,Z,13Z,16Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0113622	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/15)	C43H76NO8P	M+H	766.5381	-0.3
HMDB0113648	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/15)	C43H76NO8P	M+H	766.5381	-0.3
HMDB0114328	PE-NMe2(:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0113895	PE-NMe2(14/22:5(7Z,Z,13Z,16Z,19Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0113912	PE-NMe2(14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0113952	PE-NMe2(16/:5(5Z,8Z,11Z,14Z,17Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0113973	PE-NMe2(16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0113974	PE-NMe2(16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0114159	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0114020	PE-NMe2(18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0114047	PE-NMe2(18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0114158	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0114074	PE-NMe2(18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0114131	PE-NMe2(18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0114549	PE-NMe2(22:5(7Z,Z,13Z,16Z,19Z)/14)	C43H76NO8P	M+H	766.5381	-0.3
HMDB0114523	PE-NMe2(22:5(4Z,7Z,Z,13Z,16Z)/14)	C43H76NO8P	M+H	766.5381	-0.3
HMDB0112978	PE-NMe(15/22:5(7Z,Z,13Z,16Z,19Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0114496	PE-NMe2(22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0114384	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/16)	C43H76NO8P	M+H	766.5381	-0.3
HMDB0114356	PE-NMe2(:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0114102	PE-NMe2(18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0007951	PC(15/:5(5Z,8Z,11Z,14Z,17Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009261	PE(:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0113035	PE-NMe(15/22:5(4Z,7Z,Z,13Z,16Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009292	PE(:2(11Z,14Z)/18:3(6Z,9Z,12Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009293	PE(:2(11Z,14Z)/18:3(9Z,12Z,15Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009324	PE(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009357	PE(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009388	PE(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009389	PE(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009421	PE(:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C43H76NO8P	M+H	766.5381	-0.3

HMDB0009422	PE(:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009453	PE(:5(5Z,8Z,11Z,14Z,17Z)/18)	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009584	PE(22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009616	PE(22:5(4Z,7Z,Z,13Z,16Z)/16)	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009197	PE(18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009165	PE(18:3(9Z,12Z,15Z)/:2(11Z,14Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0008494	PC(:5(5Z,8Z,11Z,14Z,17Z)/15)	C43H76NO8P	M+H	766.5381	-0.3
HMDB0008944	PE(16/22:5(4Z,7Z,Z,13Z,16Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0008945	PE(16/22:5(7Z,Z,13Z,16Z,19Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0008976	PE(16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009005	PE(18/:5(5Z,8Z,11Z,14Z,17Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009036	PE(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009037	PE(18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009070	PE(18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009069	PE(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009101	PE(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009132	PE(18:3(6Z,9Z,12Z)/:2(11Z,14Z))	C43H76NO8P	M+H	766.5381	-0.3
HMDB0009649	PE(22:5(7Z,Z,13Z,16Z,19Z)/16)	C43H76NO8P	M+H	766.5381	-0.3
HMDB0007997	PC(16/P-18:1(9Z))	C42H82NO7P	M+Na	766.5721	2.2
HMDB0011305	PC(P-18:1(9Z)/16)	C42H82NO7P	M+Na	766.5721	2.2
HMDB0011272	PC(P-18:1(11Z)/16)	C42H82NO7P	M+Na	766.5721	2.2
HMDB0011240	PC(P-18/16:1(9Z))	C42H82NO7P	M+Na	766.5721	2.2
HMDB0011210	PC(P-16/18:1(9Z))	C42H82NO7P	M+Na	766.5721	2.2
HMDB0011209	PC(P-16/18:1(11Z))	C42H82NO7P	M+Na	766.5721	2.2
HMDB0011151	Pc(o-16/18:2(9z,12z))	C42H82NO7P	M+Na	766.5721	2.2
HMDB0008126	PC(18:1(9Z)/P-16)	C42H82NO7P	M+Na	766.5721	2.2
HMDB0008093	PC(18:1(11Z)/P-16)	C42H82NO7P	M+Na	766.5721	2.2
HMDB0008028	PC(16:1(9Z)/P-18)	C42H82NO7P	M+Na	766.5721	2.2
HMDB0007996	PC(16/P-18:1(11Z))	C42H82NO7P	M+Na	766.5721	2.2
HMDB0011311	PC(P-18:1(9Z)/18:3(6Z,9Z,12Z))	C44H80NO7P	M+H	766.5745	-0.9
HMDB0013415	PC(O-16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C44H80NO7P	M+H	766.5745	-0.9
HMDB0011312	PC(P-18:1(9Z)/18:3(9Z,12Z,15Z))	C44H80NO7P	M+H	766.5745	-0.9

766.5738

	HMDB0011278	PC(P-18:1(11Z)/18:3(6Z,9Z,12Z))	C44H80NO7P	M+H	766.5745	-0.9
	HMDB0011247	PC(P-18/18:4(6Z,9Z,12Z,15Z))	C44H80NO7P	M+H	766.5745	-0.9
	HMDB0011221	PC(P-16/:4(8Z,11Z,14Z,17Z))	C44H80NO7P	M+H	766.5745	-0.9
	HMDB0008195	PC(18:3(6Z,9Z,12Z)/P-18:1(9Z))	C44H80NO7P	M+H	766.5745	-0.9
	HMDB0008194	PC(18:3(6Z,9Z,12Z)/P-18:1(11Z))	C44H80NO7P	M+H	766.5745	-0.9
	HMDB0008228	PC(18:3(9Z,12Z,15Z)/P-18:1(9Z))	C44H80NO7P	M+H	766.5745	-0.9
	HMDB0008227	PC(18:3(9Z,12Z,15Z)/P-18:1(11Z))	C44H80NO7P	M+H	766.5745	-0.9
	HMDB0008259	PC(18:4(6Z,9Z,12Z,15Z)/P-18)	C44H80NO7P	M+H	766.5745	-0.9
	HMDB0008488	PC(:4(8Z,11Z,14Z,17Z)/P-16)	C44H80NO7P	M+H	766.5745	-0.9
	HMDB0008455	PC(:4(5Z,8Z,11Z,14Z)/P-16)	C44H80NO7P	M+H	766.5745	-0.9
	HMDB0011279	PC(P-18:1(11Z)/18:3(9Z,12Z,15Z))	C44H80NO7P	M+H	766.5745	-0.9
	HMDB0011220	PC(P-16/:4(5Z,8Z,11Z,14Z))	C44H80NO7P	M+H	766.5745	-0.9
	HMDB0039528	PC(O-16/:5(5Z,8Z,11Z,14Z,17Z))	C44H80NO7P	M+H	766.5745	-0.9
766.6917	HMDB0042128	TG(14/16/14:1(9Z))	C47H88O6	M+NH4	766.6919	-0.3
	HMDB0042995	TG(15/15/14:1(9Z))	C47H88O6	M+NH4	766.6919	-0.3
	HMDB0043834	TG(16/14/14:1(9Z))	C47H88O6	M+NH4	766.6919	-0.3
	HMDB0042069	TG(14/14/16:1(9Z))	C47H88O6	M+NH4	766.6919	-0.3
	HMDB0042301	TG(14/16:1(9Z)/14)	C47H88O6	M+NH4	766.6919	-0.3
	HMDB0043163	TG(15/14:1(9Z)/15)	C47H88O6	M+NH4	766.6919	-0.3
	HMDB0042273	TG(14/14:1(9Z)/16)	C47H88O6	M+NH4	766.6919	-0.3
	HMDB0113034	PE-NMe(15/22:4(7Z,Z,13Z,16Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0113594	PE-NMe(22:4(7Z,Z,13Z,16Z)/15)	C43H78NO8P	M+H	768.5538	0.2
	HMDB0113893	PE-NMe2(14/22:4(7Z,Z,13Z,16Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0116711	PE-NMe2(16/:4(8Z,11Z,14Z,17Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0113951	PE-NMe2(16/:4(5Z,8Z,11Z,14Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0113971	PE-NMe2(16:1(9Z)/:3(5Z,8Z,11Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0113972	PE-NMe2(16:1(9Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0113993	PE-NMe2(18/18:4(6Z,9Z,12Z,15Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0114018	PE-NMe2(18:1(11Z)/18:3(6Z,9Z,12Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0114019	PE-NMe2(18:1(11Z)/18:3(9Z,12Z,15Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0114045	PE-NMe2(18:1(9Z)/18:3(6Z,9Z,12Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0114046	PE-NMe2(18:1(9Z)/18:3(9Z,12Z,15Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0114073	PE-NMe2(18:2(9Z,12Z)/18:2(9Z,12Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0114100	PE-NMe2(18:3(6Z,9Z,12Z)/18:1(11Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0114101	PE-NMe2(18:3(6Z,9Z,12Z)/18:1(9Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0114129	PE-NMe2(18:3(9Z,12Z,15Z)/18:1(11Z))	C43H78NO8P	M+H	768.5538	0.2

768.5539

HMDB0114130	PE-NMe2(18:3(9Z,12Z,15Z)/18:1(9Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0114157	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/18)	C43H78NO8P	M+H	768.5538	0.2
HMDB0114272	PE-NMe2(:3(5Z,8Z,11Z)/16:1(9Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0114300	PE-NMe2(:3(8Z,11Z,14Z)/16:1(9Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0114327	PE-NMe2(:4(5Z,8Z,11Z,14Z)/16)	C43H78NO8P	M+H	768.5538	0.2
HMDB0114355	PE-NMe2(:4(8Z,11Z,14Z,17Z)/16)	C43H78NO8P	M+H	768.5538	0.2
HMDB0114495	PE-NMe2(22:4(7Z,Z,13Z,16Z)/14)	C43H78NO8P	M+H	768.5538	0.2
HMDB0007950	PC(15/:4(8Z,11Z,14Z,17Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0009228	PE(/18:4(6Z,9Z,12Z,15Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0009260	PE(:1(11Z)/18:3(9Z,12Z,15Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0009259	PE(:1(11Z)/18:3(6Z,9Z,12Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0009291	PE(:2(11Z,14Z)/18:2(9Z,12Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0009322	PE(:3(5Z,8Z,11Z)/18:1(11Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0009323	PE(:3(5Z,8Z,11Z)/18:1(9Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0009356	PE(:3(8Z,11Z,14Z)/18:1(9Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0009355	PE(:3(8Z,11Z,14Z)/18:1(11Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0009387	PE(:4(5Z,8Z,11Z,14Z)/18)	C43H78NO8P	M+H	768.5538	0.2
HMDB0009420	PE(:4(8Z,11Z,14Z,17Z)/18)	C43H78NO8P	M+H	768.5538	0.2
HMDB0009583	PE(22:4(7Z,Z,13Z,16Z)/16)	C43H78NO8P	M+H	768.5538	0.2
HMDB0009196	PE(18:4(6Z,9Z,12Z,15Z)/)	C43H78NO8P	M+H	768.5538	0.2
HMDB0009164	PE(18:3(9Z,12Z,15Z)/:1(11Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0007949	PC(15/:4(5Z,8Z,11Z,14Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0008428	PC(:4(5Z,8Z,11Z,14Z)/15)	C43H78NO8P	M+H	768.5538	0.2
HMDB0008461	PC(:4(8Z,11Z,14Z,17Z)/15)	C43H78NO8P	M+H	768.5538	0.2
HMDB0008943	PE(16/22:4(7Z,Z,13Z,16Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0008969	PE(16:1(9Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0009004	PE(18/:4(8Z,11Z,14Z,17Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0009003	PE(18/:4(5Z,8Z,11Z,14Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0009034	PE(18:1(11Z)/:3(5Z,8Z,11Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0009035	PE(18:1(11Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0009068	PE(18:1(9Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M+H	768.5538	0.2
HMDB0009067	PE(18:1(9Z)/:3(5Z,8Z,11Z))	C43H78NO8P	M+H	768.5538	0.2

	HMDB0009099	PE(18:2(9Z,12Z)/:2(11Z,14Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0009131	PE(18:3(6Z,9Z,12Z)/:1(11Z))	C43H78NO8P	M+H	768.5538	0.2
	HMDB0115354	PA(22:5(4Z,7Z,Z,13Z,16Z)/18)	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115330	PA(22:4(7Z,Z,13Z,16Z)/18:1(9Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115184	PA(:4(8Z,11Z,14Z,17Z)/:1(11Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115380	PA(22:5(7Z,Z,13Z,16Z,19Z)/18)	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115546	PA(:2(11Z,14Z)/:3(5Z,8Z,11Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115547	PA(:2(11Z,14Z)/:3(8Z,11Z,14Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115560	PA(:3(5Z,8Z,11Z)/:2(11Z,14Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115574	PA(:3(8Z,11Z,14Z)/:2(11Z,14Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115329	PA(22:4(7Z,Z,13Z,16Z)/18:1(11Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115306	PA(22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115305	PA(22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0114892	PA(18/22:5(7Z,Z,13Z,16Z,19Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0114915	PA(18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0114940	PA(18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0114993	PA(18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115020	PA(18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115046	PA(18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115080	PA(/:5(5Z,8Z,11Z,14Z,17Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115106	PA(:1(11Z)/:4(5Z,8Z,11Z,14Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115107	PA(:1(11Z)/:4(8Z,11Z,14Z,17Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115157	PA(:4(5Z,8Z,11Z,14Z)/:1(11Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115209	PA(:5(5Z,8Z,11Z,14Z,17Z)/)	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0115281	PA(22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C43H75O8P	M+NH4	768.5538	0.2
	HMDB0114891	PA(18/22:5(4Z,7Z,Z,13Z,16Z))	C43H75O8P	M+NH4	768.5538	0.2
768.5888	HMDB0013407	PC(O-16/:4(8Z,11Z,14Z,17Z))	C44H82NO7P	M+H	768.5902	-1.8
	HMDB0013435	PC(O-18:2(9Z,12Z)/18:2(9Z,12Z))	C44H82NO7P	M+H	768.5902	-1.8
	HMDB0011246	PC(P-18/18:3(9Z,12Z,15Z))	C44H82NO7P	M+H	768.5902	-1.8
	HMDB0011245	PC(P-18/18:3(6Z,9Z,12Z))	C44H82NO7P	M+H	768.5902	-1.8
	HMDB0011219	PC(P-16/:3(8Z,11Z,14Z))	C44H82NO7P	M+H	768.5902	-1.8
	HMDB0011218	PC(P-16/:3(5Z,8Z,11Z))	C44H82NO7P	M+H	768.5902	-1.8
	HMDB0008162	PC(18:2(9Z,12Z)/P-18:1(9Z))	C44H82NO7P	M+H	768.5902	-1.8
	HMDB0008161	PC(18:2(9Z,12Z)/P-18:1(11Z))	C44H82NO7P	M+H	768.5902	-1.8
	HMDB0008422	PC(:3(8Z,11Z,14Z)/P-16)	C44H82NO7P	M+H	768.5902	-1.8
	HMDB0008226	PC(18:3(9Z,12Z,15Z)/P-18)	C44H82NO7P	M+H	768.5902	-1.8
	HMDB0008390	PC(:3(5Z,8Z,11Z)/P-16)	C44H82NO7P	M+H	768.5902	-1.8
	HMDB0008193	PC(18:3(6Z,9Z,12Z)/P-18)	C44H82NO7P	M+H	768.5902	-1.8
	HMDB0011277	PC(P-18:1(11Z)/18:2(9Z,12Z))	C44H82NO7P	M+H	768.5902	-1.8
	HMDB0011310	PC(P-18:1(9Z)/18:2(9Z,12Z))	C44H82NO7P	M+H	768.5902	-1.8
	HMDB0007995	PC(16/P-18)	C42H84NO7P	M+Na	768.5878	1.4
	HMDB0013426	PC(O-18:1(9Z)/16)	C42H84NO7P	M+Na	768.5878	1.4
	HMDB0013424	PC(O-18:1(11Z)/16)	C42H84NO7P	M+Na	768.5878	1.4
	HMDB0013412	PC(O-16:1(9Z)/18)	C42H84NO7P	M+Na	768.5878	1.4

HMDB0011208	PC(P-16/18)	C42H84NO7P	M+Na	768.5878	1.4
HMDB0008060	PC(18/P-16)	C42H84NO7P	M+Na	768.5878	1.4
HMDB0011239	PC(P-18/16)	C42H84NO7P	M+Na	768.5878	1.4
HMDB0101963	TG(15/16/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101946	TG(a-15/16/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101947	TG(15/i-16/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101743	TG(i-15/15/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101742	TG(15/i-15/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101740	TG(a-15/i-15/14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101741	TG(i-15/15/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101739	TG(a-15/i-15/i-14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101735	TG(15/a-15/i-14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101736	TG(15/i-15/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101738	TG(a-15/15/i-14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101737	TG(a-15/15/14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101732	TG(i-15/a-15/i-14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101949	TG(a-15/16/i-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101948	TG(a-15/16/13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101950	TG(a-15/i-16/i-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101960	TG(i-15/16/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101961	TG(15/16/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101962	TG(15/16/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101958	TG(i-15/16/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101959	TG(i-15/i-16/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101956	TG(15/i-16/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101957	TG(i-15/i-16/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101955	TG(a-15/i-16/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101953	TG(i-15/i-16/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101954	TG(15/i-16/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101952	TG(i-15/16/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101951	TG(a-15/i-16/13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101733	TG(15/a-15/14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101734	TG(i-15/a-15/14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101585	TG(15/14/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101568	TG(a-15/a-15/14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101570	TG(a-15/14/15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101369	TG(15/13/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101368	TG(15/13/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101367	TG(i-15/13/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101366	TG(i-15/i-13/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101365	TG(i-15/i-13/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101364	TG(15/i-13/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101363	TG(i-15/13/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101361	TG(a-15/i-13/i-16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101362	TG(a-15/i-13/16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101359	TG(a-15/13/16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101569	TG(15/15/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101571	TG(a-15/14/i-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101572	TG(a-15/i-14/i-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101583	TG(15/15/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101584	TG(15/14/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101582	TG(i-15/14/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101581	TG(i-15/i-15/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101578	TG(15/i-14/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101580	TG(i-15/14/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101579	TG(i-15/i-14/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101577	TG(a-15/a-15/i-14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101576	TG(15/i-14/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101575	TG(i-15/i-14/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101574	TG(i-15/i-15/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101573	TG(a-15/i-14/15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101360	TG(a-15/13/i-16)[rac]	C47H90O6	M+NH4	768.7076	-1.1

HMDB0102110	TG(i-15/a-17/i-12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103776	TG(16/i-13/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103643	TG(i-16/i-12/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103641	TG(i-16/i-16/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103640	TG(16/16/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103569	TG(16//i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103567	TG(i-16//18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103566	TG(i-16//i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103568	TG(16//18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103516	TG(16/8/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103514	TG(i-16/8/i-)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103515	TG(i-16/8/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103517	TG(16/8/i-)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102874	TG(i-15/21/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103642	TG(16/i-12/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103644	TG(i-16/i-16/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103645	TG(i-16/12/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103777	TG(i-16/i-13/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103772	TG(16/i-13/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103774	TG(i-16/i-13/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103775	TG(16/i-13/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103773	TG(i-16/13/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103770	TG(i-16/a-13/15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103768	TG(i-16/a-13/i-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103771	TG(16/a-13/i-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103769	TG(16/a-13/15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103767	TG(i-16/a-13/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103766	TG(16/a-13/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103647	TG(16/12/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102875	TG(15/21/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102871	TG(a-15/21/8)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102873	TG(i-15/i-21/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102124	TG(i-15/i-17/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102122	TG(15/i-17/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102119	TG(a-15/i-17/i-12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102120	TG(a-15/i-17/12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102118	TG(a-15/17/i-12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102121	TG(i-15/17/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102116	TG(15/i-17/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102117	TG(a-15/17/12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102115	TG(a-15/a-17/i-12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102111	TG(15/a-17/12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102113	TG(a-15/a-17/12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102114	TG(15/a-17/i-12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102123	TG(i-15/i-17/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102126	TG(15/17/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102125	TG(i-15/17/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102872	TG(a-15/i-21/8)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102870	TG(15/i-21/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102868	TG(i-15/a-21/8)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102869	TG(a-15/a-21/8)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102867	TG(15/a-21/8)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102533	TG(i-15/19/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102532	TG(i-15/i-19/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102534	TG(15/19/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102531	TG(a-15/i-19/)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102530	TG(a-15/19/)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102529	TG(15/i-19/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102127	TG(15/17/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0102112	TG(i-15/a-17/12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100010	TG(14/17/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099886	TG(14/i-16/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099887	TG(i-14/i-16/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099752	TG(14/15/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099753	TG(14/15/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1

HMDB0099749	TG(i-14/15/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099748	TG(i-14/i-15/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099750	TG(i-14/i-15/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099751	TG(i-14/15/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099746	TG(14/i-15/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099744	TG(i-14/15/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099745	TG(i-14/i-15/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099747	TG(14/i-15/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099888	TG(i-14/16/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099889	TG(14/16/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099994	TG(i-14/a-17/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100009	TG(i-14/17/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100005	TG(14/i-17/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100004	TG(14/i-17/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100006	TG(i-14/i-17/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100003	TG(i-14/i-17/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100002	TG(i-14/17/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099996	TG(14/a-17/13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099999	TG(14/i-17/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099997	TG(i-14/a-17/13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099998	TG(14/a-17/i-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099993	TG(14/a-17/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099995	TG(i-14/a-17/i-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099741	TG(i-14/a-15/15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099742	TG(14/a-15/i-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099740	TG(14/a-15/15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099508	TG(i-14/i-13/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099506	TG(i-14/i-13/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099505	TG(14/i-13/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099507	TG(i-14/13/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099504	TG(14/i-13/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099503	TG(i-14/i-13/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099502	TG(i-14/13/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099501	TG(14/i-13/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099500	TG(14/a-13/i-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099499	TG(i-14/a-13/17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099498	TG(14/a-13/17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099496	TG(i-14/a-13/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099509	TG(i-14/13/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099511	TG(14/13/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099510	TG(14/13/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099743	TG(14/i-15/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099739	TG(i-14/a-15/i-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099737	TG(14/a-15/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099738	TG(i-14/a-15/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099626	TG(i-14/14/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099627	TG(14/14/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099625	TG(i-14/i-14/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099624	TG(i-14/i-14/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099622	TG(i-14/14/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099623	TG(14/i-14/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099621	TG(14/i-14/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099512	TG(14/13/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099497	TG(i-14/a-13/i-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100007	TG(i-14/17/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101356	TG(15/a-13/i-16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101156	TG(15/i-12/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101154	TG(i-15/12/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101153	TG(a-15/i-12/17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101155	TG(i-15/i-12/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101152	TG(a-15/i-12/i-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101150	TG(a-15/12/17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101151	TG(a-15/12/i-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101148	TG(a-15/12/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101149	TG(15/i-12/17)	C47H90O6	M+NH4	768.7076	-1.1

HMDB0101034	TG(i-15//19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101035	TG(15//19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101033	TG(i-15//i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101157	TG(a-15/i-12/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101160	TG(i-15/12/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101158	TG(15/i-12/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101355	TG(a-15/a-13/16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101358	TG(15/i-13/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101357	TG(a-15/a-13/i-16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101353	TG(15/a-13/16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101354	TG(i-15/a-13/16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101352	TG(i-15/a-13/i-16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101163	TG(15/12/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101162	TG(i-15/12/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101164	TG(15/12/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101165	TG(15/12/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101159	TG(i-15/i-12/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101161	TG(i-15/i-12/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101036	TG(15//i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101031	TG(a-15//19)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0101032	TG(a-15//i-19)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100376	TG(14/i-/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100377	TG(i-14/i-/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100160	TG(14/18/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100159	TG(14/18/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100158	TG(i-14/18/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100156	TG(i-14/i-18/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100157	TG(i-14/i-18/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100155	TG(14/i-18/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100154	TG(i-14/18/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100153	TG(14/i-18/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100012	TG(14/17/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100011	TG(14/17/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100378	TG(i-14//)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100379	TG(14//)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100657	TG(14/i-22/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100960	TG(15/8/i-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100961	TG(15/8/a-21)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100957	TG(i-15/8/a-21)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100958	TG(i-15/8/21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100956	TG(i-15/8/i-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100959	TG(15/8/21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100953	TG(a-15/8/a-21)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100954	TG(a-15/8/21)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100955	TG(a-15/8/i-21)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100659	TG(i-14/22/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100658	TG(i-14/i-22/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100660	TG(14/22/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0100008	TG(i-14/i-17/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103779	TG(i-16/i-13/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108236	TG(18/i-14/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108071	TG(i-18/a-13/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108073	TG(18/a-13/13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108072	TG(i-18/a-13/i-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108070	TG(18/a-13/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107959	TG(i-18/12/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107961	TG(18/12/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107960	TG(18/12/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107956	TG(18/i-12/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107955	TG(i-18/12/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107957	TG(i-18/i-12/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107958	TG(i-18/i-12/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107954	TG(18/i-12/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108074	TG(i-18/a-13/13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108076	TG(18/i-13/13)	C47H90O6	M+NH4	768.7076	-1.1

HMDB0108078	TG(i-18/i-13/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108234	TG(18/i-14/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108087	TG(18/13/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108084	TG(i-18/13/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108086	TG(18/13/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108083	TG(i-18/i-13/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108085	TG(18/13/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108079	TG(18/i-13/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108081	TG(i-18/i-13/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108080	TG(18/i-13/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108082	TG(i-18/13/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108077	TG(i-18/13/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108075	TG(18/a-13/i-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107893	TG(18//i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107892	TG(18//16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107891	TG(i-18//16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106462	TG(17/i-17/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106461	TG(i-17/a-17/)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106039	TG(17/15/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106038	TG(17/15/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106036	TG(i-17/i-15/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106035	TG(i-17/i-15/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106037	TG(i-17/15/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106033	TG(i-17/15/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106032	TG(a-17/i-15/12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106031	TG(a-17/i-15/i-12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106034	TG(17/i-15/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106028	TG(17/i-15/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106460	TG(17/a-17/)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106465	TG(i-17/17/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106463	TG(a-17/17/)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107890	TG(i-18//i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107843	TG(18/8/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107840	TG(i-18/i-18/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107841	TG(i-18/8/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0107842	TG(18/18/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106854	TG(17/19/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106853	TG(i-17/19/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106852	TG(i-17/i-19/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106851	TG(a-17/i-19/8)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106850	TG(a-17/19/8)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106849	TG(17/i-19/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106464	TG(a-17/i-17/)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106027	TG(a-17/a-15/i-12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108237	TG(i-18/i-14/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0110380	TG(19/17/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109794	TG(i-19/i-13/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109791	TG(19/i-13/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109793	TG(19/i-13/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109792	TG(i-19/13/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109789	TG(i-19/a-13/12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109788	TG(19/a-13/12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109787	TG(i-19/a-13/i-12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109790	TG(19/a-13/i-12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109680	TG(19/12/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109679	TG(i-19/12/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109682	TG(19/12/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109681	TG(19/12/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109795	TG(i-19/i-13/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109798	TG(19/13/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109797	TG(19/13/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0110379	TG(i-19/17/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0110378	TG(i-19/i-17/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0110377	TG(19/i-17/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0110376	TG(i-19/a-17/8)[rac]	C47H90O6	M+NH4	768.7076	-1.1

HMDB0110375	TG(19/a-17/8)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0110084	TG(i-19/i-15/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0110083	TG(19/i-15/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0110086	TG(19/15/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0110085	TG(i-19/15/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0110082	TG(i-19/a-15/)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0110081	TG(19/a-15/)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109796	TG(i-19/13/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109678	TG(i-19/i-12/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109676	TG(i-19/i-12/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109677	TG(i-19/12/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109564	TG(i-19/8/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109563	TG(i-19/8/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108821	TG(i-18/18/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108820	TG(18/i-18/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108527	TG(i-18/i-16/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108528	TG(i-18/16/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108526	TG(18/i-16/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108529	TG(18/16/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108241	TG(18/14/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108239	TG(i-18/14/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108240	TG(18/14/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108238	TG(i-18/i-14/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109565	TG(i-19/8/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109566	TG(19/8/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109567	TG(19/8/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109675	TG(19/i-12/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109673	TG(i-19/i-12/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109672	TG(i-19/12/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109674	TG(19/i-12/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109671	TG(19/i-12/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109618	TG(19//a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109617	TG(19//i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109615	TG(i-19//15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109616	TG(19//15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109614	TG(i-19//a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109613	TG(i-19//i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0109568	TG(19/8/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0108235	TG(i-18/14/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105428	TG(a-17/12/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104681	TG(16/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104679	TG(i-16/i-8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104680	TG(i-16//8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104678	TG(16/i-8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104456	TG(16/18/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104455	(2R)-1-(decanoyloxy)-3-[(14-methylpentadecanoyl)oxy]propan-2-yl octadecanoate	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104454	TG(i-16/i-18/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104453	TG(16/i-18/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104191	TG(16/i-16/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104192	TG(i-16/16/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104189	TG(16/i-16/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104190	TG(i-16/16/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105253	TG(i-17/8/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105251	TG(a-17/8/19)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105252	TG(a-17/8/i-19)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105332	TG(17/17/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105331	TG(i-17//17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105334	TG(17//a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105333	TG(17//i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105327	TG(a-17//17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105328	TG(a-17//i-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105329	TG(i-17/i-17/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105330	TG(i-17//a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105326	TG(a-17/a-17/)[rac]	C47H90O6	M+NH4	768.7076	-1.1

HMDB0105256	TG(17/8/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105255	TG(17/8/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105254	TG(i-17/8/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104048	TG(16/15/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104049	TG(16/15/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104047	TG(16/15/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103927	TG(16/14/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103926	TG(16/14/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103924	TG(i-16/i-14/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103925	TG(i-16/14/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103923	TG(i-16/i-14/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103922	TG(16/i-14/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103921	TG(i-16/14/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103920	TG(16/i-14/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103783	TG(16/13/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103782	TG(16/13/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103781	TG(16/13/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103780	TG(i-16/13/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104033	TG(i-16/a-15/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104032	TG(16/a-15/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104034	TG(i-16/a-15/i-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104046	TG(i-16/15/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104045	TG(i-16/i-15/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104043	TG(i-16/i-15/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104044	TG(i-16/15/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104040	TG(i-16/i-15/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104039	TG(i-16/15/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104042	TG(16/i-15/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104041	TG(16/i-15/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104035	TG(16/a-15/13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104038	TG(16/i-15/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104036	TG(i-16/a-15/13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0104037	TG(16/a-15/i-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103778	TG(i-16/13/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105430	TG(a-17/12/15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106029	TG(a-17/15/12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105856	TG(17/i-14/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105855	TG(i-17/i-14/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105853	TG(a-17/i-14/13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105852	TG(a-17/i-14/i-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105851	TG(a-17/14/i-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105854	TG(i-17/14/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105848	TG(a-17/14/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105849	TG(17/i-14/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105850	TG(a-17/14/13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105631	TG(i-17/i-13/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105632	TG(i-17/13/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105633	TG(17/13/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105857	TG(a-17/i-14/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105858	TG(17/i-14/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105859	TG(i-17/i-14/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106030	TG(a-17/15/i-12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106023	TG(17/a-15/12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106024	TG(i-17/a-15/12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106025	TG(a-17/a-15/12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106026	TG(17/a-15/i-12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0106022	TG(i-17/a-15/i-12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105865	TG(17/14/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105864	TG(17/14/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105863	TG(17/14/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105862	TG(i-17/14/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105860	TG(i-17/14/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105861	TG(i-17/i-14/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105634	TG(17/13/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105630	TG(i-17/i-13/14)	C47H90O6	M+NH4	768.7076	-1.1

HMDB0105629	TG(17/i-13/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105441	TG(i-17/i-12/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105440	TG(i-17/12/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105442	TG(i-17/12/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105439	TG(i-17/i-12/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105435	TG(i-17/i-12/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105438	TG(17/i-12/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105436	TG(17/i-12/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105437	TG(a-17/i-12/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105434	TG(i-17/12/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105432	TG(a-17/i-12/i-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105431	TG(a-17/12/i-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105433	TG(a-17/i-12/15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105445	TG(17/12/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105444	TG(17/12/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105443	TG(17/12/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105628	TG(i-17/13/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105627	TG(a-17/i-13/14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105624	TG(a-17/13/14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105626	TG(a-17/i-13/i-14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105623	TG(17/i-13/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105625	TG(a-17/13/i-14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105621	TG(17/a-13/i-14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105622	TG(a-17/a-13/i-14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105619	TG(i-17/a-13/14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105620	TG(a-17/a-13/14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105618	TG(17/a-13/14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105617	TG(i-17/a-13/i-14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0105429	TG(17/i-12/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072460	TG(8/i-24/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072144	TG(/21/a-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072137	TG(/i-15/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072101	TG(/a-21/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072089	TG(8/a-21/a-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072082	TG(8/i-21/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072078	TG(8//i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072066	TG(/a-15/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072058	TG(8/i-12/i-24)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072055	TG(8/i-17/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072029	TG(/i-16/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071978	TG(/13/a-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071979	TG(/17/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072204	TG(/17/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072218	TG(8/18/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072230	TG(8/i-15/a-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072445	TG(8/i-21/a-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072432	TG(8/a-21/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072419	TG(/i-13/21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072394	TG(8/21/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072382	TG(8/i-19/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072362	TG(8/12/i-24)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072326	TG(/i-24)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072299	TG(8/a-15/a-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072289	TG(8/i-16/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072277	TG(/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072244	TG(/a-13/i-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072237	TG(/i-21/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071952	TG(8/i-22/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071946	TG(8/a-17/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071947	TG(/a-17/a-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071694	TG(8/19/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071691	TG(/i-13/a-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071671	TG(/i-13/i-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071666	TG(/18/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071667	TG(8/19/a-17)	C47H90O6	M+NH4	768.7076	-1.1

HMDB0071657	TG(/i-12/i-22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071653	TG(8/14/22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071647	TG(8/i-14/i-22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071644	TG(8/a-21/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071637	TG(/12/i-22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071621	TG(/14/i-)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071618	TG(/19/a-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071712	TG(8/17/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071748	TG(/19/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071752	TG(/22/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071933	TG(/i-21/a-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071929	TG(/15/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071921	TG(8/18/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071900	TG(/i-22/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071868	TG(/i-22/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071846	TG(/i-19/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071825	TG(8/i-14/22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071808	TG(/i-18/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071794	TG(8/22/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071792	TG(8/21/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071756	TG(8/i-17/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071757	TG(/a-17/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071550	TG(/a-17/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072468	TG(/a-13/a-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095290	TG(12/i-14/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095020	TG(i-12/i-12/i-)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095018	TG(12/i-12/i-)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095019	TG(i-12/i-12/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095017	TG(i-12/12/i-)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095016	TG(12/i-12/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0094932	TG(i-12/22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0094933	TG(12/22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0094931	TG(i-12//i-22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0094934	TG(12//i-22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0094875	TG(i-12/8/i-24)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0094876	TG(12/8/i-24)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072816	TG(8/i-18/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095021	TG(i-12/12/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095023	TG(12/12/i-)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095160	TG(i-12/a-13/i-19)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095293	TG(i-12/i-14/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095169	TG(i-12/13/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095168	TG(i-12/i-13/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095170	TG(12/13/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095171	TG(12/13/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095165	TG(i-12/13/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095164	TG(12/i-13/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095167	TG(i-12/i-13/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095166	TG(12/i-13/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095163	TG(12/a-13/i-19)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095161	TG(12/a-13/19)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095162	TG(i-12/a-13/19)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072793	TG(8/i-/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072776	TG(8/i-24/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072761	TG(8/15/i-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072640	TG(/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072638	TG(/i-17/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072608	TG(8/a-17/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072594	TG(/a-21/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072570	TG(/19/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072565	TG(8/i-15/i-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072561	TG(8/14/i-22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072550	TG(/22/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072553	TG(/16/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072518	TG(/i-17/a-17)	C47H90O6	M+NH4	768.7076	-1.1

HMDB0072521	TG(/i-12/22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072483	TG(8/i-22/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072646	TG(/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072656	TG(/21/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072658	TG(/15/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072756	TG(8/a-15/21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072751	TG(8/i-/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072753	TG(8/i-18/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072735	TG(8/22/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072736	TG(8/21/a-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072719	TG(8/16/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072721	TG(/i-21/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072712	TG(/18/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072707	TG(/i-19/a-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072708	TG(/i-14/i-)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072670	TG(/i-14/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072668	TG(8/i-21/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072485	TG(/i-/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065219	TG(a-21/i-15/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064738	TG(21/13/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064716	TG(i-21//13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064653	TG(21//13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064571	TG(a-21/i-13/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064460	TG(i-/i-16/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064455	TG(/12/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064288	TG(/14/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064242	TG(/i-16/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064144	TG(i-/12/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0063985	TG(/i-12/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0063974	TG(i-/12/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0063940	TG(i-/14/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064752	TG(i-21/8/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064756	TG(i-21/i-13/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064783	TG(i-21//a-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065192	TG(i-21/a-15/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065187	TG(a-21/a-15/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065095	TG(a-21//i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065032	TG(i-21/15/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064986	TG(21/8/a-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064976	TG(a-21//13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064922	TG(i-21/8/a-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064910	TG(21/15/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064871	TG(i-21/a-13/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064846	TG(21/i-15/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064809	TG(a-21/8/a-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0064794	TG(i-21//i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0063830	TG(/8/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0063603	TG(i-/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0063590	TG(/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095566	TG(12/16/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095296	TG(12/14/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0042063	TG(14/14/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095022	TG(12/12/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072226	TG(/12/22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0072184	TG(/16/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071809	TG(/14/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0042960	TG(15/14/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0042121	TG(14/16/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0042092	TG(14/15/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0062860	TG(i-/8/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0063563	TG(i-/8/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0063477	TG(/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0063456	TG(i-/i-12/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0063421	TG(i-/16/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0063401	TG(/16/8)	C47H90O6	M+NH4	768.7076	-1.1

HMDB0063370	TG(/8/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0063233	TG(i-/i-12/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0063091	TG(i-/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0063026	TG(/i-14/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0062958	TG(/12/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0062946	TG(i-/i-14/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0062936	TG(/i-12/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0103646	TG(16/16/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065218	TG(i-21/13/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071520	TG(8/15/21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071217	TG(/13/i-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071195	TG(/i-17/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071188	TG(8/i-16/i-)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071179	TG(/i-15/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071176	TG(8/16/i-)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071169	TG(8/a-15/i-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071109	TG(/a-15/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0070804	TG(i-24/i-12/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0070756	TG(i-24/8/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0069903	TG(i-24/12/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0069580	TG(i-24/8/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0069478	TG(i-24//)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071216	TG(8/i-15/21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071257	TG(8/19/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071272	TG(/a-21/a-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071496	TG(8//16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071498	TG(/i-18/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071493	TG(8/15/a-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071475	TG(/13/21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071455	TG(/i-19/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071449	TG(8/i-19/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071403	TG(8/17/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071377	TG(/a-13/21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071356	TG(/i-16/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071343	TG(/17/a-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071330	TG(/21/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0071302	TG(8/i-19/a-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0069020	TG(22/12/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0068962	TG(i-22/8/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0068961	TG(22//i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0066081	TG(21//i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065966	TG(21/8/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065876	TG(i-21/8/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065791	TG(a-21/8/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065753	TG(a-21/13/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065611	TG(21/a-13/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065607	TG(21/i-13/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065571	TG(21/a-15/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065494	TG(a-21/a-13/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065479	TG(21//a-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065437	TG(i-21/i-15/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065403	TG(a-21/8/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0066118	TG(a-21/15/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0066184	TG(a-21//a-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0067704	TG(i-22/8/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0068899	TG(i-22/12/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0068851	TG(i-22/i-14/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0068845	TG(22/i-12/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0068547	TG(i-22//12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0068408	TG(22/14/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0068258	TG(i-22//i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0068016	TG(i-22/i-12/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0067999	TG(i-22/14/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0067903	TG(22/8/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0067778	TG(22//12)	C47H90O6	M+NH4	768.7076	-1.1

HMDB0067768	TG(22/8/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0067710	TG(22/i-14/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0065243	TG(21/8/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095292	TG(12/i-14/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097843	TG(a-13/i-17/14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097662	TG(a-13/i-16/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097660	TG(i-13/i-16/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097663	TG(13/i-16/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097659	TG(i-13/16/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097657	TG(a-13/i-16/i-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097658	TG(a-13/i-16/15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097656	TG(a-13/16/i-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097654	TG(13/i-16/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097655	TG(a-13/16/15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097653	TG(a-13/16/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097460	TG(13/15/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097459	TG(13/15/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097661	TG(13/i-16/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097667	TG(i-13/16/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097666	TG(i-13/i-16/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097836	TG(a-13/a-17/14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097838	TG(a-13/a-17/i-14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097839	TG(13/i-17/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097837	TG(13/a-17/i-14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097834	TG(13/a-17/14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097833	TG(i-13/a-17/i-14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097835	TG(i-13/a-17/14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097668	TG(13/16/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097670	TG(13/16/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097669	TG(13/16/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097664	TG(i-13/i-16/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097665	TG(i-13/16/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097458	TG(i-13/15/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097457	TG(i-13/i-15/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097456	TG(i-13/i-15/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097260	TG(i-13/14/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097263	TG(13/14/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097262	TG(i-13/14/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097261	TG(i-13/i-14/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097259	TG(i-13/i-14/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097256	TG(13/i-14/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097258	TG(13/i-14/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097257	TG(a-13/i-14/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097254	TG(i-13/14/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097253	TG(a-13/i-14/17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097255	TG(i-13/i-14/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097252	TG(a-13/i-14/i-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097265	TG(13/14/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097264	TG(13/14/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097443	TG(i-13/a-15/i-16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097453	TG(a-13/i-15/16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097455	TG(13/i-15/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097454	TG(i-13/15/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097452	TG(a-13/i-15/i-16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097448	TG(a-13/a-15/i-16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097449	TG(13/i-15/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097450	TG(a-13/15/16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097451	TG(a-13/15/i-16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097446	TG(a-13/a-15/16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097445	TG(i-13/a-15/16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097447	TG(13/a-15/i-16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097444	TG(13/a-15/16)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097249	TG(13/i-14/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097841	TG(a-13/17/i-14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099495	TG(14/a-13/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1

HMDB0099223	TG(i-14/8/i-22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098579	TG(13/21/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098577	TG(i-13/i-21/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098576	TG(a-13/i-21/)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098578	TG(i-13/21/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098574	TG(13/i-21/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098573	TG(a-13/a-21/)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098572	TG(i-13/a-21/)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098575	TG(a-13/21/)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098571	TG(13/a-21/)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098236	TG(13/19/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098237	TG(13/19/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099224	TG(i-14/8/22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099225	TG(14/8/22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099226	TG(14/8/i-22)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099364	TG(i-14/12/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099366	TG(14/12/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099365	TG(14/12/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099361	TG(14/i-12/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099362	TG(i-14/i-12/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099360	TG(i-14/12/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099363	TG(i-14/i-12/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099359	TG(14/i-12/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099276	TG(14/i-)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099273	TG(i-14/i-)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099275	TG(14/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0099274	TG(i-14/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098232	TG(13/i-19/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098233	TG(i-13/i-19/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098234	TG(i-13/i-19/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098066	TG(a-13/i-18/i-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098067	TG(a-13/i-18/13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098065	TG(a-13/18/i-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098064	TG(a-13/18/13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097849	TG(13/17/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097850	TG(13/17/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097848	TG(i-13/17/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097844	TG(i-13/17/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097846	TG(i-13/i-17/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097845	TG(13/i-17/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097847	TG(i-13/i-17/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097840	TG(a-13/17/14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098068	TG(i-13/i-18/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098069	TG(13/i-18/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098071	TG(i-13/i-18/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098235	TG(i-13/19/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098228	TG(a-13/19/i-12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098230	TG(a-13/i-19/12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098229	TG(a-13/i-19/i-12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098231	TG(i-13/19/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098226	TG(13/i-19/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098227	TG(a-13/19/12)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098073	TG(i-13/18/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098075	TG(13/18/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098072	TG(i-13/18/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098074	TG(13/18/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0098070	TG(13/i-18/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097842	TG(a-13/i-17/i-14)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095936	TG(12/i-19/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095690	TG(12/i-17/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095693	TG(i-12/i-17/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095692	TG(i-12/17/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095691	TG(i-12/i-17/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095689	TG(12/i-17/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095687	TG(i-12/17/i-15)	C47H90O6	M+NH4	768.7076	-1.1

HMDB0095686	TG(12/i-17/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095688	TG(i-12/i-17/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095684	TG(i-12/a-17/15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095682	TG(i-12/a-17/i-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095683	TG(12/a-17/15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095685	TG(12/a-17/i-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095697	TG(12/17/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095694	TG(i-12/17/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095696	TG(12/17/i-15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095935	TG(i-12/i-19/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095934	TG(i-12/19/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095933	TG(12/i-19/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095835	TG(i-12/18/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095836	TG(12/18/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095837	TG(12/18/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095834	TG(i-12/i-18/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095831	TG(i-12/18/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095833	TG(i-12/i-18/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095830	TG(12/i-18/14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095832	TG(12/i-18/i-14)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095695	TG(12/17/15)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095681	TG(i-12/a-17/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095680	TG(12/a-17/a-15)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095567	TG(12/16/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095430	TG(12/i-15/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095428	TG(i-12/i-15/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095425	TG(12/a-15/i-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095424	TG(i-12/a-15/17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095426	TG(12/i-15/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095423	TG(12/a-15/17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095421	TG(i-12/a-15/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095422	TG(i-12/a-15/i-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095420	TG(12/a-15/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095295	TG(i-12/14/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095297	TG(12/14/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095294	TG(i-12/i-14/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095427	TG(i-12/15/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095429	TG(12/i-15/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095434	TG(i-12/15/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095563	TG(i-12/i-16/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095564	TG(i-12/i-16/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095562	TG(12/i-16/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095565	TG(i-12/16/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095561	TG(i-12/16/i-16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095560	TG(12/i-16/16)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095436	TG(12/15/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095437	TG(12/15/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095435	TG(12/15/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095432	TG(i-12/15/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095433	TG(i-12/i-15/i-17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095431	TG(i-12/i-15/17)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095291	TG(i-12/14/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095937	TG(12/i-19/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097250	TG(a-13/14/17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097057	TG(13/a-13/i-18)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097056	TG(a-13/a-13/18)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097055	TG(i-13/a-13/18)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097054	TG(13/a-13/18)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097053	TG(i-13/a-13/i-18)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096864	TG(13/12/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096862	TG(i-13/12/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096861	TG(i-13/i-12/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096863	TG(13/12/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096860	TG(i-13/i-12/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096857	TG(a-13/i-12/19)[rac]	C47H90O6	M+NH4	768.7076	-1.1

HMDB0096856	TG(a-13/i-12/i-19)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097059	TG(13/i-13/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097058	TG(a-13/a-13/i-18)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097060	TG(a-13/13/18)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097251	TG(a-13/14/i-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097248	TG(a-13/14/a-17)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097069	TG(13/13/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097068	TG(i-13/13/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097070	TG(13/13/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097065	TG(13/i-13/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097067	TG(i-13/i-13/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097066	TG(i-13/i-13/18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097064	TG(i-13/13/i-18)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097063	TG(a-13/i-13/18)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097062	TG(a-13/i-13/i-18)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0097061	TG(a-13/13/i-18)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096858	TG(i-13/12/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096859	TG(13/i-12/i-19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096855	TG(a-13/12/i-19)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096332	TG(i-12/i-22/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096331	TG(12/i-22/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096045	TG(12/i-/i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096047	TG(i-12//12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096046	TG(i-12/i-/12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096048	TG(12//i-12)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095941	TG(i-12/19/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095942	TG(12/19/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095944	TG(12/19/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095943	TG(12/19/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095938	TG(i-12/i-19/13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095940	TG(i-12/i-19/i-13)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096334	TG(12/22/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096333	TG(i-12/22/)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096443	TG(12/i-24/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096854	TG(a-13/12/19)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096853	TG(13/i-12/19)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096724	TG(13//21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096726	TG(13//a-21)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096725	TG(13//i-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096721	TG(i-13//i-21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096720	TG(a-13//i-21)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096722	TG(i-13//a-21)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096723	TG(i-13//21)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096718	TG(a-13//a-21)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096719	TG(a-13//21)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0096444	TG(i-12/i-24/8)	C47H90O6	M+NH4	768.7076	-1.1
HMDB0095939	TG(i-12/19/a-13)[rac]	C47H90O6	M+NH4	768.7076	-1.1
HMDB0168100	3,4,5-trihydroxy-6-[-(5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-7-yl)-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-5-yl]oxy]oxane-2-carboxylic acid	C38H34O16	M+Na	769.1739	1.7
HMDB0162320	3,4,5-trihydroxy-6-[(6-{5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl}-8,-dimethoxy-2-methyl-4-oxo-4H-benzo[h]chromen-5-yl)oxy]oxane-2-carboxylic acid	C38H34O16	M+Na	769.1739	1.7
HMDB0162321	3,4,5-trihydroxy-6-[-(5-hydroxy-8,-dimethoxy-2-methyl-4-oxo-4H-benzo[h]chromen-6-yl)-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-5-yl]oxy]oxane-2-carboxylic acid	C38H34O16	M+Na	769.1739	1.7
HMDB0162266	3,4,5-trihydroxy-6-[-(5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen--yl)-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-5-yl]oxy]oxane-2-carboxylic acid	C38H34O16	M+Na	769.1739	1.7

769.1752	HMDB0162208	3,4,5-trihydroxy-6-[(7-{6-hydroxy-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-yl}-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-6-yl)oxy]oxane-2-carboxylic acid	C38H34O16	M+Na	769.1739	1.7
	HMDB0162209	3,4,5-trihydroxy-6-[(6-hydroxy-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-7-yl)-5,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-6-yl]oxy]oxane-2-carboxylic acid	C38H34O16	M+Na	769.1739	1.7
	HMDB0168099	3,4,5-trihydroxy-6-[(7-{5-hydroxy-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-yl}-6,8-dimethoxy-2-methyl-4-oxo-4H-benzo[g]chromen-5-yl)oxy]oxane-2-carboxylic acid	C38H34O16	M+Na	769.1739	1.7
	HMDB0150848	6-({2-[4-(2,4-dihydroxyphenyl)-,18-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-8-yl]-1-benzofuran-6-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H32O16	M+H	769.1763	-1.4
	HMDB0150849	6-{[4-(2,4-dihydroxyphenyl)-18-hydroxy-8-(6-hydroxy-1-benzofuran-2-yl)-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H32O16	M+H	769.1763	-1.4
	HMDB0150850	6-{[4-(2,4-dihydroxyphenyl)-hydroxy-8-(6-hydroxy-1-benzofuran-2-yl)-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-18-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H32O16	M+H	769.1763	-1.4
	HMDB0150847	6-{2-[1,18-dihydroxy-8-(6-hydroxy-1-benzofuran-2-yl)-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-4-yl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H32O16	M+H	769.1763	-1.4
	HMDB0150846	6-{4-[1,18-dihydroxy-8-(6-hydroxy-1-benzofuran-2-yl)-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-4-yl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H32O16	M+H	769.1763	-1.4
769.2446	HMDB0137633	3,4,5-trihydroxy-6-({1-hydroxy-4-[8-(2-hydroxypropan-2-yl)-2-oxo-2H,8H,9H-furo[2,3-h]chromen-9-yl]-3,5,6-trimethoxy--methyl-9-oxo-9,-dihydroacridin-2-yl}oxy)oxane-2-carboxylic acid	C37H37NO16	M+NH4	769.2451	-0.6
	HMDB0137634	3,4,5-trihydroxy-6-({2-hydroxy-4-[8-(2-hydroxypropan-2-yl)-2-oxo-2H,8H,9H-furo[2,3-h]chromen-9-yl]-3,5,6-trimethoxy--methyl-9-oxo-9,-dihydroacridin-1-yl}oxy)oxane-2-carboxylic acid	C37H37NO16	M+NH4	769.2451	-0.6
	HMDB0137635	3,4,5-trihydroxy-6-({8-hydroxy-5-[8-(2-hydroxypropan-2-yl)-2-oxo-2H,8H,9H-furo[2,3-h]chromen-9-yl]-3,4,6-trimethoxy--methyl-9-oxo-9,-dihydroacridin-2-yl}oxy)oxane-2-carboxylic acid	C37H37NO16	M+NH4	769.2451	-0.6
	HMDB0137636	3,4,5-trihydroxy-6-({7-hydroxy-4-[8-(2-hydroxypropan-2-yl)-2-oxo-2H,8H,9H-furo[2,3-h]chromen-9-yl]-3,5,6-trimethoxy--methyl-9-oxo-9,-dihydroacridin-1-yl}oxy)oxane-2-carboxylic acid	C37H37NO16	M+NH4	769.2451	-0.6
	HMDB0137637	6-({4-[8-(1,2-dihydroxypropan-2-yl)-2-oxo-2H,8H,9H-furo[2,3-h]chromen-9-yl]-3,5,6-trimethoxy--methyl-9-oxo-9,-dihydroacridin-1-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C37H37NO16	M+NH4	769.2451	-0.6
	HMDB0010595	PG(16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C42H73O10P	M+H	769.5014	-2.5
	HMDB0010651	PG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C42H73O10P	M+H	769.5014	-2.5
	HMDB0010652	PG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C42H73O10P	M+H	769.5014	-2.5
	HMDB0010665	PG(18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C42H73O10P	M+H	769.5014	-2.5

769.4995	HMDB0010680	PG(18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C42H73O10P	M+H	769.5014	-2.5
	HMDB0116608	PG(:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C42H73O10P	M+H	769.5014	-2.5
	HMDB0010631	PG(18:1(9Z)/16:1(9Z))	C40H75O10P	M+Na	769.4990	0.6
	HMDB0010645	PG(18:2(9Z,12Z)/16)	C40H75O10P	M+Na	769.4990	0.6
	HMDB0010616	PG(18:1(11Z)/16:1(9Z))	C40H75O10P	M+Na	769.4990	0.6
	HMDB0010589	PG(16:1(9Z)/18:1(9Z))	C40H75O10P	M+Na	769.4990	0.6
	HMDB0010588	PG(16:1(9Z)/18:1(11Z))	C40H75O10P	M+Na	769.4990	0.6
	HMDB0010575	PG(16/18:2(9Z,12Z))	C40H75O10P	M+Na	769.4990	0.6
770.1765	HMDB0169799	6-{2-[4,5-dihydroxy-6-(hydroxymethyl)-3-(3,4,5-trihydroxybenzoyloxy)oxan-2-yl]-6-(3,4-dihydroxybenzoyl)-3,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H32O21	M+NH4	770.1774	-1.2
	HMDB0170030	6-{5-[(6-[3-(3,4-dihydroxybenzoyl)-2,4,6-trihydroxyphenyl]-3,4,5-trihydroxyoxan-2-yl)methoxy]carbonyl]-2,3-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H32O21	M+NH4	770.1774	-1.2
	HMDB0170029	6-[4-(3,4-dihydroxybenzoyl)-3,5-dihydroxy-2-{3,4,5-trihydroxy-6-[(3,4,5-trihydroxybenzoyloxy)methyl]oxan-2-yl}phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H32O21	M+NH4	770.1774	-1.2
	HMDB0170026	3,4,5-trihydroxy-6-[2-hydroxy-4-(2,4,6-trihydroxy-3-{3,4,5-trihydroxy-6-[(3,4,5-trihydroxybenzoyloxy)methyl]oxan-2-yl}benzoyl)phenoxy]oxane-2-carboxylic acid	C32H32O21	M+NH4	770.1774	-1.2
	HMDB0170025	6-[2-(3,4-dihydroxybenzoyl)-3,5-dihydroxy-6-{3,4,5-trihydroxy-6-[(3,4,5-trihydroxybenzoyloxy)methyl]oxan-2-yl}phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H32O21	M+NH4	770.1774	-1.2
	HMDB0170027	3,4,5-trihydroxy-6-[2-hydroxy-5-(2,4,6-trihydroxy-3-{3,4,5-trihydroxy-6-[(3,4,5-trihydroxybenzoyloxy)methyl]oxan-2-yl}benzoyl)phenoxy]oxane-2-carboxylic acid	C32H32O21	M+NH4	770.1774	-1.2
	HMDB0170028	6-[2-(3,4-dihydroxybenzoyl)-3,5-dihydroxy-4-{3,4,5-trihydroxy-6-[(3,4,5-trihydroxybenzoyloxy)methyl]oxan-2-yl}phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H32O21	M+NH4	770.1774	-1.2
	HMDB0169805	6-{4-[(2-[3-(3,4-dihydroxybenzoyl)-2,4,6-trihydroxyphenyl]-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy)carbonyl]-2,6-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H32O21	M+NH4	770.1774	-1.2
	HMDB0169804	6-{5-[(2-[3-(3,4-dihydroxybenzoyl)-2,4,6-trihydroxyphenyl]-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy)carbonyl]-2,3-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H32O21	M+NH4	770.1774	-1.2
	HMDB0169802	6-{4-[4,5-dihydroxy-6-(hydroxymethyl)-3-(3,4,5-trihydroxybenzoyloxy)oxan-2-yl]-2-(3,4-dihydroxybenzoyl)-3,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H32O21	M+NH4	770.1774	-1.2
	HMDB0169803	6-{2-[4,5-dihydroxy-6-(hydroxymethyl)-3-(3,4,5-trihydroxybenzoyloxy)oxan-2-yl]-4-(3,4-dihydroxybenzoyl)-3,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H32O21	M+NH4	770.1774	-1.2

	HMDB0169801	6-(5-{3-[4,5-dihydroxy-6-(hydroxymethyl)-3-(3,4,5-trihydroxybenzoyloxy)oxan-2-yl]-2,4,6-trihydroxybenzoyl}-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H32O21	M+NH4	770.1774	-1.2
	HMDB0169800	6-(4-{3-[4,5-dihydroxy-6-(hydroxymethyl)-3-(3,4,5-trihydroxybenzoyloxy)oxan-2-yl]-2,4,6-trihydroxybenzoyl}-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H32O21	M+NH4	770.1774	-1.2
	HMDB0170031	6-{4-[(6-{3-(3,4-dihydroxybenzoyl)-2,4,6-trihydroxyphenyl}-3,4,5-trihydroxyoxan-2-yl)methoxy]carbonyl}-2,6-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H32O21	M+NH4	770.1774	-1.2
770.5094	HMDB0005780	PE(P-16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H74NO7P	M+Na	770.5095	-0.1
	HMDB0011453	PE(P-18:1(9Z))/:5(5Z,8Z,11Z,14Z,17Z))	C43H74NO7P	M+Na	770.5095	-0.1
	HMDB0011420	PE(P-18:1(11Z))/:5(5Z,8Z,11Z,14Z,17Z))	C43H74NO7P	M+Na	770.5095	-0.1
	HMDB0009708	PE(22:6(4Z,7Z,Z,13Z,16Z,19Z)/P-16)	C43H74NO7P	M+Na	770.5095	-0.1
	HMDB0009479	PE(:5(5Z,8Z,11Z,14Z,17Z)/P-18:1(11Z))	C43H74NO7P	M+Na	770.5095	-0.1
	HMDB0009480	PE(:5(5Z,8Z,11Z,14Z,17Z)/P-18:1(9Z))	C43H74NO7P	M+Na	770.5095	-0.1
	HMDB0113911	PE-NMe2(14:1(9Z)/22:2(13Z,16Z))	C43H80NO8P	M+H	770.5694	0.3
	HMDB0113949	PE-NMe2(16/:3(5Z,8Z,11Z))	C43H80NO8P	M+H	770.5694	0.3
	HMDB0113950	PE-NMe2(16/:3(8Z,11Z,14Z))	C43H80NO8P	M+H	770.5694	0.3
	HMDB0113992	PE-NMe2(18/18:3(9Z,12Z,15Z))	C43H80NO8P	M+H	770.5694	0.3
	HMDB0113991	PE-NMe2(18/18:3(6Z,9Z,12Z))	C43H80NO8P	M+H	770.5694	0.3
	HMDB0114017	PE-NMe2(18:1(11Z)/18:2(9Z,12Z))	C43H80NO8P	M+H	770.5694	0.3
	HMDB0114044	PE-NMe2(18:1(9Z)/18:2(9Z,12Z))	C43H80NO8P	M+H	770.5694	0.3
	HMDB0114071	PE-NMe2(18:2(9Z,12Z)/18:1(11Z))	C43H80NO8P	M+H	770.5694	0.3
	HMDB0114072	PE-NMe2(18:2(9Z,12Z)/18:1(9Z))	C43H80NO8P	M+H	770.5694	0.3
	HMDB0114099	PE-NMe2(18:3(6Z,9Z,12Z)/18)	C43H80NO8P	M+H	770.5694	0.3
	HMDB0114128	PE-NMe2(18:3(9Z,12Z,15Z)/18)	C43H80NO8P	M+H	770.5694	0.3
	HMDB0114271	PE-NMe2(:3(5Z,8Z,11Z)/16)	C43H80NO8P	M+H	770.5694	0.3
	HMDB0114299	PE-NMe2(:3(8Z,11Z,14Z)/16)	C43H80NO8P	M+H	770.5694	0.3
	HMDB0114467	PE-NMe2(22:2(13Z,16Z)/14:1(9Z))	C43H80NO8P	M+H	770.5694	0.3
	HMDB0113970	PE-NMe2(16:1(9Z)/:2(11Z,14Z))	C43H80NO8P	M+H	770.5694	0.3
	HMDB0114243	PE-NMe2(:2(11Z,14Z)/16:1(9Z))	C43H80NO8P	M+H	770.5694	0.3
	HMDB0009258	PE(:1(11Z)/18:2(9Z,12Z))	C43H80NO8P	M+H	770.5694	0.3
	HMDB0007948	PC(15/:3(8Z,11Z,14Z))	C43H80NO8P	M+H	770.5694	0.3
	HMDB0009354	PE(:3(8Z,11Z,14Z)/18)	C43H80NO8P	M+H	770.5694	0.3
	HMDB0009321	PE(:3(5Z,8Z,11Z)/18)	C43H80NO8P	M+H	770.5694	0.3

770.5697

HMDB0009289	PE(:2(11Z,14Z)/18:1(11Z))	C43H80NO8P	M+H	770.5694	0.3
HMDB0009290	PE(:2(11Z,14Z)/18:1(9Z))	C43H80NO8P	M+H	770.5694	0.3
HMDB0009226	PE(/18:3(6Z,9Z,12Z))	C43H80NO8P	M+H	770.5694	0.3
HMDB0009227	PE(/18:3(9Z,12Z,15Z))	C43H80NO8P	M+H	770.5694	0.3
HMDB0009163	PE(18:3(9Z,12Z,15Z)/)	C43H80NO8P	M+H	770.5694	0.3
HMDB0009130	PE(18:3(6Z,9Z,12Z)/)	C43H80NO8P	M+H	770.5694	0.3
HMDB0009001	PE(18/:3(5Z,8Z,11Z))	C43H80NO8P	M+H	770.5694	0.3
HMDB0009098	PE(18:2(9Z,12Z)/:1(11Z))	C43H80NO8P	M+H	770.5694	0.3
HMDB0009066	PE(18:1(9Z)/:2(11Z,14Z))	C43H80NO8P	M+H	770.5694	0.3
HMDB0009033	PE(18:1(11Z)/:2(11Z,14Z))	C43H80NO8P	M+H	770.5694	0.3
HMDB0009002	PE(18/:3(8Z,11Z,14Z))	C43H80NO8P	M+H	770.5694	0.3
HMDB0008975	PE(16:1(9Z)/22:2(13Z,16Z))	C43H80NO8P	M+H	770.5694	0.3
HMDB0008396	PC(:3(8Z,11Z,14Z)/15)	C43H80NO8P	M+H	770.5694	0.3
HMDB0008363	PC(:3(5Z,8Z,11Z)/15)	C43H80NO8P	M+H	770.5694	0.3
HMDB0007947	PC(15/:3(5Z,8Z,11Z))	C43H80NO8P	M+H	770.5694	0.3
HMDB0009551	PE(22:2(13Z,16Z)/16:1(9Z))	C43H80NO8P	M+H	770.5694	0.3
HMDB0115328	PA(22:4(7Z,Z,13Z,16Z)/18)	C43H77O8P	M+NH4	770.5694	0.4
HMDB0115573	PA(:3(8Z,11Z,14Z)/:1(11Z))	C43H77O8P	M+NH4	770.5694	0.4
HMDB0115545	PA(:2(11Z,14Z)/:2(11Z,14Z))	C43H77O8P	M+NH4	770.5694	0.4
HMDB0115531	PA(:1(11Z)/:3(8Z,11Z,14Z))	C43H77O8P	M+NH4	770.5694	0.4
HMDB0115304	PA(22:2(13Z,16Z)/18:2(9Z,12Z))	C43H77O8P	M+NH4	770.5694	0.4
HMDB0114890	PA(18/22:4(7Z,Z,13Z,16Z))	C43H77O8P	M+NH4	770.5694	0.4
HMDB0114992	PA(18:3(6Z,9Z,12Z)/22:1(13Z))	C43H77O8P	M+NH4	770.5694	0.4
HMDB0115019	PA(18:3(9Z,12Z,15Z)/22:1(13Z))	C43H77O8P	M+NH4	770.5694	0.4
HMDB0115045	PA(18:4(6Z,9Z,12Z,15Z)/22)	C43H77O8P	M+NH4	770.5694	0.4
HMDB0115078	PA(/:4(5Z,8Z,11Z,14Z))	C43H77O8P	M+NH4	770.5694	0.4
HMDB0115079	PA(/:4(8Z,11Z,14Z,17Z))	C43H77O8P	M+NH4	770.5694	0.4
HMDB0115105	PA(:1(11Z)/:3(5Z,8Z,11Z))	C43H77O8P	M+NH4	770.5694	0.4
HMDB0115131	PA(:3(5Z,8Z,11Z)/:1(11Z))	C43H77O8P	M+NH4	770.5694	0.4
HMDB0115156	PA(:4(5Z,8Z,11Z,14Z)/)	C43H77O8P	M+NH4	770.5694	0.4
HMDB0115183	PA(:4(8Z,11Z,14Z,17Z)/)	C43H77O8P	M+NH4	770.5694	0.4
HMDB0115251	PA(22/18:4(6Z,9Z,12Z,15Z))	C43H77O8P	M+NH4	770.5694	0.4
HMDB0115279	PA(22:1(13Z)/18:3(6Z,9Z,12Z))	C43H77O8P	M+NH4	770.5694	0.4
HMDB0115280	PA(22:1(13Z)/18:3(9Z,12Z,15Z))	C43H77O8P	M+NH4	770.5694	0.4
HMDB0114966	PA(18:2(9Z,12Z)/22:2(13Z,16Z))	C43H77O8P	M+NH4	770.5694	0.4
HMDB0013405	PC(O-16/18)	C42H86NO7P	M+Na	770.6034	2.1
HMDB0013429	PC(O-18:1(9Z)/18:2(9Z,12Z))	C44H84NO7P	M+H	770.6058	-1.1
HMDB0013425	PC(O-18:1(11Z)/18:2(9Z,12Z))	C44H84NO7P	M+H	770.6058	-1.1
HMDB0039527	PC(O-16/:3(8Z,11Z,14Z))	C44H84NO7P	M+H	770.6058	-1.1
HMDB0011309	PC(P-18:1(9Z)/18:1(9Z))	C44H84NO7P	M+H	770.6058	-1.1
HMDB0011308	PC(P-18:1(9Z)/18:1(11Z))	C44H84NO7P	M+H	770.6058	-1.1
HMDB0011276	PC(P-18:1(11Z)/18:1(9Z))	C44H84NO7P	M+H	770.6058	-1.1

770.6050	HMDB0011275	PC(P-18:1(11Z)/18:1(11Z))	C44H84NO7P	M+H	770.6058	-1.1
	HMDB0011244	PC(P-18/18:2(9Z,12Z))	C44H84NO7P	M+H	770.6058	-1.1
	HMDB0011217	PC(P-16/:2(11Z,14Z))	C44H84NO7P	M+H	770.6058	-1.1
	HMDB0008357	PC(:2(11Z,14Z)/P-16)	C44H84NO7P	M+H	770.6058	-1.1
	HMDB0008160	PC(18:2(9Z,12Z)/P-18)	C44H84NO7P	M+H	770.6058	-1.1
	HMDB0008129	PC(18:1(9Z)/P-18:1(9Z))	C44H84NO7P	M+H	770.6058	-1.1
	HMDB0008128	PC(18:1(9Z)/P-18:1(11Z))	C44H84NO7P	M+H	770.6058	-1.1
	HMDB0008096	PC(18:1(11Z)/P-18:1(9Z))	C44H84NO7P	M+H	770.6058	-1.1
	HMDB0008095	PC(18:1(11Z)/P-18:1(11Z))	C44H84NO7P	M+H	770.6058	-1.1
771.2197	HMDB0163002	3,4,5-trihydroxy-2-(2,3,4,5,6-pentahydroxy-1-{2,3,4-trihydroxy-6-oxo-3-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]cyclohexa-1,4-dien-1-yl}hexyl)-4-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]cyclohexa-2,5-dien-1-one	C30H42O23	M+H	771.2190	1.0
771.5125	HMDB0010573	PG(16/18:1(11Z))	C40H77O10P	M+Na	771.5147	-2.8
	HMDB0010574	PG(16/18:1(9Z))	C40H77O10P	M+Na	771.5147	-2.8
	HMDB0010587	PG(16:1(9Z)/18)	C40H77O10P	M+Na	771.5147	-2.8
	HMDB0010601	PG(18/16:1(9Z))	C40H77O10P	M+Na	771.5147	-2.8
	HMDB0010615	PG(18:1(11Z)/16)	C40H77O10P	M+Na	771.5147	-2.8
	HMDB0010630	PG(18:1(9Z)/16)	C40H77O10P	M+Na	771.5147	-2.8
772.2666	HMDB0030335	1,2-Disinapoylgentiobiose	C34H42O19	M+NH4	772.2659	1.0
	HMDB0040838	3',6'-Disinapoylsucrose	C34H42O19	M+NH4	772.2659	1.0
	HMDB0040804	Kaempferide 3-[rhamnopyranosyl-(1->6)-glucoside] 7-rhamnoside	C34H42O19	M+NH4	772.2659	1.0
	HMDB0039175	Raphanusol A	C34H42O19	M+NH4	772.2659	1.0
772.4219	HMDB0186057	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{3-hydroxy-3-methyl-1,4-dioxo-2-(3,7,11,15-tetramethylhexadeca-2,15-dien-1-yl)-1,2,3,4-tetrahydronaphthalen-2-yl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C41H61N3O9S	M+H	772.4201	2.3
	HMDB0186058	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{3-hydroxy-2-methyl-1,4-dioxo-3-(3,7,11,15-tetramethylhexadeca-2,15-dien-1-yl)-1,2,3,4-tetrahydronaphthalen-2-yl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C41H61N3O9S	M+H	772.4201	2.3
	HMDB0186056	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{3-hydroxy-2-methyl-1,4-dioxo-3-(3,7,15-trimethyl-11-methylidenehexadec-2-en-1-yl)-1,2,3,4-tetrahydronaphthalen-2-yl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C41H61N3O9S	M+H	772.4201	2.3
	HMDB0186053	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{3-hydroxy-3-methyl-1,4-dioxo-2-(3,11,15-trimethyl-7-methylidenehexadec-2-en-1-yl)-1,2,3,4-tetrahydronaphthalen-2-yl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C41H61N3O9S	M+H	772.4201	2.3

	HMDB0186054	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{[3-hydroxy-2-methyl-1,4-dioxo-3-(3,11,15-trimethyl-7-methylidenehexadec-2-en-1-yl)-1,2,3,4-tetrahydronaphthalen-2-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C41H61N3O9S	M+H	772.4201	2.3
	HMDB0186055	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{[3-hydroxy-3-methyl-1,4-dioxo-2-(3,7,15-trimethyl-11-methylidenehexadec-2-en-1-yl)-1,2,3,4-tetrahydronaphthalen-2-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C41H61N3O9S	M+H	772.4201	2.3
772.5846	HMDB0115530	PA(:1(11Z):2(11Z,14Z))	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0115572	PA(:3(8Z,11Z,14Z)/)	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0115544	PA(:2(11Z,14Z):1(11Z))	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0115529	PA(/:3(8Z,11Z,14Z))	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0115303	PA(22:2(13Z,16Z)/18:1(9Z))	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0115302	PA(22:2(13Z,16Z)/18:1(11Z))	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0115278	PA(22:1(13Z)/18:2(9Z,12Z))	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0115250	PA(22/18:3(9Z,12Z,15Z))	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0115249	PA(22/18:3(6Z,9Z,12Z))	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0115130	PA(:3(5Z,8Z,11Z)/)	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0114914	PA(18:1(11Z)/22:2(13Z,16Z))	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0114939	PA(18:1(9Z)/22:2(13Z,16Z))	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0114965	PA(18:2(9Z,12Z)/22:1(13Z))	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0114991	PA(18:3(6Z,9Z,12Z)/22)	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0115018	PA(18:3(9Z,12Z,15Z)/22)	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0115077	PA(/:3(5Z,8Z,11Z))	C43H79O8P	M+NH4	772.5851	-0.6
	HMDB0009097	PE(18:2(9Z,12Z)/)	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0008942	PE(16/22:2(13Z,16Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0009288	PE(:2(11Z,14Z)/18)	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0009257	PE(:1(11Z)/18:1(9Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0009256	PE(:1(11Z)/18:1(11Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0009225	PE(/18:2(9Z,12Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0009065	PE(18:1(9Z):1(11Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0009032	PE(18:1(11Z):1(11Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0009000	PE(18/:2(11Z,14Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0008974	PE(16:1(9Z)/22:1(13Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0008882	PE(14:1(9Z)/24:1(15Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0008330	PC(:2(11Z,14Z)/15)	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0007946	PC(15/:2(11Z,14Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0009518	PE(22:1(13Z)/16:1(9Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0009550	PE(22:2(13Z,16Z)/16)	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0009746	PE(24:1(15Z)/14:1(9Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0010564	PE-NMe2(18:1(9Z)/18:1(9Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0113565	PE-NMe(22:2(13Z,16Z)/15)	C43H82NO8P	M+H	772.5851	-0.6

	HMDB0113990	PE-NMe2(18/18:2(9Z,12Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0113910	PE-NMe2(14:1(9Z)/22:1(13Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0113033	PE-NMe(15/22:2(13Z,16Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0113892	PE-NMe2(14/22:2(13Z,16Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0114214	PE-NMe2(:1(11Z)/16:1(9Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0114438	PE-NMe2(22:1(13Z)/14:1(9Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0114070	PE-NMe2(18:2(9Z,12Z)/18)	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0114242	PE-NMe2(:2(11Z,14Z)/16)	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0113948	PE-NMe2(16/:2(11Z,14Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0114466	PE-NMe2(22:2(13Z,16Z)/14)	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0113870	PE-NMe2(18:1(11Z)/18:1(11Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0113869	PE-NMe2(18:1(11Z)/18:1(9Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0113868	PE-NMe2(18:1(9Z)/18:1(11Z))	C43H82NO8P	M+H	772.5851	-0.6
	HMDB0113867	PE-NMe2(16:1(9Z)/:1(11Z))	C43H82NO8P	M+H	772.5851	-0.6
773.0811	HMDB0134693	2,3,4,7,8,9,15,21,22,23,28-undecahydroxy-14-(hydroxymethyl)-12,27,31,34-tetraoxo-13,25,32,35-tetraoxaoctacyclo[14.13.3.3?????]pentatriaconta-1,3,5(),6,8,,19,21,23-nonaene--carboxylic acid	C33H24O22	M+H	773.0832	-2.7
	HMDB0134699	2,3,4,7,8,9,15,22,23,28,33-undecahydroxy-14-(hydroxymethyl)-12,27,31,34-tetraoxo-13,25,32,35-tetraoxaoctacyclo[14.13.3.3?????]pentatriaconta-1,3,5(),6,8,,19(24),,22-nonaene--carboxylic acid	C33H24O22	M+H	773.0832	-2.7
773.2158	HMDB0125130	3-{[4,5-dihydroxy-6-(hydroxymethyl)-3-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}oxan-2-yl]oxy}-2-(3,4-dihydroxyphenyl)-7-hydroxy-5-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-1-yl?chromen-1-ylum	C33H41O21	M+H	773.2135	3.0
	HMDB0032008	kaempferol 3-O-beta-D-glucosyl-(1->2)-beta-D-glucosyl-(1->2)-beta-D-glucoside	C33H40O21	M+H	773.2135	3.0
	HMDB0177369	3,4,5-trihydroxy-6-[(8-methoxy-2-methyl-4-oxo--{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}methyl)oxan-2-yl]oxy}-4H-benzo[h]chromen-5-yl]oxy]oxane-2-	C33H40O21	M+H	773.2135	3.0
	HMDB0176662	3,4,5-trihydroxy-6-[(8-methoxy-2-methyl-4-oxo-6-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}methyl)oxan-2-yl]oxy}-4H-benzof[g]chromen-5-yl]oxy]oxane-2-	C33H40O21	M+H	773.2135	3.0
	HMDB0141985	6-({2-[3,4-bis(2-hydroxyethoxy)phenyl]-7-(2-hydroxyethoxy)-4-oxo-3-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-4H-chromen-5-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C33H40O21	M+H	773.2135	3.0
	HMDB0136152	7-{[3,4-dihydroxy-6-(hydroxymethyl)-5-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}oxan-2-yl]oxy}-5-hydroxy-2-(4-hydroxyphenyl)-3-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-4H-chromen-4-one	C33H40O21	M+H	773.2135	3.0
	HMDB0135148	3-[(3,4-dihydroxy-6-methyl-5-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}oxan-2-yl]oxy]-2-(3,4-dihydroxyphenyl)-5-hydroxy-7-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-4H-chromen-4-one	C33H40O21	M+H	773.2135	3.0

	HMDB0126863	3,4,5-trihydroxy-6-[[7-hydroxy-2-(4-hydroxyphenyl)-4-oxo-6,8-bis[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-3,4-dihydro-2H-1-benzopyran-5-yl]oxy]oxane-2-carboxylic acid	C33H40O21	M+H	773.2135	3.0
	HMDB0126862	6-(4-{5,7-dihydroxy-4-oxo-6,8-bis[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-3,4-dihydro-2H-1-benzopyran-2-yl}phenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C33H40O21	M+H	773.2135	3.0
	HMDB0126861	3,4,5-trihydroxy-6-[[5-hydroxy-2-(4-hydroxyphenyl)-4-oxo-6,8-bis[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-3,4-dihydro-2H-1-benzopyran-7-yl]oxy]oxane-2-carboxylic acid	C33H40O21	M+H	773.2135	3.0
	HMDB0037957	Quercetin 3-rutinoside 7-galactoside	C33H40O21	M+H	773.2135	3.0
	HMDB0037960	Quercetin 3-(2G-glucosylrutinoside)	C33H40O21	M+H	773.2135	3.0
	HMDB0039363	Quercetin 3-(3R-glucosylrutinoside)	C33H40O21	M+H	773.2135	3.0
	HMDB0039375	Hyperin 6"-[glucosyl-(1->3)-rhamnoside]	C33H40O21	M+H	773.2135	3.0
	HMDB0037936	Quercetin 3-(2G-rhamnosylgentiobioside)	C33H40O21	M+H	773.2135	3.0
	HMDB0041771	Quercetin 3-O-glucosyl-rutinoside	C33H40O21	M+H	773.2135	3.0
	HMDB0037207	Kaempferol 3-sophoroside 7-glucoside	C33H40O21	M+H	773.2135	3.0
	HMDB0037995	Cyanidin 3-sophorotrioside	C33H41O21	M+H	773.2140	2.3
	HMDB0041716	Cyanidin 3-diglucoside 5-glucoside	C33H41O21	M+H	773.2140	2.3
	HMDB0037973	Cyanidin 3,3',5-triglucoside	C33H41O21	M+H	773.2140	2.3
	HMDB0038487	Cyanidin 3-sophoroside 5-glucoside	C33H41O21	M+H	773.2140	2.3
773.5348	HMDB0010579	PG(16/:3(8Z,11Z,14Z))	C42H77O10P	M+H	773.5327	2.7
	HMDB0010607	PG(18/18:3(9Z,12Z,15Z))	C42H77O10P	M+H	773.5327	2.7
	HMDB0010606	PG(18/18:3(6Z,9Z,12Z))	C42H77O10P	M+H	773.5327	2.7
	HMDB0010620	PG(18:1(11Z)/18:2(9Z,12Z))	C42H77O10P	M+H	773.5327	2.7
	HMDB0010635	PG(18:1(9Z)/18:2(9Z,12Z))	C42H77O10P	M+H	773.5327	2.7
	HMDB0010648	PG(18:2(9Z,12Z)/18:1(11Z))	C42H77O10P	M+H	773.5327	2.7
	HMDB0010649	PG(18:2(9Z,12Z)/18:1(9Z))	C42H77O10P	M+H	773.5327	2.7
	HMDB0010662	PG(18:3(6Z,9Z,12Z)/18)	C42H77O10P	M+H	773.5327	2.7
	HMDB0010677	PG(18:3(9Z,12Z,15Z)/18)	C42H77O10P	M+H	773.5327	2.7
	HMDB0010578	PG(16/:3(5Z,8Z,11Z))	C42H77O10P	M+H	773.5327	2.7
	HMDB0115459	PA(24:1(15Z)/16:1(9Z))	C43H81O8P	M+NH4	774.6007	-0.2
	HMDB0115543	PA(:2(11Z,14Z)/)	C43H81O8P	M+NH4	774.6007	-0.2
	HMDB0115528	PA(/:2(11Z,14Z))	C43H81O8P	M+NH4	774.6007	-0.2
	HMDB0115301	PA(22:2(13Z,16Z)/18)	C43H81O8P	M+NH4	774.6007	-0.2
	HMDB0115276	PA(22:1(13Z)/18:1(11Z))	C43H81O8P	M+NH4	774.6007	-0.2
	HMDB0115277	PA(22:1(13Z)/18:1(9Z))	C43H81O8P	M+NH4	774.6007	-0.2
	HMDB0115248	PA(22/18:2(9Z,12Z))	C43H81O8P	M+NH4	774.6007	-0.2
	HMDB0114872	PA(16:1(9Z)/24:1(15Z))	C43H81O8P	M+NH4	774.6007	-0.2
	HMDB0114889	PA(18/22:2(13Z,16Z))	C43H81O8P	M+NH4	774.6007	-0.2
	HMDB0114913	PA(18:1(11Z)/22:1(13Z))	C43H81O8P	M+NH4	774.6007	-0.2
	HMDB0114938	PA(18:1(9Z)/22:1(13Z))	C43H81O8P	M+NH4	774.6007	-0.2
	HMDB0114964	PA(18:2(9Z,12Z)/22)	C43H81O8P	M+NH4	774.6007	-0.2
	HMDB0115104	PA(:1(11Z)/:1(11Z))	C43H81O8P	M+NH4	774.6007	-0.2
	HMDB0007945	PC(15/:1(11Z))	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0009485	PE(22/16:1(9Z))	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0009255	PE(:1(11Z)/18)	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0008999	PE(18/:1(11Z))	C43H84NO8P	M+H	774.6007	-0.2

774.6006	HMDB0009223	PE(/18:1(11Z))	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0009224	PE(/18:1(9Z))	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0009064	PE(18:1(9Z)/)	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0009031	PE(18:1(11Z)/)	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0008973	PE(16:1(9Z)/22)	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0008941	PE(16/22:1(13Z))	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0008881	PE(14:1(9Z)/24)	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0008849	PE(14/24:1(15Z))	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0008297	PC(:1(11Z)/15)	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0009517	PE(22:1(13Z)/16)	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0009745	PE(24:1(15Z)/14)	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0009713	PE(24/14:1(9Z))	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0114411	PE-NMe2(22/14:1(9Z))	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0113032	PE-NMe(15/22:1(13Z))	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0113537	PE-NMe(22:1(13Z)/15)	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0113891	PE-NMe2(14/22:1(13Z))	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0114016	PE-NMe2(18:1(11Z)/18)	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0114043	PE-NMe2(18:1(9Z)/18)	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0114185	PE-NMe2(/16:1(9Z))	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0114437	PE-NMe2(22:1(13Z)/14)	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0114213	PE-NMe2(:1(11Z)/16)	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0113875	PE-NMe2(16:1(9Z)/)	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0113873	PE-NMe2(14:1(9Z)/22)	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0113874	PE-NMe2(16/:1(11Z))	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0113872	PE-NMe2(18/18:1(11Z))	C43H84NO8P	M+H	774.6007	-0.2
	HMDB0113871	PE-NMe2(18/18:1(9Z))	C43H84NO8P	M+H	774.6007	-0.2
775.1457	HMDB0129146	{2-hydroxy-5-[7,15,23-trihydroxy-11,19-bis(4-hydroxyphenyl)-4,12,-trioxahaptacyclo[16.6.1.1,?1?,??heptacosa-1(25),5,7,9(27),13,15,17(26),21,23-nonaen-3-yl]phenyl}oxidanesulfonic acid	C42H30O13S	M+H	775.1480	-3.0
775.9539	HMDB0240386	Cangrelor	C17H25Cl2F3N5O12P3S2	M+H	775.9556	-2.2
	HMDB0030915	1-Hydroxyepiacorone	C39H62O14	M+Na	777.4032	-2.9

777.4009	HMDB0166548	2-([4,5-dihydroxy-6-(hydroxymethyl)-2-[5-(hydroxymethyl)-5,7',9',13'-tetramethyl-5'-oxaspiro[oxolane-2,6'-pentacyclo[.8,?,甾icosan]-18'-eneoxy]oxan-3-yl]oxy]-6-(hydroxymethyl)oxane-3,4,5-triol	C39H62O14	M+Na	777.4032	-2.9
	HMDB0036251	Schidigerasaponin C2	C39H62O14	M+Na	777.4032	-2.9
	HMDB0034211	Agavoside B	C39H62O14	M+Na	777.4032	-2.9
	HMDB0166660	2-(hydroxymethyl)-6-([5,7',9',13'-tetramethyl-16'-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-5'-oxaspiro[oxolane-2,6'-pentacyclo[.8,?,甾icosan]-18'-en-5-yl]methoxy]oxane-3,4,5-triol	C39H62O14	M+Na	777.4032	-2.9
	HMDB0113090	PE-NMe(18/18:3(6Z,9Z,12Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113011	PE-NMe(14:1(9Z)/22:2(13Z,16Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113048	PE-NMe(16/:3(5Z,8Z,11Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113049	PE-NMe(16/:3(8Z,11Z,14Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113341	PE-NMe(:2(11Z,14Z)/16:1(9Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113116	PE-NMe(18:1(11Z)/18:2(9Z,12Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113170	PE-NMe(18:2(9Z,12Z)/18:1(11Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113171	PE-NMe(18:2(9Z,12Z)/18:1(9Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113226	PE-NMe(18:3(9Z,12Z,15Z)/18)	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113369	PE-NMe(:3(5Z,8Z,11Z)/16)	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113397	PE-NMe(:3(8Z,11Z,14Z)/16)	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113564	PE-NMe(22:2(13Z,16Z)/14:1(9Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113926	PE-NMe2(15/:3(5Z,8Z,11Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113198	PE-NMe(18:3(6Z,9Z,12Z)/18)	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113927	PE-NMe2(15/:3(8Z,11Z,14Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0114270	PE-NMe2(:3(5Z,8Z,11Z)/15)	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0114298	PE-NMe2(:3(8Z,11Z,14Z)/15)	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113069	PE-NMe(16:1(9Z)/:2(11Z,14Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113091	PE-NMe(18/18:3(9Z,12Z,15Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0113143	PE-NMe(18:1(9Z)/18:2(9Z,12Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0008394	PC(:3(8Z,11Z,14Z)/14)	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0008361	PC(:3(5Z,8Z,11Z)/14)	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0008329	PC(:2(11Z,14Z)/14:1(9Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0008199	PC(18:3(9Z,12Z,15Z)/16)	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0008166	PC(18:3(6Z,9Z,12Z)/16)	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0008134	PC(18:2(9Z,12Z)/16:1(9Z))	C42H78NO8P	M+Na	778.5357	2.4
	HMDB0008006	PC(16:1(9Z)/18:2(9Z,12Z))	C42H78NO8P	M+Na	778.5357	2.4

778.5376

HMDB0007974	PC(16/18:3(6Z,9Z,12Z))	C42H78NO8P	M+Na	778.5357	2.4
HMDB0007975	PC(16/18:3(9Z,12Z,15Z))	C42H78NO8P	M+Na	778.5357	2.4
HMDB0007913	PC(14:1(9Z)/:2(11Z,14Z))	C42H78NO8P	M+Na	778.5357	2.4
HMDB0007882	PC(14/:3(8Z,11Z,14Z))	C42H78NO8P	M+Na	778.5357	2.4
HMDB0007881	PC(14/:3(5Z,8Z,11Z))	C42H78NO8P	M+Na	778.5357	2.4
HMDB0113058	PE-NMe(16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113079	PE-NMe(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113127	PE-NMe(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113154	PE-NMe(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113181	PE-NMe(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113182	PE-NMe(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113207	PE-NMe(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113208	PE-NMe(18:3(6Z,9Z,12Z)/:3(8Z,11Z,14Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113676	PE-NMe(22:6(4Z,7Z,Z,13Z,16Z,19Z)/16)	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113937	PE-NMe2(15/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0114578	PE-NMe2(22:6(4Z,7Z,Z,13Z,16Z,19Z)/15)	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113264	PE-NMe(18:4(6Z,9Z,12Z,15Z)/:2(11Z,14Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113348	PE-NMe(:2(11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113650	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113623	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113486	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113236	PE-NMe(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113237	PE-NMe(18:3(9Z,12Z,15Z)/:3(8Z,11Z,14Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113375	PE-NMe(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113376	PE-NMe(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113403	PE-NMe(:3(8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113404	PE-NMe(:3(8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113430	PE-NMe(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113458	PE-NMe(:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0113485	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0007923	PC(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C44H76NO8P	M+H	778.5381	-0.7
HMDB0008173	PC(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C44H76NO8P	M+H	778.5381	-0.7

	HMDB0007924	PC(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C44H76NO8P	M+H	778.5381	-0.7
	HMDB0008722	PC(22:6(4Z,7Z,Z,13Z,16Z,19Z)/14)	C44H76NO8P	M+H	778.5381	-0.7
	HMDB0008690	PC(22:5(7Z,Z,13Z,16Z,19Z)/14:1(9Z))	C44H76NO8P	M+H	778.5381	-0.7
	HMDB0008657	PC(22:5(4Z,7Z,Z,13Z,16Z)/14:1(9Z))	C44H76NO8P	M+H	778.5381	-0.7
	HMDB0008496	PC(:5(5Z,8Z,11Z,14Z,17Z)/16:1(9Z))	C44H76NO8P	M+H	778.5381	-0.7
	HMDB0008237	PC(18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C44H76NO8P	M+H	778.5381	-0.7
	HMDB0113080	PE-NMe(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C44H76NO8P	M+H	778.5381	-0.7
	HMDB0008205	PC(18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C44H76NO8P	M+H	778.5381	-0.7
	HMDB0008017	PC(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C44H76NO8P	M+H	778.5381	-0.7
	HMDB0008172	PC(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C44H76NO8P	M+H	778.5381	-0.7
	HMDB0007892	PC(14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C44H76NO8P	M+H	778.5381	-0.7
	HMDB0008142	PC(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C44H76NO8P	M+H	778.5381	-0.7
	HMDB0008206	PC(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C44H76NO8P	M+H	778.5381	-0.7
778.5740	HMDB0009313	PE(:2(11Z,14Z)/P-18)	C43H82NO7P	M+Na	778.5721	2.4
	HMDB0009576	PE(22:2(13Z,16Z)/P-16)	C43H82NO7P	M+Na	778.5721	2.4
	HMDB0011357	PE(P-16/22:2(13Z,16Z))	C43H82NO7P	M+Na	778.5721	2.4
	HMDB0011382	PE(P-18/:2(11Z,14Z))	C43H82NO7P	M+Na	778.5721	2.4
	HMDB0011414	PE(P-18:1(11Z)/:1(11Z))	C43H82NO7P	M+Na	778.5721	2.4
	HMDB0009281	PE(:1(11Z)/P-18:1(11Z))	C43H82NO7P	M+Na	778.5721	2.4
	HMDB0011447	PE(P-18:1(9Z)/:1(11Z))	C43H82NO7P	M+Na	778.5721	2.4
	HMDB0009282	PE(:1(11Z)/P-18:1(9Z))	C43H82NO7P	M+Na	778.5721	2.4
	HMDB0009643	PE(22:5(4Z,7Z,Z,13Z,16Z)/P-18)	C45H80NO7P	M+H	778.5745	-0.7
	HMDB0011457	PE(P-18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C45H80NO7P	M+H	778.5745	-0.7
	HMDB0011424	PE(P-18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C45H80NO7P	M+H	778.5745	-0.7
	HMDB0011393	PE(P-18/22:5(7Z,Z,13Z,16Z,19Z))	C45H80NO7P	M+H	778.5745	-0.7
	HMDB0009611	PE(22:4(7Z,Z,13Z,16Z)/P-18:1(11Z))	C45H80NO7P	M+H	778.5745	-0.7
	HMDB0009676	PE(22:5(7Z,Z,13Z,16Z,19Z)/P-18)	C45H80NO7P	M+H	778.5745	-0.7
	HMDB0009612	PE(22:4(7Z,Z,13Z,16Z)/P-18:1(9Z))	C45H80NO7P	M+H	778.5745	-0.7
	HMDB0011392	PE(P-18/22:5(4Z,7Z,Z,13Z,16Z))	C45H80NO7P	M+H	778.5745	-0.7
	HMDB0030581	(3S,3'R,4xi)-beta,beta-Carotene-3,3',4-triol	C36H37O18	M+Na	779.1799	-0.3
	HMDB0146178	[(6-{[2-(3,4-dihydroxyphenyl)-7-hydroxy-5-oxo-5H-chromen-3-yl]oxy}-3,4-dihydroxy-5-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}oxan-2-yl)methyl][1-hydroxy-3-(4-hydroxyphenyl)prop-2-en-1-ylidene]oxidanium	C36H37O18	M+Na	779.1794	0.4

HMDB0125124	({6-([2-([2-(3,4-dihydroxyphenyl)-7-hydroxy-5-oxo-5H-chromen-3-yl]oxy)-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy)-3,4,5-trihydroxyoxan-2-yl] methyl)[1-hydroxy-3-(4-hydroxyphenyl)prop-2-en-1-ylidene]oxidanium	C36H37O18	M+Na	779.1794	0.4
HMDB0154479	6-(3-{3-[2-(3,5-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-2-hydroxy-3-(2,4,6-trihydroxyphenyl)propyl}-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0149743	6-{3,5-dihydroxy-4-[2-hydroxy-3-(3-hydroxyphenyl)-1-[3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-8-yl]propyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0149744	6-([3,5-dihydroxy-8-[2-hydroxy-3-(3-hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)propyl]-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-7-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0149741	3,4,5-trihydroxy-6-(3-{2-hydroxy-3-[3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-8-yl]-3-(2,4,6-trihydroxyphenyl)propyl}phenoxy)oxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0149742	6-{3,5-dihydroxy-2-[2-hydroxy-3-(3-hydroxyphenyl)-1-[3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-8-yl]propyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0149740	6-(2,3-dihydroxy-5-{3,5,7-trihydroxy-8-[2-hydroxy-3-(3-hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)propyl]-3,4-dihydro-2H-1-benzopyran-2-yl}phenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0149736	6-{[2-(3,5-dihydroxyphenyl)-8-[3-(3,4-dihydroxyphenyl)-2-hydroxy-1-(2,4,6-trihydroxyphenyl)propyl]-3,5-dihydroxy-3,4-dihydro-2H-1-benzopyran-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0149735	6-{4-[3-(3,4-dihydroxyphenyl)-1-[2-(3,5-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-2-hydroxypropyl]-3,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0149732	6-(5-{3-[2-(3,5-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-2-hydroxy-3-(2,4,6-trihydroxyphenyl)propyl]-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0149731	6-(3-{8-[3-(3,4-dihydroxyphenyl)-2-hydroxy-1-(2,4,6-trihydroxyphenyl)propyl]-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-2-yl]-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0149734	6-{2-[3-(3,4-dihydroxyphenyl)-1-[2-(3,5-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-2-hydroxypropyl]-3,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0149733	6-(4-{3-[2-(3,5-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-2-hydroxy-3-(2,4,6-trihydroxyphenyl)propyl]-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0154481	6-{[2-(3,5-dihydroxyphenyl)-8-[3-(3,5-dihydroxyphenyl)-2-hydroxy-1-(2,4,6-trihydroxyphenyl)propyl]-3,5-dihydroxy-3,4-dihydro-2H-1-benzopyran-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4

779.1797

HMDB0154480	6-(3-{8-[3-(3,5-dihydroxyphenyl)-2-hydroxy-1-(2,4,6-trihydroxyphenyl)propyl]-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-2-yl}-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0154482	6-{2-[3-(3,5-dihydroxyphenyl)-1-[2-(3,5-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-2-hydroxypropyl]-3,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0154534	6-{2-[3-(3,5-dihydroxyphenyl)-1-[2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-2-hydroxypropyl]-3,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0154533	6-(3-{3-[2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-2-hydroxy-3-(2,4,6-trihydroxyphenyl)propyl]-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0154535	6-{4-[3-(3,5-dihydroxyphenyl)-1-[2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-2-hydroxypropyl]-3,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0154536	6-(5-{8-[3-(3,5-dihydroxyphenyl)-2-hydroxy-1-(2,4,6-trihydroxyphenyl)propyl]-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-2-yl]-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0154532	6-{[2-(3,4-dihydroxyphenyl)-8-[3-(3,5-dihydroxyphenyl)propyl]-3,5-dihydroxy-3,4-dihydro-2H-1-benzopyran-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0154490	6-(3,5-dihydroxy-4-{2-hydroxy-1-[3,5,7-trihydroxy-2-(3-hydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-8-yl]-3-(3,4,5-trihydroxyphenyl)propyl}phenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0154487	3,4,5-trihydroxy-6-(3-{3,5,7-trihydroxy-8-[2-hydroxy-1-(2,4,6-trihydroxyphenyl)-3-(3,4,5-trihydroxyphenyl)propyl]-3,4-dihydro-2H-1-benzopyran-2-yl}phenoxy)oxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0154489	6-(3,5-dihydroxy-2-{2-hydroxy-1-[3,5,7-trihydroxy-2-(3-hydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-8-yl]-3-(3,4,5-trihydroxyphenyl)propyl}phenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0154488	6-(3,5-dihydroxy-8-[2-hydroxy-1-(2,4,6-trihydroxyphenyl)-3-(3,4,5-trihydroxyphenyl)propyl]-2-(3-hydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-7-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0154485	6-(2,3-dihydroxy-5-{2-hydroxy-3-[3,5,7-trihydroxy-2-(3-hydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-8-yl]-3-(2,4,6-trihydroxyphenyl)propyl}phenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0154483	6-{4-[3-(3,5-dihydroxyphenyl)-1-[2-(3,5-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-2-hydroxypropyl]-3,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
HMDB0154486	6-(2,6-dihydroxy-4-{2-hydroxy-3-[3,5,7-trihydroxy-2-(3-hydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-8-yl]-3-(2,4,6-trihydroxyphenyl)propyl}phenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4

	HMDB0142338	6-{4-[3-(3,4-dihydroxyphenyl)-1-[2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-2-hydroxypropyl]-3,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
	HMDB0142337	6-{2-[3-(3,4-dihydroxyphenyl)-1-[2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-2-hydroxypropyl]-3,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
	HMDB0032910	Isoorientin 2"-[p-coumaroyl(->6)-glucoside]	C36H36O18	M+Na	779.1794	0.4
	HMDB0037437	6''-(4-Hydroxycinnamoyl)astragalin 4'-glucoside	C36H36O18	M+Na	779.1794	0.4
	HMDB0142336	6-(5-{3-[2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-2-hydroxy-3-(2,4,6-trihydroxyphenyl)propyl]-2-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
	HMDB0142333	6-(5-{8-[3-(3,4-dihydroxyphenyl)-2-hydroxy-1-(2,4,6-trihydroxyphenyl)propyl]-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-2-yl]-2-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
	HMDB0142335	6-(4-{3-[2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-2-hydroxy-3-(2,4,6-trihydroxyphenyl)propyl]-2-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
	HMDB0142334	6-{2-(3,4-dihydroxyphenyl)-8-[3-(3,4-dihydroxyphenyl)-2-hydroxy-1-(2,4,6-trihydroxyphenyl)propyl]-3,5-dihydroxy-3,4-dihydro-2H-1-benzopyran-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H36O18	M+Na	779.1794	0.4
	HMDB0039332	2''-(6''-p-Coumaroylglucosyl)quercitrin	C36H36O18	M+Na	779.1794	0.4
779.5779	HMDB0116435	(2S)-1-{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C47H80O7	M+Na	779.5796	-2.2
	HMDB0116379	(2S)-1-{[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C47H80O7	M+Na	779.5796	-2.2
	HMDB0116401	(2S)-1-hydroxy-3-{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C47H80O7	M+Na	779.5796	-2.2
	HMDB0116405	(2S)-2-{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C47H80O7	M+Na	779.5796	-2.2
	HMDB0116412	(2S)-2-{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C47H80O7	M+Na	779.5796	-2.2
	HMDB0116417	(2S)-3-hydroxy-2-{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C47H80O7	M+Na	779.5796	-2.2
	HMDB0116373	(2S)-1-{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C47H80O7	M+Na	779.5796	-2.2
	HMDB0116671	PG(i-12/i-24)	C42H83O10P	M+H	779.5797	-2.3
	HMDB0010602	PG(18/18)	C42H83O10P	M+H	779.5797	-2.3
	HMDB0112968	PE-NMe(18:1(11Z)/18:1(9Z))	C42H80NO8P	M+Na	780.5514	2.5
	HMDB0112967	PE-NMe(18:1(9Z)/18:1(11Z))	C42H80NO8P	M+Na	780.5514	2.5
	HMDB0112969	PE-NMe(18:1(11Z)/18:1(11Z))	C42H80NO8P	M+Na	780.5514	2.5
	HMDB0112966	PE-NMe(16:1(9Z)/1(11Z))	C42H80NO8P	M+Na	780.5514	2.5
	HMDB0112992	PE-NMe(14/22:2(13Z,16Z))	C42H80NO8P	M+Na	780.5514	2.5

HMDB0113089	PE-NMe(18/18:2(9Z,12Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0113169	PE-NMe(18:2(9Z,12Z)/18)	C42H80NO8P	M+Na	780.5514	2.5
HMDB0113312	PE-NMe(:1(11Z)/16:1(9Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0113563	PE-NMe(22:2(13Z,16Z)/14)	C42H80NO8P	M+Na	780.5514	2.5
HMDB0113047	PE-NMe(16/:2(11Z,14Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0114241	PE-NMe2(:2(11Z,14Z)/15)	C42H80NO8P	M+Na	780.5514	2.5
HMDB0113925	PE-NMe2(15/:2(11Z,14Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0113340	PE-NMe(:2(11Z,14Z)/16)	C42H80NO8P	M+Na	780.5514	2.5
HMDB0113536	PE-NMe(22:1(13Z)/14:1(9Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0113010	PE-NMe(14:1(9Z)/22:1(13Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0010565	PE-NMe(18:1(9Z)/18:1(9Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0007912	PC(14:1(9Z)/:1(11Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0007973	PC(16/18:2(9Z,12Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0008005	PC(16:1(9Z)/18:1(9Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0008004	PC(16:1(9Z)/18:1(11Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0008068	PC(18:1(11Z)/16:1(9Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0008101	PC(18:1(9Z)/16:1(9Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0008133	PC(18:2(9Z,12Z)/16)	C42H80NO8P	M+Na	780.5514	2.5
HMDB0008296	PC(:1(11Z)/14:1(9Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0008328	PC(:2(11Z,14Z)/14)	C42H80NO8P	M+Na	780.5514	2.5
HMDB0008909	PE(15/22:2(13Z,16Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0009549	PE(22:2(13Z,16Z)/15)	C42H80NO8P	M+Na	780.5514	2.5
HMDB0007880	PC(14/:2(11Z,14Z))	C42H80NO8P	M+Na	780.5514	2.5
HMDB0113056	PE-NMe(16/22:5(4Z,7Z,Z,13Z,16Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113057	PE-NMe(16/22:5(7Z,Z,13Z,16Z,19Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113078	PE-NMe(16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113100	PE-NMe(18/:5(5Z,8Z,11Z,14Z,17Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113125	PE-NMe(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113126	PE-NMe(18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113153	PE-NMe(18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113152	PE-NMe(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113179	PE-NMe(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C44H78NO8P	M+H	780.5538	-0.6

780.5533

HMDB0113180	PE-NMe(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113263	PE-NMe(18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0114525	PE-NMe2(22:5(4Z,7Z,Z,13Z,16Z)/15)	C44H78NO8P	M+H	780.5538	-0.6
HMDB0114551	PE-NMe2(22:5(7Z,Z,13Z,16Z,19Z)/15)	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113206	PE-NMe(18:3(6Z,9Z,12Z)/:2(11Z,14Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113235	PE-NMe(18:3(9Z,12Z,15Z)/:2(11Z,14Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113347	PE-NMe(:2(11Z,14Z)/18:3(9Z,12Z,15Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113346	PE-NMe(:2(11Z,14Z)/18:3(6Z,9Z,12Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113319	PE-NMe(:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113374	PE-NMe(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113402	PE-NMe(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113428	PE-NMe(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113429	PE-NMe(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113456	PE-NMe(:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113457	PE-NMe(:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113484	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/18)	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113596	PE-NMe(22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0116733	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/16)	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113649	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/16)	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113935	PE-NMe2(15/22:5(4Z,7Z,Z,13Z,16Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0113936	PE-NMe2(15/22:5(7Z,Z,13Z,16Z,19Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0007890	PC(14/22:5(4Z,7Z,Z,13Z,16Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0008430	PC(:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0008463	PC(:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0008495	PC(:5(5Z,8Z,11Z,14Z,17Z)/16)	C44H78NO8P	M+H	780.5538	-0.6
HMDB0008624	PC(22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0008656	PC(22:5(4Z,7Z,Z,13Z,16Z)/14)	C44H78NO8P	M+H	780.5538	-0.6
HMDB0008689	PC(22:5(7Z,Z,13Z,16Z,19Z)/14)	C44H78NO8P	M+H	780.5538	-0.6
HMDB0008235	PC(18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0008236	PC(18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0008204	PC(18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C44H78NO8P	M+H	780.5538	-0.6
HMDB0007891	PC(14/22:5(7Z,Z,13Z,16Z,19Z))	C44H78NO8P	M+H	780.5538	-0.6

	HMDB0007984	PC(16/:5(5Z,8Z,11Z,14Z,17Z))	C44H78NO8P	M+H	780.5538	-0.6
	HMDB0008015	PC(16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C44H78NO8P	M+H	780.5538	-0.6
	HMDB0008016	PC(16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C44H78NO8P	M+H	780.5538	-0.6
	HMDB0008075	PC(18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C44H78NO8P	M+H	780.5538	-0.6
	HMDB0008108	PC(18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C44H78NO8P	M+H	780.5538	-0.6
	HMDB0008140	PC(18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C44H78NO8P	M+H	780.5538	-0.6
	HMDB0008141	PC(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C44H78NO8P	M+H	780.5538	-0.6
	HMDB0008171	PC(18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C44H78NO8P	M+H	780.5538	-0.6
	HMDB0007922	PC(14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C44H78NO8P	M+H	780.5538	-0.6
780.7066	HMDB0042099	TG(14/15/16:1(9Z))	C48H90O6	M+NH4	780.7076	-1.2
	HMDB0042302	TG(14/16:1(9Z)/15)	C48H90O6	M+NH4	780.7076	-1.2
	HMDB0042967	TG(15/14/16:1(9Z))	C48H90O6	M+NH4	780.7076	-1.2
	HMDB0043024	TG(15/16/14:1(9Z))	C48H90O6	M+NH4	780.7076	-1.2
	HMDB0043164	TG(15/14:1(9Z)/16)	C48H90O6	M+NH4	780.7076	-1.2
	HMDB0043862	TG(16/15/14:1(9Z))	C48H90O6	M+NH4	780.7076	-1.2
782.5132	HMDB0186563	2-[(2-amino-3-{[(7E,9E,11Z,14Z)-1-{[(8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraen-1-yl]oxy}-5-hydroxy-1-oxoicosa-7,9,11,14-tetraen-6-yl]sulfanyl}-1-hydroxypropylidene)amino]acetic acid	C45H68N2O6S	M+NH4	782.5136	-0.6
	HMDB0112974	PE-NMe(16:1(9Z)/)	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0113864	PE-NMe2(15/:1(11Z))	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0112970	PE-NMe(18/18:1(9Z))	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0112971	PE-NMe(18/18:1(11Z))	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0112972	PE-NMe(14:1(9Z)/22)	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0112973	PE-NMe(16/:1(11Z))	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0114212	PE-NMe2(:1(11Z)/15)	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0113535	PE-NMe(22:1(13Z)/14)	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0113509	PE-NMe(22/14:1(9Z))	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0113311	PE-NMe(:1(11Z)/16)	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0113283	PE-NMe(/16:1(9Z))	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0113142	PE-NMe(18:1(9Z)/18)	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0113115	PE-NMe(18:1(11Z)/18)	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0112991	PE-NMe(14/22:1(13Z))	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0007911	PC(14:1(9Z)/)	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0007879	PC(14/:1(11Z))	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0008263	PC(/14:1(9Z))	C42H82NO8P	M+Na	782.5670	2.4
	HMDB0007972	PC(16/18:1(9Z))	C42H82NO8P	M+Na	782.5670	2.4

782.5689

HMDB0008003	PC(16:1(9Z)/18)	C42H82NO8P	M+Na	782.5670	2.4
HMDB0008035	PC(18/16:1(9Z))	C42H82NO8P	M+Na	782.5670	2.4
HMDB0008067	PC(18:1(11Z)/16)	C42H82NO8P	M+Na	782.5670	2.4
HMDB0008100	PC(18:1(9Z)/16)	C42H82NO8P	M+Na	782.5670	2.4
HMDB0008295	PC(:1(11Z)/14)	C42H82NO8P	M+Na	782.5670	2.4
HMDB0008908	PE(15/22:1(13Z))	C42H82NO8P	M+Na	782.5670	2.4
HMDB0009516	PE(22:1(13Z)/15)	C42H82NO8P	M+Na	782.5670	2.4
HMDB0007971	PC(16/18:1(11Z))	C42H82NO8P	M+Na	782.5670	2.4
HMDB0008623	PC(22:4(7Z,Z,13Z,16Z)/14)	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008462	PC(:4(8Z,11Z,14Z,17Z)/16)	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008429	PC(:4(5Z,8Z,11Z,14Z)/16)	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008398	PC(:3(8Z,11Z,14Z)/16:1(9Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008365	PC(:3(5Z,8Z,11Z)/16:1(9Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008138	PC(18:2(9Z,12Z)/18:2(9Z,12Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0007889	PC(14/22:4(7Z,Z,13Z,16Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008013	PC(16:1(9Z)/:3(5Z,8Z,11Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008074	PC(18:1(11Z)/18:3(9Z,12Z,15Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008073	PC(18:1(11Z)/18:3(6Z,9Z,12Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0007982	PC(16/:4(5Z,8Z,11Z,14Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008042	PC(18/18:4(6Z,9Z,12Z,15Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0007983	PC(16/:4(8Z,11Z,14Z,17Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008014	PC(16:1(9Z)/:3(8Z,11Z,14Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008107	PC(18:1(9Z)/18:3(9Z,12Z,15Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008106	PC(18:1(9Z)/18:3(6Z,9Z,12Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008234	PC(18:4(6Z,9Z,12Z,15Z)/18)	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008203	PC(18:3(9Z,12Z,15Z)/18:1(9Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008202	PC(18:3(9Z,12Z,15Z)/18:1(11Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008169	PC(18:3(6Z,9Z,12Z)/18:1(11Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0008170	PC(18:3(6Z,9Z,12Z)/18:1(9Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0113234	PE-NMe(18:3(9Z,12Z,15Z)/:1(11Z))	C44H80NO8P	M+H	782.5694	-0.7
HMDB0113262	PE-NMe(18:4(6Z,9Z,12Z,15Z)/)	C44H80NO8P	M+H	782.5694	-0.7
HMDB0113205	PE-NMe(18:3(6Z,9Z,12Z)/:1(11Z))	C44H80NO8P	M+H	782.5694	-0.7

	HMDB0113290	PE-NMe(/18:4(6Z,9Z,12Z,15Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113318	PE-NMe(:1(11Z)/18:3(9Z,12Z,15Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113150	PE-NMe(18:1(9Z):3(5Z,8Z,11Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113317	PE-NMe(:1(11Z)/18:3(6Z,9Z,12Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113151	PE-NMe(18:1(9Z):3(8Z,11Z,14Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113055	PE-NMe(16/22:4(7Z,Z,13Z,16Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113099	PE-NMe(18/:4(8Z,11Z,14Z,17Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113098	PE-NMe(18/:4(5Z,8Z,11Z,14Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113123	PE-NMe(18:1(11Z):3(5Z,8Z,11Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113124	PE-NMe(18:1(11Z):3(8Z,11Z,14Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113373	PE-NMe(:3(5Z,8Z,11Z)/18:1(9Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113934	PE-NMe2(15/22:4(7Z,Z,13Z,16Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0114497	PE-NMe2(22:4(7Z,Z,13Z,16Z)/15)	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113178	PE-NMe(18:2(9Z,12Z):2(11Z,14Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113345	PE-NMe(:2(11Z,14Z)/18:2(9Z,12Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113455	PE-NMe(:4(8Z,11Z,14Z,17Z)/18)	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113427	PE-NMe(:4(5Z,8Z,11Z,14Z)/18)	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113372	PE-NMe(:3(5Z,8Z,11Z)/18:1(11Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113401	PE-NMe(:3(8Z,11Z,14Z)/18:1(9Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113400	PE-NMe(:3(8Z,11Z,14Z)/18:1(11Z))	C44H80NO8P	M+H	782.5694	-0.7
	HMDB0113595	PE-NMe(22:4(7Z,Z,13Z,16Z)/16)	C44H80NO8P	M+H	782.5694	-0.7
783.2365	HMDB0040541	Kaempferol 3-(2"-rhamnosyl-6"-acetylgalactoside) 7-rhamnoside	C35H42O20	M+H	783.2342	2.9
784.1945	HMDB0148814	5-({5-[(2-carboxyacetyl)oxy]-6-[(2-carboxyacetyl)oxy]methyl}-3,4-dihydroxyoxan-2-yl)oxy)-7-hydroxy-2-(4-hydroxyphenyl)-3-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-1-yl?chromen-1-ylum	C33H35O21	M+NH4	784.1931	1.8
	HMDB0112990	PE-NMe(14/22)	C42H84NO8P	M+Na	784.5827	2.5
	HMDB0113282	PE-NMe(/16)	C42H84NO8P	M+Na	784.5827	2.5
	HMDB0113046	PE-NMe(16/)	C42H84NO8P	M+Na	784.5827	2.5
	HMDB0113508	PE-NMe(22/14)	C42H84NO8P	M+Na	784.5827	2.5
	HMDB0113924	PE-NMe2(15/)	C42H84NO8P	M+Na	784.5827	2.5
	HMDB0114183	PE-NMe2(/15)	C42H84NO8P	M+Na	784.5827	2.5
	HMDB0112975	PE-NMe(18/18)	C42H84NO8P	M+Na	784.5827	2.5
	HMDB0009483	PE(22/15)	C42H84NO8P	M+Na	784.5827	2.5

784.5846

HMDB0008907	PE(15/22)	C42H84NO8P	M+Na	784.5827	2.5
HMDB0007878	PC(14/)	C42H84NO8P	M+Na	784.5827	2.5
HMDB0008262	PC(/14)	C42H84NO8P	M+Na	784.5827	2.5
HMDB0007970	PC(16/18)	C42H84NO8P	M+Na	784.5827	2.5
HMDB0008034	PC(18/16)	C42H84NO8P	M+Na	784.5827	2.5
HMDB0008591	PC(22:2(13Z,16Z)/14:1(9Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0008397	PC(:3(8Z,11Z,14Z)/16)	C44H82NO8P	M+H	784.5851	-0.6
HMDB0008364	PC(:3(5Z,8Z,11Z)/16)	C44H82NO8P	M+H	784.5851	-0.6
HMDB0008332	PC(:2(11Z,14Z)/16:1(9Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0007921	PC(14:1(9Z)/22:2(13Z,16Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0007980	PC(16/:3(5Z,8Z,11Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0007981	PC(16/:3(8Z,11Z,14Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0008012	PC(16:1(9Z)/:2(11Z,14Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0008137	PC(18:2(9Z,12Z)/18:1(9Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0008040	PC(18/18:3(6Z,9Z,12Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0008041	PC(18/18:3(9Z,12Z,15Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0008072	PC(18:1(11Z)/18:2(9Z,12Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0008105	PC(18:1(9Z)/18:2(9Z,12Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0008136	PC(18:2(9Z,12Z)/18:1(11Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0008168	PC(18:3(6Z,9Z,12Z)/18)	C44H82NO8P	M+H	784.5851	-0.6
HMDB0008201	PC(18:3(9Z,12Z,15Z)/18)	C44H82NO8P	M+H	784.5851	-0.6
HMDB0113399	PE-NMe(:3(8Z,11Z,14Z)/18)	C44H82NO8P	M+H	784.5851	-0.6
HMDB0113371	PE-NMe(:3(5Z,8Z,11Z)/18)	C44H82NO8P	M+H	784.5851	-0.6
HMDB0113316	PE-NMe(:1(11Z)/18:2(9Z,12Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0113289	PE-NMe(/18:3(9Z,12Z,15Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0113288	PE-NMe(/18:3(6Z,9Z,12Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0113233	PE-NMe(18:3(9Z,12Z,15Z)/)	C44H82NO8P	M+H	784.5851	-0.6
HMDB0113204	PE-NMe(18:3(6Z,9Z,12Z)/)	C44H82NO8P	M+H	784.5851	-0.6
HMDB0113177	PE-NMe(18:2(9Z,12Z)/:1(11Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0113096	PE-NMe(18/:3(5Z,8Z,11Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0113567	PE-NMe(22:2(13Z,16Z)/16:1(9Z))	C44H82NO8P	M+H	784.5851	-0.6
HMDB0113149	PE-NMe(18:1(9Z)/:2(11Z,14Z))	C44H82NO8P	M+H	784.5851	-0.6

	HMDB0113344	PE-NMe(:2(11Z,14Z)/18:1(9Z))	C44H82NO8P	M+H	784.5851	-0.6
	HMDB0113343	PE-NMe(:2(11Z,14Z)/18:1(11Z))	C44H82NO8P	M+H	784.5851	-0.6
	HMDB0113122	PE-NMe(18:1(11Z):2(11Z,14Z))	C44H82NO8P	M+H	784.5851	-0.6
	HMDB0113097	PE-NMe(18:3(8Z,11Z,14Z))	C44H82NO8P	M+H	784.5851	-0.6
	HMDB0113077	PE-NMe(16:1(9Z)/22:2(13Z,16Z))	C44H82NO8P	M+H	784.5851	-0.6
786.1888	HMDB0149911	6-{[5-(3,5-dihydroxyphenyl)-6,9,19,21-tetrahydroxy-13-(3,4,5-trihydroxyphenyl)-4,12,14-trioxapentacyclo[11.7.1,,?癩henicosa-2(11),3(8),9,15,17,19-hexaen-17-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H32O19	M+NH4	786.1876	1.5
	HMDB0149912	6-{[5-(3,5-dihydroxyphenyl)-6,17,19,21-tetrahydroxy-13-(3,4,5-trihydroxyphenyl)-4,12,14-trioxapentacyclo[11.7.1,,?癩henicosa-2(11),3(8),9,15,17,19-hexaen-9-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H32O19	M+NH4	786.1876	1.5
	HMDB0149910	6-{[5-(3,5-dihydroxyphenyl)-6,9,17,21-tetrahydroxy-13-(3,4,5-trihydroxyphenyl)-4,12,14-trioxapentacyclo[11.7.1,,?癩henicosa-2(11),3(8),9,15,17,19-hexaen-19-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H32O19	M+NH4	786.1876	1.5
	HMDB0149908	6-{4-[5-(3,5-dihydroxyphenyl)-6,9,17,19,21-pentahydroxy-4,12,14-trioxapentacyclo[11.7.1,,?癩henicosa-2(11),3(8),9,15,17,19-hexaen-13-yl]-2,6-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H32O19	M+NH4	786.1876	1.5
	HMDB0149907	6-{5-[5-(3,5-dihydroxyphenyl)-6,9,17,19,21-pentahydroxy-4,12,14-trioxapentacyclo[11.7.1,,?癩henicosa-2(11),3(8),9,15,17,19-hexaen-13-yl]-2,3-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H32O19	M+NH4	786.1876	1.5
	HMDB0149903	6-{[13-(3,5-dihydroxyphenyl)-6,17,19,21-tetrahydroxy-5-(3,4,5-trihydroxyphenyl)-4,12,14-trioxapentacyclo[11.7.1,,?癩henicosa-2(11),3(8),9,15,17,19-hexaen-9-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H32O19	M+NH4	786.1876	1.5
	HMDB0149902	6-{[13-(3,5-dihydroxyphenyl)-6,9,19,21-tetrahydroxy-5-(3,4,5-trihydroxyphenyl)-4,12,14-trioxapentacyclo[11.7.1,,?癩henicosa-2(11),3(8),9,15,17,19-hexaen-17-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H32O19	M+NH4	786.1876	1.5
	HMDB0149901	6-{[13-(3,5-dihydroxyphenyl)-6,9,17,21-tetrahydroxy-5-(3,4,5-trihydroxyphenyl)-4,12,14-trioxapentacyclo[11.7.1,,?癩henicosa-2(11),3(8),9,15,17,19-hexaen-19-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H32O19	M+NH4	786.1876	1.5
	HMDB0149898	3,4,5-trihydroxy-6-{3-hydroxy-5-[6,9,17,19,21-pentahydroxy-5-(3,4,5-trihydroxyphenyl)-4,12,14-trioxapentacyclo[11.7.1,,?癩henicosa-2(11),3(8),9,15,17,19-hexaen-13-yl]phenoxy}oxane-2-carboxylic acid	C36H32O19	M+NH4	786.1876	1.5
	HMDB0149900	6-{4-[13-(3,5-dihydroxyphenyl)-6,9,17,19,21-pentahydroxy-4,12,14-trioxapentacyclo[11.7.1,,?癩henicosa-2(11),3(8),9,15,17,19-hexaen-5-yl]-2,6-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H32O19	M+NH4	786.1876	1.5
	HMDB0149899	6-{5-[13-(3,5-dihydroxyphenyl)-6,9,17,19,21-pentahydroxy-4,12,14-trioxapentacyclo[11.7.1,,?癩henicosa-2(11),3(8),9,15,17,19-hexaen-5-yl]-2,3-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H32O19	M+NH4	786.1876	1.5

	HMDB0149909	3,4,5-trihydroxy-6-{3-hydroxy-5-[6,9,17,19,21-pentahydroxy-13-(3,4,5-trihydroxyphenyl)-4,12,14-trioxapentacyclo[11.7.1.,?癩henicosa-2(11),3(8),9,15,17,19-hexaen-5-yl]phenoxy}oxane-2-carboxylic acid	C36H32O19	M+NH4	786.1876	1.5
786.2430	HMDB0124931	6-[(2-{4-[(3-{[4-(acetyloxy)-3-hydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy}-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}phenyl]-4-oxo-3,4-dihydro-2H-1-benzopyran-7-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H40O20	M+NH4	786.2451	-2.7
	HMDB0127086	3,4,5-trihydroxy-6-({7-methoxy-4-oxo-2-phenyl-6,8-bis[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-4H-chromen-5-yl}oxy)oxane-2-carboxylic acid	C34H40O20	M+NH4	786.2451	-2.7
	HMDB0140784	2-{4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]phenyl}-3-[(3-{[4,5-dihydroxy-6-(hydroxymethyl)-3-methyloxan-2-yl]oxy}-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl)oxy]-5,7-dihydroxy-1位?chromen-1-ylum	C34H41O20	M+NH4	786.2451	-2.7
	HMDB0140785	5-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-3-[(3-{[4,5-dihydroxy-6-(hydroxymethyl)-3-methyloxan-2-yl]oxy}-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl)oxy]-7-hydroxy-2-(4-hydroxyphenyl)-1位?chromen-1-ylum	C34H41O20	M+NH4	786.2451	-2.7
	HMDB0140786	7-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-3-[(3-{[4,5-dihydroxy-6-(hydroxymethyl)-3-methyloxan-2-yl]oxy}-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl)oxy]-5-hydroxy-2-(4-hydroxyphenyl)-1位?chromen-1-ylum	C34H41O20	M+NH4	786.2451	-2.7
786.3884	HMDB0034713	Fumonisin A1	C36H61NO16	M+Na	786.3883	0.2
786.5998	HMDB0115591	PA(22:1(13Z)/19:2(Z,13Z))	C44H81O8P	M+NH4	786.6007	-1.2
	HMDB0062690	1,2-dioleoyl-sn-glycero-3-phosphocholine	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0000593	1,2-dioleoyl-sn-glycero-3-phosphocholine	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0007888	PC(14/22:2(13Z,16Z))	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0007920	PC(14:1(9Z)/22:1(13Z))	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0007979	PC(16/:2(11Z,14Z))	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0008011	PC(16:1(9Z)/:1(11Z))	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0008039	PC(18/18:2(9Z,12Z))	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0008071	PC(18:1(11Z)/18:1(9Z))	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0008070	PC(18:1(11Z)/18:1(11Z))	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0008590	PC(22:2(13Z,16Z)/14)	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0008559	PC(22:1(13Z)/14:1(9Z))	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0008331	PC(:2(11Z,14Z)/16)	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0008299	PC(:1(11Z)/16:1(9Z))	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0008135	PC(18:2(9Z,12Z)/18)	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0008103	PC(18:1(9Z)/18:1(11Z))	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0113566	PE-NMe(22:2(13Z,16Z)/16)	C44H84NO8P	M+H	786.6007	-1.2
	HMDB0113539	PE-NMe(22:1(13Z)/16:1(9Z))	C44H84NO8P	M+H	786.6007	-1.2

HMDB0113315	PE-NMe(1(11Z)/18:1(9Z))	C44H84NO8P	M+H	786.6007	-1.2
HMDB0113314	PE-NMe(1(11Z)/18:1(11Z))	C44H84NO8P	M+H	786.6007	-1.2
HMDB0113287	PE-NMe(/18:2(9Z,12Z))	C44H84NO8P	M+H	786.6007	-1.2
HMDB0113176	PE-NMe(18:2(9Z,12Z)/)	C44H84NO8P	M+H	786.6007	-1.2
HMDB0113148	PE-NMe(18:1(9Z):1(11Z))	C44H84NO8P	M+H	786.6007	-1.2
HMDB0113121	PE-NMe(18:1(11Z):1(11Z))	C44H84NO8P	M+H	786.6007	-1.2
HMDB0113729	PE-NMe(24:1(15Z)/14:1(9Z))	C44H84NO8P	M+H	786.6007	-1.2
HMDB0113933	PE-NMe2(15/22:2(13Z,16Z))	C44H84NO8P	M+H	786.6007	-1.2
HMDB0113342	PE-NMe(2(11Z,14Z)/18)	C44H84NO8P	M+H	786.6007	-1.2
HMDB0113095	PE-NMe(18:2(11Z,14Z))	C44H84NO8P	M+H	786.6007	-1.2
HMDB0114468	PE-NMe2(22:2(13Z,16Z)/15)	C44H84NO8P	M+H	786.6007	-1.2
HMDB0113076	PE-NMe(16:1(9Z)/22:1(13Z))	C44H84NO8P	M+H	786.6007	-1.2
HMDB0113054	PE-NMe(16/22:2(13Z,16Z))	C44H84NO8P	M+H	786.6007	-1.2
HMDB0112977	PE-NMe(14:1(9Z)/24:1(15Z))	C44H84NO8P	M+H	786.6007	-1.2
HMDB0138453	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,12-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-18-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138436	6-{4-[(E)-2-[,18-dihydroxy-14-methyl-13-oxo-4-(2,4,5-trihydroxyphenyl)-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-8-yl]ethenyl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138433	6-(4-{8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,18-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-4-yl}-2,5-dihydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138434	6-(2-{8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,18-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-4-yl}-4,5-dihydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138435	6-({8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-18-hydroxy-14-methyl-13-oxo-4-(2,4,5-trihydroxyphenyl)-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen--yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138432	6-(5-{8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,18-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-4-yl}-2,4-dihydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138430	6-{2-[(E)-2-[4-(2,4-dihydroxyphenyl)-,18,-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16,18,-hexaen-8-yl]ethenyl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6

HMDB0138429	6-{4-[(E)-2-[4-(2,4-dihydroxyphenyl)-,18,-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahehexacyclo[12.7.1.,??]docosa-6,8,,16,18,-hexaen-8-yl]ethenyl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138428	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-18,-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahehexacyclo[12.7.1.,??]docosa-6,8,,16,18,-hexaen--yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138431	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahehexacyclo[12.7.1.,??]docosa-6,8,,16,18,-hexaen-18-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138425	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,18-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahehexacyclo[12.7.1.,??]docosa-6,8,,16,18,-hexaen--yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138424	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,17-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahehexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-18-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138438	6-({8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]--hydroxy-14-methyl-13-oxo-4-(2,4,5-trihydroxyphenyl)-3,5,15-trioxahehexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-18-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138437	6-{2-[(E)-2-[18-dihydroxy-14-methyl-13-oxo-4-(2,4,5-trihydroxyphenyl)-3,5,15-trioxahehexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-8-yl]ethenyl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138443	6-{[4-(2,4-dihydroxyphenyl)-18-hydroxy-14-methyl-13-oxo-8-[(E)-2-(2,4,5-trihydroxyphenyl)ethenyl]-3,5,15-trioxahehexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen--yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138452	6-{2-[(E)-2-[4-(2,4-dihydroxyphenyl)-,12,18-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahehexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-8-yl]ethenyl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138450	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-12,18-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahehexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen--yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138451	6-{4-[(E)-2-[4-(2,4-dihydroxyphenyl)-,12,18-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahehexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-8-yl]ethenyl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138449	6-(2-{8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,12,18-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahehexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-4-yl}-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138448	6-(4-{8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,12,18-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahehexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-4-yl}-3-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6

HMDB0138444	6-{4-[(E)-2-[4-(2,4-dihydroxyphenyl)-,18-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-8-yl]ethenyl]-2,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138446	6-{[4-(2,4-dihydroxyphenyl)--hydroxy-14-methyl-13-oxo-8-[(E)-2-(2,4,5-trihydroxyphenyl)ethenyl]-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-18-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138445	6-{2-[(E)-2-[4-(2,4-dihydroxyphenyl)-,18-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-8-yl]ethenyl]-4,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138442	6-(2-{,18-dihydroxy-14-methyl-13-oxo-8-[(E)-2-(2,4,5-trihydroxyphenyl)ethenyl]-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-4-yl}-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138441	6-(4-{,18-dihydroxy-14-methyl-13-oxo-8-[(E)-2-(2,4,5-trihydroxyphenyl)ethenyl]-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-4-yl}-3-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138440	6-{5-[(E)-2-[4-(2,4-dihydroxyphenyl)-,18-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-8-yl]ethenyl]-2,4-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138426	6-(4-{8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,18,-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16,18,-hexaen-4-yl}-3-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138427	6-(2-{8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,18,-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16,18,-hexaen-4-yl}-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138408	6-{4-[(E)-2-[4-(2,4-dihydroxyphenyl)-9,,18-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6(11),7,9,16(21),17,19-hexaen-8-yl]ethenyl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138409	6-{2-[(E)-2-[4-(2,4-dihydroxyphenyl)-9,,18-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6(11),7,9,16(21),17,19-hexaen-8-yl]ethenyl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138405	6-(4-{8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-9,,18-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6(11),7,9,16(21),17,19-hexaen-4-yl}-3-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138406	6-(2-{8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-9,,18-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6(11),7,9,16(21),17,19-hexaen-4-yl}-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6

HMDB0138407	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-9,18-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6(11),7,9,16(21),17,19-hexaen--yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138404	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,18-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6(11),7,9,16(21),17,19-hexaen-9-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138402	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-hydroxy-14-(hydroxymethyl)-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-18-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138401	6-{2-[(E)-2-[4-(2,4-dihydroxyphenyl)-,18-dihydroxy-14-(hydroxymethyl)-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-8-yl]ethenyl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138400	6-{4-[(E)-2-[4-(2,4-dihydroxyphenyl)-,18-dihydroxy-14-(hydroxymethyl)-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-8-yl]ethenyl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138397	6-(4-{8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,18-dihydroxy-14-(hydroxymethyl)-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-4-yl}-3-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138398	6-(2-{8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,18-dihydroxy-14-(hydroxymethyl)-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-4-yl}-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138410	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-9,-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6(11),7,9,16(21),17,19-hexaen-18-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138411	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,18-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16,18,-hexaen-19-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138415	6-{4-[(E)-2-[4-(2,4-dihydroxyphenyl)-,18,19-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-8-yl]ethenyl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138421	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-17,18-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen--yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138423	6-{2-[(E)-2-[4-(2,4-dihydroxyphenyl)-,17,18-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-8-yl]ethenyl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6

HMDB0138422	6-{4-[(E)-2-[4-(2,4-dihydroxyphenyl)-,17,18-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-8-yl]ethenyl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138420	6-(2-{8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,17,18-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-4-yl}-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138418	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,18-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-17-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138419	6-(4-{8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,17,18-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-4-yl}-3-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138417	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,19-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16,18,-hexaen-18-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138416	6-{2-[(E)-2-[4-(2,4-dihydroxyphenyl)-,18,19-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-8-yl]ethenyl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138414	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-18,19-dihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen--yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138413	6-(2-{8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,18,19-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-4-yl}-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138412	6-(4-{8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-,18,19-trihydroxy-14-methyl-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen-4-yl}-3-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0138399	6-{[4-(2,4-dihydroxyphenyl)-8-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]-18-hydroxy-14-(hydroxymethyl)-13-oxo-3,5,15-trioxahexacyclo[12.7.1.,??]docosa-6,8,,16(21),17,19-hexaen--yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H34O17	M+H	787.1869	2.6
HMDB0034871	Spinacoside D	C40H60O14	M+Na	787.3875	0.2
HMDB0175659	6-{[1,11-bis(acetyloxy)-4a-carboxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahdropicen-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H60O14	M+Na	787.3875	0.2
HMDB0175660	6-[1,11-bis(acetyloxy)-1-hydroxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahdropicene-4a-carbonyloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H60O14	M+Na	787.3875	0.2

787.3877	HMDB0175655	6-[11-(acetyloxy)-9-[(acetyloxy)methyl]-1,-dihydroxy-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carbonyloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H60O14	M+Na	787.3875	0.2
	HMDB0175653	6-{[2-(acetyloxy)-4-[(acetyloxy)methyl]-8a-carboxy-12-hydroxy-4,6a,6b,11,11,14b-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H60O14	M+Na	787.3875	0.2
	HMDB0175654	6-{[11-(acetyloxy)-9-[(acetyloxy)methyl]-4a-carboxy--hydroxy-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H60O14	M+Na	787.3875	0.2
	HMDB0175649	6-{[-(acetyloxy)-9-[(acetyloxy)methyl]-4a-carboxy-11-hydroxy-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H60O14	M+Na	787.3875	0.2
	HMDB0175650	6-[-(acetyloxy)-9-[(acetyloxy)methyl]-1,11-dihydroxy-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carbonyloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H60O14	M+Na	787.3875	0.2
	HMDB0175648	6-{[3-(acetyloxy)-4-[(acetyloxy)methyl]-8a-carboxy-12-hydroxy-4,6a,6b,11,11,14b-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H60O14	M+Na	787.3875	0.2
	HMDB0175658	6-{[2,3-bis(acetyloxy)-8a-carboxy-12-hydroxy-4,6a,6b,11,11,14b-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-4-yl]methoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H60O14	M+Na	787.3875	0.2
788.5439	HMDB0112288	PS(16:1(9Z):1(11Z))	C42H78NO10P	M+H	788.5436	0.4
	HMDB0112302	PS(14/22:2(13Z,16Z))	C42H78NO10P	M+H	788.5436	0.4
	HMDB0112570	PS(:2(11Z,14Z)/16)	C42H78NO10P	M+H	788.5436	0.4
	HMDB0112346	PS(16/:2(11Z,14Z))	C42H78NO10P	M+H	788.5436	0.4
	HMDB0112761	PS(22:2(13Z,16Z)/14)	C42H78NO10P	M+H	788.5436	0.4
	HMDB0112737	PS(22:1(13Z)/14:1(9Z))	C42H78NO10P	M+H	788.5436	0.4
	HMDB0112272	PS(18:1(11Z)/18:1(11Z))	C42H78NO10P	M+H	788.5436	0.4
	HMDB0112291	PS(18:1(9Z)/18:1(11Z))	C42H78NO10P	M+H	788.5436	0.4
	HMDB0112544	PS(:1(11Z)/16:1(9Z))	C42H78NO10P	M+H	788.5436	0.4
	HMDB0112314	PS(14:1(9Z)/22:1(13Z))	C42H78NO10P	M+H	788.5436	0.4
	HMDB0012390	PS(18:1(9Z)/18:1(9Z))	C42H78NO10P	M+H	788.5436	0.4
	HMDB0112290	PS(18:1(11Z)/18:1(9Z))	C42H78NO10P	M+H	788.5436	0.4
	HMDB0012400	PS(18:2(9Z,12Z)/18)	C42H78NO10P	M+H	788.5436	0.4
	HMDB0012380	PS(18/18:2(9Z,12Z))	C42H78NO10P	M+H	788.5436	0.4
	HMDB0116606	PG(:4(5Z,8Z,11Z,14Z)/16)	C42H75O10P	M+NH4	788.5436	0.4

	HMDB0010678	PG(18:3(9Z,12Z,15Z)/18:1(11Z))	C42H75O10P	M+NH4	788.5436	0.4
	HMDB0010664	PG(18:3(6Z,9Z,12Z)/18:1(9Z))	C42H75O10P	M+NH4	788.5436	0.4
	HMDB0010663	PG(18:3(6Z,9Z,12Z)/18:1(11Z))	C42H75O10P	M+NH4	788.5436	0.4
	HMDB0010650	PG(18:2(9Z,12Z)/18:2(9Z,12Z))	C42H75O10P	M+NH4	788.5436	0.4
	HMDB0010637	PG(18:1(9Z)/18:3(9Z,12Z,15Z))	C42H75O10P	M+NH4	788.5436	0.4
	HMDB0010636	PG(18:1(9Z)/18:3(6Z,9Z,12Z))	C42H75O10P	M+NH4	788.5436	0.4
	HMDB0010622	PG(18:1(11Z)/18:3(9Z,12Z,15Z))	C42H75O10P	M+NH4	788.5436	0.4
	HMDB0010621	PG(18:1(11Z)/18:3(6Z,9Z,12Z))	C42H75O10P	M+NH4	788.5436	0.4
	HMDB0010594	PG(16:1(9Z)/:3(8Z,11Z,14Z))	C42H75O10P	M+NH4	788.5436	0.4
	HMDB0010593	PG(16:1(9Z)/:3(5Z,8Z,11Z))	C42H75O10P	M+NH4	788.5436	0.4
	HMDB0010679	PG(18:3(9Z,12Z,15Z)/18:1(9Z))	C42H75O10P	M+NH4	788.5436	0.4
	HMDB0010580	PG(16/:4(5Z,8Z,11Z,14Z))	C42H75O10P	M+NH4	788.5436	0.4
789.1165	HMDB0039371	1,2',3,5-Tetra-O-galloylhamamelofuranose	C34H28O22	M+H	789.1145	2.5
	HMDB0039186	2,3,4,6-Tetragalloyl-D-glucopyranose	C34H28O22	M+H	789.1145	2.5
	HMDB0039191	1,2,4,6-Tetragalloyl-beta-D-glucopyranose	C34H28O22	M+H	789.1145	2.5
	HMDB0039188	1,2,3,6-Tetragalloyl-beta-D-glucopyranose	C34H28O22	M+H	789.1145	2.5
789.2071	HMDB0037220	Quercetin 3-(2"-glucosylgalactoside) 7-glucoside	C33H40O22	M+H	789.2084	-1.6
	HMDB0128226	3,4,5-trihydroxy-6-{4-[(1E)-3-oxo-3-{2,3,4-trihydroxy-5-[hydroxy(3,4,5-trihydroxyoxan-2-yl)methyl]-6-oxo-3-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]cyclohexa-1,4-dien-1-yl}prop-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C33H40O22	M+H	789.2084	-1.6
	HMDB0128285	6-{4-[(1E)-3-{4,5-dihydroxy-3-[hydroxy(3,4,5-trihydroxyoxan-2-yl)methyl]-2,6-dioxo-5-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]cyclohex-3-en-1-yl]-3-oxoprop-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C33H40O22	M+H	789.2084	-1.6
	HMDB0128295	6-{4-[(1E)-3-{2,3-dihydroxy-5-[hydroxy(3,4,5-trihydroxyoxan-2-yl)methyl]-4,6-dioxo-3-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]cyclohex-1-en-1-yl]-3-oxoprop-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C33H40O22	M+H	789.2084	-1.6
	HMDB0040487	Moracetin	C33H40O22	M+H	789.2084	-1.6
	HMDB0037937	Quercetin 3-(2G-glucosylgentiobioside)	C33H40O22	M+H	789.2084	-1.6
	HMDB0030414	Quercetin 3-glucosyl-(1->2)-galactosyl-(1->2)-	C33H40O22	M+H	789.2084	-1.6
	HMDB0133720	3-[(3-{[(4S)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy}-4,5-dihydroxy-6-({[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}methyl)oxan-2-yl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-methoxy-4H-chromen-4-one	C33H40O22	M+H	789.2084	-1.6
	HMDB0037542	Patuletin 3-(2"-apiosylgentiobioside)	C33H40O22	M+H	789.2084	-1.6
	HMDB0029262	Quercetin 3,7,4'-O-triglucoside	C33H40O22	M+H	789.2084	-1.6
	HMDB0039118	Delphinidin 3-sophoroside 5-glucoside	C33H41O22	M+H	789.2089	-2.3
789.4024	HMDB0041185	(3b,5a,25R)-3-Hydroxyspirostan-6-one 3-[2-acetyl-arabinosyl-(1->6)-glucoside]	C40H62O14	M+Na	789.4032	-1.0
789.5492	HMDB0183271	6-[(13-{[2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-yl]oxy}-13-oxotridecanoyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C46H76O10	M+H	789.5511	-2.4
789.7326	HMDB0007848	DG(24:1(15Z)/24:1(15Z))	C51H96O5	M+H	789.7331	-0.6
	HMDB0048588	TG(16:1(9Z)/14:1(9Z)/O-18)	C51H96O5	M+H	789.7331	-0.6
	HMDB0048392	TG(14:1(9Z)/O-18/16:1(9Z))	C51H96O5	M+H	789.7331	-0.6
	HMDB0047930	TG(14:1(9Z)/16:1(9Z)/O-18)	C51H96O5	M+H	789.7331	-0.6

	HMDB0056267	DG(24:1n9/24:1n9)	C51H96O5	M+H	789.7331	-0.6
790.4588	HMDB0034595	(S)-Codamine	C39H64O15	M+NH4	790.4583	0.6
790.5809	HMDB0175703	6-{[-(decanoyloxy)-2,2,6a,6b,9,9,12a-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-4a-yl]methoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C46H76O9	M+NH4	790.5828	-2.3
790.6908	HMDB0042286	TG(14/14:1(9Z)/18:2(9Z,12Z))	C49H88O6	M+NH4	790.6919	-1.4
	HMDB0047887	TG(14:1(9Z)/14:1(9Z)/18:1(11Z))	C49H88O6	M+NH4	790.6919	-1.4
	HMDB0047909	TG(14:1(9Z)/16:1(9Z)/16:1(9Z))	C49H88O6	M+NH4	790.6919	-1.4
	HMDB0047732	TG(14:1(9Z)/14/18:2(9Z,12Z))	C49H88O6	M+NH4	790.6919	-1.4
	HMDB0047888	TG(14:1(9Z)/14:1(9Z)/18:1(9Z))	C49H88O6	M+NH4	790.6919	-1.4
	HMDB0042084	TG(14/14/18:3(9Z,12Z,15Z))	C49H88O6	M+NH4	790.6919	-1.4
	HMDB0042077	TG(14/14/18:3(6Z,9Z,12Z))	C49H88O6	M+NH4	790.6919	-1.4
	HMDB0048567	TG(16:1(9Z)/14:1(9Z)/16:1(9Z))	C49H88O6	M+NH4	790.6919	-1.4
	HMDB0047954	TG(14:1(9Z)/18:1(9Z)/14:1(9Z))	C49H88O6	M+NH4	790.6919	-1.4
	HMDB0047931	TG(14:1(9Z)/18:1(11Z)/14:1(9Z))	C49H88O6	M+NH4	790.6919	-1.4
	HMDB0042751	TG(14/18:3(9Z,12Z,15Z)/14)	C49H88O6	M+NH4	790.6919	-1.4
	HMDB0042541	TG(14/18:3(6Z,9Z,12Z)/14)	C49H88O6	M+NH4	790.6919	-1.4
	HMDB0042518	TG(14/18:2(9Z,12Z)/14:1(9Z))	C49H88O6	M+NH4	790.6919	-1.4
791.5544	HMDB0115591	PA(22:1(13Z)/19:2(Z,13Z))	C44H81O8P	M+Na	791.5561	-2.2
	HMDB0174781	21-(2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl)sulfanyl)-22-hydroxytriacontanoic acid	C40H75N3O9S	M+NH4	791.5562	-2.3
	HMDB0174782	22-(2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl)sulfanyl)-21-hydroxytriacontanoic acid	C40H75N3O9S	M+NH4	791.5562	-2.3
	HMDB0112328	PS(15/:2(11Z,14Z))	C41H76NO10P	M+NH4	791.5545	-0.1
	HMDB0112569	PS(:2(11Z,14Z)/15)	C41H76NO10P	M+NH4	791.5545	-0.1
791.6258	HMDB0009745	PE(24:1(15Z)/14)	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0007945	PC(15/:1(11Z))	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0008297	PC(:1(11Z)/15)	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0008849	PE(14/24:1(15Z))	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0008881	PE(14:1(9Z)/24)	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0008941	PE(16/22:1(13Z))	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0008973	PE(16:1(9Z)/22)	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0008999	PE(18/:1(11Z))	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0009031	PE(18:1(11Z)/)	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0009064	PE(18:1(9Z)/)	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0009713	PE(24/14:1(9Z))	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0009517	PE(22:1(13Z)/16)	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0009485	PE(22/16:1(9Z))	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0009255	PE(:1(11Z)/18)	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0009223	PE(/18:1(11Z))	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0009224	PE(/18:1(9Z))	C43H84NO8P	M+NH4	791.6273	-1.9

	HMDB0113891	PE-NMe2(14/22:1(13Z))	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0113537	PE-NMe(22:1(13Z)/15)	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0113032	PE-NMe(15/22:1(13Z))	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0113875	PE-NMe2(16:1(9Z)/)	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0114016	PE-NMe2(18:1(11Z)/18)	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0114043	PE-NMe2(18:1(9Z)/18)	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0114437	PE-NMe2(22:1(13Z)/14)	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0114411	PE-NMe2(22/14:1(9Z))	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0114213	PE-NMe2(:1(11Z)/16)	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0114185	PE-NMe2(/16:1(9Z))	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0113874	PE-NMe2(16/:1(11Z))	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0113873	PE-NMe2(14:1(9Z)/22)	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0113872	PE-NMe2(18/18:1(11Z))	C43H84NO8P	M+NH4	791.6273	-1.9
	HMDB0113871	PE-NMe2(18/18:1(9Z))	C43H84NO8P	M+NH4	791.6273	-1.9
792.5899	HMDB0039527	PC(O-16/:3(8Z,11Z,14Z))	C44H84NO7P	M+Na	792.5878	2.7
	HMDB0008095	PC(18:1(11Z)/P-18:1(11Z))	C44H84NO7P	M+Na	792.5878	2.7
	HMDB0011309	PC(P-18:1(9Z)/18:1(9Z))	C44H84NO7P	M+Na	792.5878	2.7
	HMDB0011308	PC(P-18:1(9Z)/18:1(11Z))	C44H84NO7P	M+Na	792.5878	2.7
	HMDB0011276	PC(P-18:1(11Z)/18:1(9Z))	C44H84NO7P	M+Na	792.5878	2.7
	HMDB0011275	PC(P-18:1(11Z)/18:1(11Z))	C44H84NO7P	M+Na	792.5878	2.7
	HMDB0011244	PC(P-18/18:2(9Z,12Z))	C44H84NO7P	M+Na	792.5878	2.7
	HMDB0011217	PC(P-16/:2(11Z,14Z))	C44H84NO7P	M+Na	792.5878	2.7
	HMDB0008357	PC(:2(11Z,14Z)/P-16)	C44H84NO7P	M+Na	792.5878	2.7
	HMDB0008160	PC(18:2(9Z,12Z)/P-18)	C44H84NO7P	M+Na	792.5878	2.7
	HMDB0008129	PC(18:1(9Z)/P-18:1(9Z))	C44H84NO7P	M+Na	792.5878	2.7
	HMDB0008128	PC(18:1(9Z)/P-18:1(11Z))	C44H84NO7P	M+Na	792.5878	2.7
	HMDB0013429	PC(O-18:1(9Z)/18:2(9Z,12Z))	C44H84NO7P	M+Na	792.5878	2.7
	HMDB0013425	PC(O-18:1(11Z)/18:2(9Z,12Z))	C44H84NO7P	M+Na	792.5878	2.7
	HMDB0008096	PC(18:1(11Z)/P-18:1(9Z))	C44H84NO7P	M+Na	792.5878	2.7
	HMDB0039529	2-O-(4,7,,13,16,19-Docosahexaenoyl)-1-O-hexadecylglycero-3-phosphocholine	C46H82NO7P	M+H	792.5902	-0.3
	HMDB0011319	PC(P-18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C46H82NO7P	M+H	792.5902	-0.3
	HMDB0011286	PC(P-18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C46H82NO7P	M+H	792.5902	-0.3

	HMDB0013409	PC(O-16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C46H82NO7P	M+H	792.5902	-0.3
	HMDB0011287	PC(P-18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C46H82NO7P	M+H	792.5902	-0.3
	HMDB0011255	PC(P-18/:5(5Z,8Z,11Z,14Z,17Z))	C46H82NO7P	M+H	792.5902	-0.3
	HMDB0008685	PC(22:5(4Z,7Z,Z,13Z,16Z)/P-16)	C46H82NO7P	M+H	792.5902	-0.3
	HMDB0008490	PC(:4(8Z,11Z,14Z,17Z)/P-18:1(11Z))	C46H82NO7P	M+H	792.5902	-0.3
	HMDB0008491	PC(:4(8Z,11Z,14Z,17Z)/P-18:1(9Z))	C46H82NO7P	M+H	792.5902	-0.3
	HMDB0008718	PC(22:5(7Z,Z,13Z,16Z,19Z)/P-16)	C46H82NO7P	M+H	792.5902	-0.3
	HMDB0008458	PC(:4(5Z,8Z,11Z,14Z)/P-18:1(9Z))	C46H82NO7P	M+H	792.5902	-0.3
	HMDB0011227	PC(P-16/22:5(4Z,7Z,Z,13Z,16Z))	C46H82NO7P	M+H	792.5902	-0.3
	HMDB0011228	PC(P-16/22:5(7Z,Z,13Z,16Z,19Z))	C46H82NO7P	M+H	792.5902	-0.3
	HMDB0008522	PC(:5(5Z,8Z,11Z,14Z,17Z)/P-18)	C46H82NO7P	M+H	792.5902	-0.3
	HMDB0008457	PC(:4(5Z,8Z,11Z,14Z)/P-18:1(11Z))	C46H82NO7P	M+H	792.5902	-0.3
	HMDB0011320	PC(P-18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C46H82NO7P	M+H	792.5902	-0.3
792.7065	HMDB0044031	TG(16/14:1(9Z)/16:1(9Z))	C49H90O6	M+NH4	792.7076	-1.3
	HMDB0042511	TG(14/18:2(9Z,12Z)/14)	C49H90O6	M+NH4	792.7076	-1.3
	HMDB0047727	TG(14:1(9Z)/14/18:1(9Z))	C49H90O6	M+NH4	792.7076	-1.3
	HMDB0042368	TG(14/18:1(9Z)/14:1(9Z))	C49H90O6	M+NH4	792.7076	-1.3
	HMDB0047726	TG(14:1(9Z)/14/18:1(11Z))	C49H90O6	M+NH4	792.7076	-1.3
	HMDB0042076	TG(14/14/18:2(9Z,12Z))	C49H90O6	M+NH4	792.7076	-1.3
	HMDB0044861	TG(18/14:1(9Z)/14:1(9Z))	C49H90O6	M+NH4	792.7076	-1.3
	HMDB0042338	TG(14/18:1(11Z)/14:1(9Z))	C49H90O6	M+NH4	792.7076	-1.3
	HMDB0042280	TG(14/14:1(9Z)/18:1(11Z))	C49H90O6	M+NH4	792.7076	-1.3
	HMDB0044058	TG(16/16:1(9Z)/14:1(9Z))	C49H90O6	M+NH4	792.7076	-1.3
	HMDB0047771	TG(14:1(9Z)/16/16:1(9Z))	C49H90O6	M+NH4	792.7076	-1.3
	HMDB0042281	TG(14/14:1(9Z)/18:1(9Z))	C49H90O6	M+NH4	792.7076	-1.3
	HMDB0042309	TG(14/16:1(9Z)/16:1(9Z))	C49H90O6	M+NH4	792.7076	-1.3
	HMDB0047793	TG(14:1(9Z)/18/14:1(9Z))	C49H90O6	M+NH4	792.7076	-1.3
	HMDB0010419	TG(16:1(9Z)/14/16:1(9Z))	C49H90O6	M+NH4	792.7076	-1.3
793.5933	HMDB0116653	PG(a-13/i-24)	C43H85O10P	M+H	793.5953	-2.5
	HMDB0116689	PG(i-13/i-24)	C43H85O10P	M+H	793.5953	-2.5
	HMDB0116659	PG(i-12/a-25)	C43H85O10P	M+H	793.5953	-2.5
	HMDB0116408	(2S)-3-hydroxy-2-{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C48H82O7	M+Na	793.5953	-2.5
	HMDB0116400	(2S)-1-hydroxy-3-{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C48H82O7	M+Na	793.5953	-2.5
	HMDB0116383	(2S)-1- {[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C48H82O7	M+Na	793.5953	-2.5
	HMDB0116415	(2S)-2- {[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C48H82O7	M+Na	793.5953	-2.5
	HMDB0011216	PC(P-16/:1(11Z))	C44H86NO7P	M+Na	794.6034	2.1
	HMDB0008062	PC(18/P-18:1(11Z))	C44H86NO7P	M+Na	794.6034	2.1
	HMDB0011307	PC(P-18:1(9Z)/18)	C44H86NO7P	M+Na	794.6034	2.1

794.6051	HMDB0011274	PC(P-18:1(11Z)/18)	C44H86NO7P	M+Na	794.6034	2.1
	HMDB0011243	PC(P-18/18:1(9Z))	C44H86NO7P	M+Na	794.6034	2.1
	HMDB0011242	PC(P-18/18:1(11Z))	C44H86NO7P	M+Na	794.6034	2.1
	HMDB0008324	PC(:1(11Z)/P-16)	C44H86NO7P	M+Na	794.6034	2.1
	HMDB0008127	PC(18:1(9Z)/P-18)	C44H86NO7P	M+Na	794.6034	2.1
	HMDB0008094	PC(18:1(11Z)/P-18)	C44H86NO7P	M+Na	794.6034	2.1
	HMDB0013428	PC(O-18:1(9Z)/18:1(11Z))	C44H86NO7P	M+Na	794.6034	2.1
	HMDB0013418	PC(O-18/18:2(9Z,12Z))	C44H86NO7P	M+Na	794.6034	2.1
	HMDB0008063	PC(18/P-18:1(9Z))	C44H86NO7P	M+Na	794.6034	2.1
	HMDB0013432	PC(O-18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C46H84NO7P	M+H	794.6058	-0.9
	HMDB0011450	PE(P-18:1(9Z)/:3(8Z,11Z,14Z))	C46H84NO7P	M+H	794.6058	-0.9
	HMDB0011253	PC(P-18/:4(5Z,8Z,11Z,14Z))	C46H84NO7P	M+H	794.6058	-0.9
	HMDB0011226	PC(P-16/22:4(7Z,Z,13Z,16Z))	C46H84NO7P	M+H	794.6058	-0.9
	HMDB0008652	PC(22:4(7Z,Z,13Z,16Z)/P-16)	C46H84NO7P	M+H	794.6058	-0.9
	HMDB0008489	PC(:4(8Z,11Z,14Z,17Z)/P-18)	C46H84NO7P	M+H	794.6058	-0.9
	HMDB0008456	PC(:4(5Z,8Z,11Z,14Z)/P-18)	C46H84NO7P	M+H	794.6058	-0.9
	HMDB0008425	PC(:3(8Z,11Z,14Z)/P-18:1(9Z))	C46H84NO7P	M+H	794.6058	-0.9
	HMDB0008424	PC(:3(8Z,11Z,14Z)/P-18:1(11Z))	C46H84NO7P	M+H	794.6058	-0.9
	HMDB0008393	PC(:3(5Z,8Z,11Z)/P-18:1(9Z))	C46H84NO7P	M+H	794.6058	-0.9
	HMDB0008392	PC(:3(5Z,8Z,11Z)/P-18:1(11Z))	C46H84NO7P	M+H	794.6058	-0.9
	HMDB0011254	PC(P-18/:4(8Z,11Z,14Z,17Z))	C46H84NO7P	M+H	794.6058	-0.9
	HMDB0011318	PC(P-18:1(9Z)/:3(8Z,11Z,14Z))	C46H84NO7P	M+H	794.6058	-0.9
	HMDB0011317	PC(P-18:1(9Z)/:3(5Z,8Z,11Z))	C46H84NO7P	M+H	794.6058	-0.9
	HMDB0011285	PC(P-18:1(11Z)/:3(8Z,11Z,14Z))	C46H84NO7P	M+H	794.6058	-0.9
	HMDB0011284	PC(P-18:1(11Z)/:3(5Z,8Z,11Z))	C46H84NO7P	M+H	794.6058	-0.9
794.7226	HMDB0014651	Dextrothyroxine	C15H11I4NO ₄	M+NH4	794.7205	2.6
	HMDB0000248	Thyroxine	C15H11I4NO ₄	M+NH4	794.7205	2.6
	HMDB0185011	Thyroxine	C15H11I4NO ₄	M+NH4	794.7205	2.6
	HMDB0042071	TG(14/14/18:1(9Z))	C49H92O6	M+NH4	794.7232	-0.8
	HMDB0042274	TG(14/14:1(9Z)/18)	C49H92O6	M+NH4	794.7232	-0.8
	HMDB0043890	TG(16/16/14:1(9Z))	C49H92O6	M+NH4	794.7232	-0.8
	HMDB0010412	TG(16/14/16:1(9Z))	C49H92O6	M+NH4	794.7232	-0.8
	HMDB0044672	TG(18/14/14:1(9Z))	C49H92O6	M+NH4	794.7232	-0.8
	HMDB0042303	TG(14/16:1(9Z)/16)	C49H92O6	M+NH4	794.7232	-0.8
	HMDB0042158	TG(14/18/14:1(9Z))	C49H92O6	M+NH4	794.7232	-0.8
	HMDB0042129	TG(14/16/16:1(9Z))	C49H92O6	M+NH4	794.7232	-0.8
	HMDB0042996	TG(15/15/16:1(9Z))	C49H92O6	M+NH4	794.7232	-0.8

	HMDB0042070	TG(14/14/18:1(11Z))	C49H92O6	M+NH4	794.7232	-0.8
	HMDB0031123	Glycerol 1,3-ditetradecanoate 2-(9Z-octadecenoate)	C49H92O6	M+NH4	794.7232	-0.8
	HMDB0044025	TG(16/14:1(9Z)/16)	C49H92O6	M+NH4	794.7232	-0.8
	HMDB0043192	TG(15/16:1(9Z)/15)	C49H92O6	M+NH4	794.7232	-0.8
	HMDB0042361	TG(14/18:1(9Z)/14)	C49H92O6	M+NH4	794.7232	-0.8
	HMDB0042331	TG(14/18:1(11Z)/14)	C49H92O6	M+NH4	794.7232	-0.8
795.4168	HMDB0031025	Betavulgaroside IV	C41H62O15	M+H	795.4161	0.8
	HMDB0163754	6-[(8a-carboxy-4-formyl-8-hydroxy-4,6a,6b,11,11,14b-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-3-yl)oxy]-3,5-dihydroxy-4-[(3,4,5-trihydroxyoxan-2-yl)oxy]oxane-2-carboxylic acid	C41H62O15	M+H	795.4161	0.8
795.5176	HMDB0116575	PG(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C44H75O10P	M+H	795.5171	0.7
	HMDB0116584	PG(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C44H75O10P	M+H	795.5171	0.7
	HMDB0116591	PG(:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C44H75O10P	M+H	795.5171	0.7
	HMDB0116615	PG(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C44H75O10P	M+H	795.5171	0.7
	HMDB0116623	PG(22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C44H75O10P	M+H	795.5171	0.7
	HMDB0116629	PG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/16)	C44H75O10P	M+H	795.5171	0.7
	HMDB0010597	PG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C44H75O10P	M+H	795.5171	0.7
	HMDB0010598	PG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C44H75O10P	M+H	795.5171	0.7
	HMDB0010655	PG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C44H75O10P	M+H	795.5171	0.7
	HMDB0010668	PG(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C44H75O10P	M+H	795.5171	0.7
	HMDB0010669	PG(18:3(6Z,9Z,12Z)/:3(8Z,11Z,14Z))	C44H75O10P	M+H	795.5171	0.7
	HMDB0010683	PG(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C44H75O10P	M+H	795.5171	0.7
	HMDB0010684	PG(18:3(9Z,12Z,15Z)/:3(8Z,11Z,14Z))	C44H75O10P	M+H	795.5171	0.7
	HMDB0010584	PG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C44H75O10P	M+H	795.5171	0.7
796.5248	HMDB0009710	PE(22:6(4Z,7Z,Z,13Z,16Z,19Z)/P-18:1(11Z))	C45H76NO7P	M+Na	796.5252	-0.4
	HMDB0011460	PE(P-18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C45H76NO7P	M+Na	796.5252	-0.4
	HMDB0011427	PE(P-18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C45H76NO7P	M+Na	796.5252	-0.4
	HMDB0009711	PE(22:6(4Z,7Z,Z,13Z,16Z,19Z)/P-18:1(9Z))	C45H76NO7P	M+Na	796.5252	-0.4
796.6191	HMDB0008423	PC(:3(8Z,11Z,14Z)/P-18)	C46H86NO7P	M+H	796.6215	-3.0
	HMDB0008391	PC(:3(5Z,8Z,11Z)/P-18)	C46H86NO7P	M+H	796.6215	-3.0
	HMDB0008359	PC(:2(11Z,14Z)/P-18:1(11Z))	C46H86NO7P	M+H	796.6215	-3.0
	HMDB0008360	PC(:2(11Z,14Z)/P-18:1(9Z))	C46H86NO7P	M+H	796.6215	-3.0
	HMDB0011252	PC(P-18/:3(8Z,11Z,14Z))	C46H86NO7P	M+H	796.6215	-3.0
	HMDB0011316	PC(P-18:1(9Z)/:2(11Z,14Z))	C46H86NO7P	M+H	796.6215	-3.0
	HMDB0013420	PC(O-18/:4(8Z,11Z,14Z,17Z))	C46H86NO7P	M+H	796.6215	-3.0
	HMDB0011283	PC(P-18:1(11Z)/:2(11Z,14Z))	C46H86NO7P	M+H	796.6215	-3.0

HMDB0011251	PC(P-18/:3(5Z,8Z,11Z))	C46H86NO7P	M+H	796.6215	-3.0
HMDB0013414	PC(O-16:1(9Z)/)	C44H88NO7P	M+Na	796.6191	0.1
HMDB0013427	PC(O-18:1(9Z)/18)	C44H88NO7P	M+Na	796.6191	0.1
HMDB0008061	PC(18/P-18)	C44H88NO7P	M+Na	796.6191	0.1
HMDB0011241	PC(P-18/18)	C44H88NO7P	M+Na	796.6191	0.1
HMDB0011215	PC(P-16/)	C44H88NO7P	M+Na	796.6191	0.1
HMDB0008291	PC(/P-16)	C44H88NO7P	M+Na	796.6191	0.1
HMDB0010411	TG(16/14/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0062638	TG(16/16/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0042151	TG(14/18/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0043018	TG(15/16/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071765	TG(/16/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072284	TG(/14/22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095312	TG(12/14/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071144	TG(/18/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095586	TG(12/16/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095042	TG(12/12/22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0042123	TG(14/16/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0042064	TG(14/14/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0042990	TG(15/15/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108536	TG(18/16/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0062699	TG(16/18/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0062862	TG(i-/14/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0062886	TG(/14/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0062960	TG(/a-13/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063046	TG(/i-14/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063083	TG(/i-13/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063141	TG(/i-12/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063166	TG(/i-13/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063174	TG(/8/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063237	TG(i-/8/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063257	TG(/12/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063287	TG(/16/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063286	TG(/i-14/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063288	TG(i-/12/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063293	TG(/a-13/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063298	TG(i-/13/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063400	TG(i-/i-13/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063417	TG(/18/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063441	TG(/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063474	TG(i-/i-13/a-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063553	TG(i-/18/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063557	TG(/i-13/a-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063617	TG(/14/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063638	TG(i-/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063708	TG(i-/13/a-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063724	TG(i-/16/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063778	TG(/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063780	TG(i-/14/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063794	TG(i-/a-13/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063871	TG(i-/a-13/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063897	TG(/i-18/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063917	TG(/a-13/a-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063928	TG(i-/i-18/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063978	TG(i-/i-12/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0063995	TG(i-/8/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064051	TG(/12/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064086	TG(i-/i-13/i-13)	C49H94O6	M+NH4	796.7389	-2.1

HMDB0064110	TG(/8/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064143	TG(i-/13/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064228	TG(i-/i-14/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064257	TG(i-/i-16/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064278	TG(i-/i-12/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064292	TG(/13/a-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064361	TG(/13/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064366	TG(/i-12/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064443	TG(i-/i-14/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064449	TG(/i-16/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064526	TG(/13/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064537	TG(i-/12/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064536	TG(i-//i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064539	TG(i-/a-13/a-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064619	TG(i-21/i-13/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064621	TG(i-21/a-17/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064715	TG(i-21/12/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064789	TG(i-21/a-15/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064798	TG(21/12/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064803	TG(a-21//i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064849	TG(i-21/a-13/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064862	TG(21/12/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064935	TG(a-21/15/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064951	TG(a-21/a-13/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0064964	TG(i-21/i-12/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065054	TG(a-21/i-17/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065075	TG(a-21/i-13/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065091	TG(a-21/i-15/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065109	TG(a-21/8/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065113	TG(21/a-15/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065120	TG(i-21//a-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065126	TG(a-21/12/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065178	TG(i-21/13/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065206	TG(i-21/8/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065213	TG(i-21/a-13/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065214	TG(i-21/12/a-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065217	TG(a-21/a-15/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065263	TG(21/i-12/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065279	TG(21/a-13/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065303	TG(a-21/8/a-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065322	TG(a-21/i-12/a-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065335	TG(a-21/i-12/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065348	TG(a-21//15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065364	TG(i-21/12/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065366	TG(i-21/17/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065395	TG(a-21//a-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065418	TG(21/i-15/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065506	TG(i-21/i-12/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065525	TG(a-21/a-13/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065526	TG(21/15/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065546	TG(i-21/i-13/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065576	TG(21/13/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065612	TG(21//i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065663	TG(21/a-13/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065715	TG(21//15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065727	TG(21/i-13/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065732	TG(a-21/i-13/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065755	TG(a-21/8/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065820	TG(21/17/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065832	TG(i-21/8/a-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065833	TG(21/8/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065849	TG(i-21/i-17/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065884	TG(21//a-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065882	TG(i-21/8/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065925	TG(i-21//15)	C49H94O6	M+NH4	796.7389	-2.1

HMDB0065956	TG(21/i-12/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065981	TG(a-21/12/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0065995	TG(a-21/17/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066010	TG(a-21/12/a-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066019	TG(i-21/13/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066045	TG(i-21/i-12/a-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066069	TG(a-21/a-17/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066075	TG(21/13/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066121	TG(21/12/a-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066131	TG(a-21/13/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066140	TG(21/8/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066213	TG(21/i-17/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066216	TG(21/a-17/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066277	TG(i-21/15/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066280	TG(21/8/a-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066290	TG(21/i-12/a-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066295	TG(a-21/i-12/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066310	TG(21/i-13/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066316	TG(i-21//i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066318	TG(i-21/i-15/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0066339	TG(a-21/13/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0067672	TG(22/12/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0067845	TG(i-22/12/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068145	TG(i-22/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068142	TG(i-22/i-16/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068185	TG(22/8/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068194	TG(22/8/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068199	TG(22/i-12/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068204	TG(i-22/i-14/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068210	TG(22/i-12/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068248	TG(i-22/i-12/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068284	TG(22/16/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068302	TG(i-22/i-12/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068307	TG(i-22/12/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068361	TG(i-22//14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068366	TG(22/12/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068382	TG(i-22/8/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068412	TG(22/i-14/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068467	TG(i-22/14/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068740	TG(22//i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068809	TG(i-22/8/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068900	TG(22/14/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0068921	TG(22//14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0069000	TG(22/i-16/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0069087	TG(i-22/16/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0069388	TG(i-24/12/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0069390	TG(a-25/a-13/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0069751	TG(i-24/8/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0070079	TG(a-25/8/a-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0070106	TG(i-24/14/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0070119	TG(i-24//12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0070132	TG(i-24/i-12/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0070215	TG(i-24/i-14/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0070219	TG(a-25/8/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0070350	TG(a-25/i-13/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0070451	TG(i-24//i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0070709	TG(a-25/8/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0070799	TG(i-24/8/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071087	TG(a-25/13/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071126	TG(/21/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071129	TG(/21/a-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071136	TG(/12/i-24)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071160	TG(8/a-25/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071168	TG(//16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071172	TG(8/a-25/a-13)	C49H94O6	M+NH4	796.7389	-2.1

HMDB0071182	TG(/16/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071230	TG(8/a-21/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071235	TG(/i-24/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071240	TG(/i-18/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071244	TG(/a-21/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071264	TG(8/a-21/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071269	TG(8/i-17/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071291	TG(8//i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071304	TG(8/i-16/22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071329	TG(8/16/i-22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071337	TG(8/i-24/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071369	TG(/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071379	TG(8/i-/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071438	TG(8/17/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071514	TG(8/18/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071516	TG(8/i-17/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071531	TG(8/18/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071547	TG(/i-21/a-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071544	TG(8/13/a-25)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071578	TG(/i-22/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071597	TG(/22/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071615	TG(8/i-14/i-24)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071633	TG(8/17/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071649	TG(/i-16/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071658	TG(/i-14/22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071678	TG(/i-21/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071737	TG(/18/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071755	TG(8/i-21/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071771	TG(8/i-16/i-22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071788	TG(/i-17/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071793	TG(8/17/a-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071800	TG(/a-15/a-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071824	TG(/a-21/a-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071830	TG(8/19/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071841	TG(8/a-17/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071849	TG(/a-15/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071853	TG(8/i-18/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071895	TG(8/a-21/a-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071903	TG(/22/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071901	TG(/i-19/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071969	TG(/a-15/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071975	TG(8/i-21/a-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071977	TG(/i-17/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071993	TG(8/a-17/a-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0071995	TG(/a-17/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072028	TG(/i-15/a-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072054	TG(/i-18/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072065	TG(/21/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072079	TG(/i-19/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072098	TG(8/21/a-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072103	TG(8/22/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072107	TG(/i-15/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072133	TG(/14/i-22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072148	TG(8/21/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072170	TG(8/i-13/a-25)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072175	TG(/i-/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072223	TG(/19/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072229	TG(/19/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072269	TG(/15/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072273	TG(/i-15/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072278	TG(/15/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072298	TG(8/i-19/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072370	TG(8/i-19/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072399	TG(8/i-24/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072423	TG(/15/a-21)	C49H94O6	M+NH4	796.7389	-2.1

HMDB0072421	TG(8/a-25/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072427	TG(/i-22/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072455	TG(8/22/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072454	TG(/17/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072466	TG(8/i-22/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072476	TG(8/21/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072481	TG(/i-21/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072492	TG(8//18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072539	TG(8/i-17/a-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072560	TG(/a-17/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072578	TG(/i-24/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072588	TG(/19/a-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072596	TG(8/i-18/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072605	TG(/17/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072621	TG(8/16/22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072619	TG(8/19/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072634	TG(8/a-13/a-25)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072648	TG(/a-21/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072674	TG(/i-16/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072696	TG(8/a-17/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072704	TG(/i-/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072738	TG(/i-19/a-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072749	TG(/i-12/i-24)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072763	TG(8/14/i-24)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072767	TG(/i-14/i-22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072783	TG(8/i-/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072796	TG(8/i-22/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0072837	TG(8/i-21/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0094936	TG(12//i-24)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0094935	TG(i-12//i-24)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095036	TG(12/i-12/22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095037	TG(i-12/12/i-22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095038	TG(12/i-12/i-22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095039	TG(i-12/i-12/22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095041	TG(i-12/12/22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095040	TG(i-12/i-12/i-22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095043	TG(12/12/i-22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095185	TG(i-12/a-13/a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095184	TG(12/a-13/a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095187	TG(12/a-13/21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095186	TG(i-12/a-13/i-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095190	TG(12/i-13/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095189	TG(12/a-13/i-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095191	TG(i-12/13/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095188	TG(i-12/a-13/21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095192	TG(i-12/i-13/a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095193	TG(12/i-13/a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095195	TG(i-12/i-13/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095194	TG(12/i-13/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095196	TG(i-12/13/a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095199	TG(12/13/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095198	TG(i-12/13/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095197	TG(i-12/i-13/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095201	TG(12/13/a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095200	TG(12/13/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095306	TG(12/i-14/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095307	TG(i-12/14/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095310	TG(i-12/i-14/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095309	TG(i-12/i-14/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095308	TG(12/i-14/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095311	TG(i-12/14/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095313	TG(12/14/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095451	TG(12/a-15/19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095450	TG(i-12/a-15/i-19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095452	TG(i-12/a-15/19)[rac]	C49H94O6	M+NH4	796.7389	-2.1

HMDB0095455	TG(i-12/15/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095454	TG(12/i-15/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095453	TG(12/a-15/i-19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095456	TG(12/i-15/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095459	TG(i-12/15/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095457	TG(i-12/i-15/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095458	TG(i-12/i-15/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095461	TG(12/15/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095460	TG(12/15/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095580	TG(12/i-16/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095582	TG(12/i-16/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095581	TG(i-12/16/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095584	TG(i-12/i-16/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095587	TG(12/16/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095585	TG(i-12/16/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095583	TG(i-12/i-16/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095712	TG(i-12/a-17/i-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095710	TG(12/a-17/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095713	TG(12/a-17/17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095711	TG(i-12/a-17/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095715	TG(12/a-17/i-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095716	TG(12/i-17/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095714	TG(i-12/a-17/17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095717	TG(i-12/17/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095721	TG(i-12/i-17/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095719	TG(12/i-17/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095718	TG(i-12/i-17/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095720	TG(12/i-17/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095725	TG(12/17/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095722	TG(i-12/17/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095723	TG(i-12/i-17/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095724	TG(i-12/17/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095726	TG(12/17/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095727	TG(12/17/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095850	TG(12/i-18/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095851	TG(i-12/18/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095853	TG(i-12/i-18/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095852	TG(12/i-18/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095856	TG(12/18/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095854	TG(i-12/i-18/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095855	TG(i-12/18/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095956	TG(12/i-19/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095955	TG(i-12/i-19/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095954	TG(i-12/19/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095953	TG(12/i-19/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095957	TG(12/i-19/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095958	TG(i-12/i-19/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095959	TG(i-12/19/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095960	TG(i-12/i-19/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095964	TG(12/19/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095961	TG(i-12/19/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095963	TG(12/19/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0095962	TG(12/19/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096062	TG(i-12//i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096064	TG(i-12/i-/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096063	TG(12/i-/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096061	TG(12/i-/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096065	TG(i-12/i-/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096068	TG(12//i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096067	TG(12//14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096066	TG(i-12//14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096171	TG(12/a-21/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096173	TG(i-12/a-21/i-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096174	TG(12/a-21/13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096172	TG(i-12/a-21/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1

HMDB0096177	TG(12/i-21/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096175	TG(i-12/a-21/13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096178	TG(i-12/21/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096176	TG(12/a-21/i-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096182	TG(i-12/i-21/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096180	TG(12/i-21/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096181	TG(12/i-21/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096179	TG(i-12/i-21/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096186	TG(12/21/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096183	TG(i-12/21/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096185	TG(i-12/21/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096184	TG(i-12/i-21/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096187	TG(12/21/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096188	TG(12/21/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096335	TG(12/i-22/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096337	TG(i-12/22/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096338	TG(12/22/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096336	TG(i-12/i-22/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096446	TG(i-12/i-24/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096445	TG(12/i-24/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096646	TG(a-13/8/a-25)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096647	TG(i-13/8/a-25)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096648	TG(13/8/a-25)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096877	TG(a-13/12/a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096878	TG(13/i-12/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096879	TG(a-13/12/21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096883	TG(i-13/12/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096881	TG(a-13/i-12/i-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096880	TG(a-13/12/i-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096882	TG(a-13/i-12/21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096884	TG(i-13/i-12/a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096886	TG(a-13/i-12/a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096887	TG(13/i-12/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096885	TG(13/i-12/a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096889	TG(i-13/12/a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096890	TG(i-13/i-12/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096891	TG(i-13/12/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096888	TG(i-13/i-12/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096892	TG(13/12/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096894	TG(13/12/a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0096893	TG(13/12/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097091	TG(i-13/a-13/)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097089	TG(i-13/a-13/i-)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097090	TG(13/a-13/)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097095	TG(13/i-13/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097094	TG(a-13/a-13/i-)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097092	TG(a-13/a-13/)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097093	TG(13/a-13/i-)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097096	TG(a-13/13/)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097098	TG(a-13/i-13/i-)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097099	TG(a-13/i-13/)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097097	TG(a-13/13/i-)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097102	TG(i-13/i-13/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097100	TG(i-13/13/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097103	TG(i-13/i-13/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097101	TG(13/i-13/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097104	TG(i-13/13/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097105	TG(13/13/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097106	TG(13/13/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097278	TG(13/i-14/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097279	TG(a-13/14/19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097280	TG(a-13/14/i-19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097281	TG(a-13/i-14/i-19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097282	TG(a-13/i-14/19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097283	TG(i-13/14/i-19)	C49H94O6	M+NH4	796.7389	-2.1

HMDB0097284	TG(13/i-14/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097287	TG(i-13/14/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097286	TG(i-13/i-14/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097285	TG(i-13/i-14/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097289	TG(13/14/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097288	TG(13/14/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097488	TG(i-13/a-15/i-18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097489	TG(13/a-15/18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097490	TG(i-13/a-15/18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097491	TG(a-13/a-15/18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097492	TG(13/a-15/i-18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097495	TG(a-13/15/18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097493	TG(a-13/a-15/i-18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097494	TG(13/i-15/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097497	TG(a-13/i-15/i-18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097499	TG(i-13/15/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097496	TG(a-13/15/i-18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097498	TG(a-13/i-15/18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097503	TG(i-13/15/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097502	TG(i-13/i-15/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097500	TG(13/i-15/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097501	TG(i-13/i-15/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097504	TG(13/15/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097505	TG(13/15/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097683	TG(a-13/16/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097685	TG(a-13/16/17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097687	TG(a-13/i-16/i-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097684	TG(13/i-16/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097686	TG(a-13/16/i-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097689	TG(i-13/16/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097690	TG(i-13/i-16/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097688	TG(a-13/i-16/17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097691	TG(13/i-16/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097692	TG(a-13/i-16/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097693	TG(13/i-16/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097694	TG(i-13/i-16/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097695	TG(i-13/16/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097698	TG(13/16/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097699	TG(13/16/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097696	TG(i-13/i-16/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097697	TG(i-13/16/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097700	TG(13/16/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097879	TG(13/a-17/16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097878	TG(i-13/a-17/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097880	TG(i-13/a-17/16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097883	TG(a-13/a-17/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097881	TG(a-13/a-17/16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097882	TG(13/a-17/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097886	TG(a-13/17/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097887	TG(a-13/i-17/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097885	TG(a-13/17/16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097884	TG(13/i-17/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097890	TG(13/i-17/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097891	TG(i-13/i-17/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097888	TG(a-13/i-17/16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097889	TG(i-13/17/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097892	TG(i-13/i-17/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097893	TG(i-13/17/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097895	TG(13/17/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0097894	TG(13/17/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098089	TG(13/i-18/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098088	TG(a-13/18/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098091	TG(a-13/18/i-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098090	TG(a-13/18/15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098094	TG(i-13/18/i-15)	C49H94O6	M+NH4	796.7389	-2.1

HMDB0098093	TG(a-13/i-18/15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098095	TG(i-13/i-18/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098092	TG(a-13/i-18/i-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098096	TG(13/i-18/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098097	TG(a-13/i-18/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098099	TG(i-13/i-18/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098098	TG(13/i-18/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098102	TG(i-13/18/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098100	TG(i-13/18/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098103	TG(13/18/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098101	TG(i-13/i-18/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098105	TG(13/18/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098104	TG(13/18/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098251	TG(a-13/19/14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098250	TG(13/i-19/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098253	TG(a-13/i-19/i-14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098254	TG(a-13/i-19/14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098255	TG(i-13/19/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098252	TG(a-13/19/i-14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098259	TG(i-13/19/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098257	TG(i-13/i-19/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098258	TG(i-13/i-19/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098256	TG(13/i-19/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098261	TG(13/19/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098260	TG(13/19/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098415	TG(a-13/i-/13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098413	TG(a-13//i-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098412	TG(a-13//13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098414	TG(a-13/i-/i-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098417	TG(13/i-/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098419	TG(i-13/i-/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098416	TG(i-13/i-/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098418	TG(13/i-/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098421	TG(i-13//13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098422	TG(13//i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098423	TG(13//a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098420	TG(i-13//a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098580	TG(i-13/a-21/i-12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098582	TG(i-13/a-21/12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098581	TG(13/a-21/12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098583	TG(a-13/a-21/12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098586	TG(13/i-21/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098587	TG(a-13/21/12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098585	TG(a-13/a-21/i-12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098584	TG(13/a-21/i-12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098588	TG(a-13/21/i-12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098591	TG(i-13/21/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098589	TG(a-13/i-21/i-12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098590	TG(a-13/i-21/12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098595	TG(i-13/21/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098593	TG(i-13/i-21/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098592	TG(13/i-21/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098594	TG(i-13/i-21/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098597	TG(13/21/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0098596	TG(13/21/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099086	TG(a-13/a-25/8)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099084	TG(13/a-25/8)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099085	TG(i-13/a-25/8)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099227	TG(i-14/8/i-24)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099228	TG(14/8/i-24)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099283	TG(i-14//i-22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099286	TG(14//i-22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099284	TG(i-14//22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099285	TG(14//22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099375	TG(14/i-12/)	C49H94O6	M+NH4	796.7389	-2.1

796.7372

HMDB0099377	TG(14/i-12/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099379	TG(i-14/i-12/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099376	TG(i-14/12/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099378	TG(i-14/i-12/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099382	TG(14/12/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099380	TG(i-14/12/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099381	TG(14/12/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099526	TG(14/a-13/19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099527	TG(i-14/a-13/19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099525	TG(i-14/a-13/i-19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099528	TG(14/a-13/i-19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099529	TG(14/i-13/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099531	TG(14/i-13/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099530	TG(i-14/13/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099535	TG(14/13/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099532	TG(i-14/i-13/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099534	TG(i-14/13/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099533	TG(i-14/i-13/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099536	TG(14/13/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099642	TG(14/i-14/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099643	TG(i-14/i-14/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099641	TG(i-14/14/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099640	TG(14/i-14/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099645	TG(i-14/14/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099646	TG(14/14/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099644	TG(i-14/i-14/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099765	TG(14/a-15/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099766	TG(i-14/a-15/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099767	TG(i-14/a-15/i-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099770	TG(14/a-15/i-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099771	TG(14/i-15/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099769	TG(i-14/a-15/17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099768	TG(14/a-15/17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099772	TG(i-14/15/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099775	TG(14/i-15/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099773	TG(i-14/i-15/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099774	TG(14/i-15/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099778	TG(i-14/i-15/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099779	TG(i-14/15/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099777	TG(i-14/15/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099776	TG(i-14/i-15/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099780	TG(14/15/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099781	TG(14/15/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099782	TG(14/15/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099901	TG(14/i-16/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099903	TG(14/i-16/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099902	TG(i-14/16/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099907	TG(14/16/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099905	TG(i-14/i-16/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099904	TG(i-14/i-16/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0099906	TG(i-14/16/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100019	TG(14/a-17/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100020	TG(i-14/a-17/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100022	TG(14/a-17/15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100021	TG(i-14/a-17/i-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100025	TG(14/i-17/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100023	TG(i-14/a-17/15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100024	TG(14/a-17/i-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100026	TG(i-14/17/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100030	TG(i-14/i-17/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100029	TG(14/i-17/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100028	TG(14/i-17/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100027	TG(i-14/i-17/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100033	TG(i-14/17/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100032	TG(i-14/i-17/i-15)	C49H94O6	M+NH4	796.7389	-2.1

HMDB0100031	TG(i-14/17/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100034	TG(14/17/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100036	TG(14/17/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100035	TG(14/17/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100173	TG(14/i-18/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100174	TG(i-14/i-18/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100176	TG(14/18/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100175	TG(i-14/18/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100272	TG(14/i-19/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100274	TG(i-14/i-19/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100273	TG(i-14/19/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100275	TG(14/i-19/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100276	TG(14/i-19/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100278	TG(i-14/19/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100277	TG(i-14/i-19/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100282	TG(14/19/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100279	TG(i-14/i-19/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100281	TG(14/19/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100280	TG(i-14/19/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100283	TG(14/19/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100380	TG(14/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100381	TG(i-14//i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100382	TG(14/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100385	TG(i-14//12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100383	TG(i-14/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100384	TG(i-14/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100386	TG(14//12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100387	TG(14//i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100662	TG(i-14/i-22/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100663	TG(i-14/22/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100664	TG(14/22/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100661	TG(14/i-22/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100768	TG(14/i-24/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0100769	TG(i-14/i-24/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101044	TG(a-15//21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101043	TG(a-15//a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101045	TG(a-15//i-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101047	TG(i-15//a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101048	TG(i-15//21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101046	TG(i-15//i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101051	TG(15//a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101049	TG(15//21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101050	TG(15//i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101178	TG(15/i-12/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101179	TG(a-15/12/19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101180	TG(a-15/12/i-19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101184	TG(15/i-12/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101181	TG(a-15/i-12/i-19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101182	TG(a-15/i-12/19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101183	TG(i-15/12/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101188	TG(15/12/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101187	TG(i-15/12/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101186	TG(i-15/i-12/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101185	TG(i-15/i-12/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101189	TG(15/12/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101397	TG(i-15/a-13/i-18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101398	TG(15/a-13/18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101399	TG(i-15/a-13/18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101400	TG(a-15/a-13/18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101402	TG(a-15/a-13/i-18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101401	TG(15/a-13/i-18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101403	TG(15/i-13/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101405	TG(a-15/13/i-18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101404	TG(a-15/13/18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101408	TG(i-15/13/i-18)	C49H94O6	M+NH4	796.7389	-2.1

HMDB0101406	TG(a-15/i-13/i-18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101407	TG(a-15/i-13/18)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101411	TG(i-15/i-13/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101409	TG(15/i-13/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101410	TG(i-15/i-13/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101412	TG(i-15/13/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101413	TG(15/13/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101414	TG(15/13/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101597	TG(a-15/14/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101598	TG(15/i-14/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101599	TG(a-15/14/17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101600	TG(a-15/14/i-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101601	TG(a-15/i-14/i-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101602	TG(a-15/i-14/17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101603	TG(i-15/14/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101605	TG(15/i-14/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101604	TG(i-15/i-14/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101606	TG(a-15/i-14/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101609	TG(i-15/14/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101608	TG(i-15/i-14/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101607	TG(15/i-14/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101610	TG(i-15/i-14/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101611	TG(i-15/14/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101613	TG(15/14/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101612	TG(15/14/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101614	TG(15/14/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101766	TG(i-15/a-15/16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101764	TG(i-15/a-15/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101765	TG(15/a-15/16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101768	TG(15/a-15/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101767	TG(a-15/a-15/16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101769	TG(a-15/a-15/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101770	TG(15/i-15/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101771	TG(a-15/15/16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101772	TG(a-15/15/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101773	TG(a-15/i-15/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101774	TG(a-15/i-15/16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101775	TG(i-15/15/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101776	TG(15/i-15/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101777	TG(i-15/i-15/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101778	TG(i-15/i-15/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101780	TG(15/15/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101779	TG(i-15/15/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101976	TG(a-15/16/15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101977	TG(a-15/16/i-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101978	TG(a-15/i-16/i-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101979	TG(a-15/i-16/15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101981	TG(15/i-16/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101980	TG(i-15/i-16/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101982	TG(15/i-16/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101983	TG(i-15/i-16/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101984	TG(i-15/16/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101986	TG(15/16/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101985	TG(i-15/16/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0101987	TG(15/16/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102155	TG(i-15/a-17/i-14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102156	TG(15/a-17/14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102160	TG(a-15/a-17/i-14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102157	TG(i-15/a-17/14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102159	TG(15/a-17/i-14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102158	TG(a-15/a-17/14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102161	TG(15/i-17/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102163	TG(a-15/17/i-14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102162	TG(a-15/17/14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102166	TG(i-15/17/i-14)	C49H94O6	M+NH4	796.7389	-2.1

HMDB0102165	TG(a-15/i-17/14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102167	TG(15/i-17/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102164	TG(a-15/i-17/i-14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102171	TG(15/17/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102168	TG(i-15/i-17/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102170	TG(i-15/17/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102169	TG(i-15/i-17/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102172	TG(15/17/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102378	TG(15/i-18/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102379	TG(a-15/18/13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102377	TG(a-15/18/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102380	TG(a-15/18/i-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102383	TG(i-15/18/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102382	TG(a-15/i-18/13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102381	TG(a-15/i-18/i-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102386	TG(a-15/i-18/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102384	TG(i-15/i-18/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102387	TG(15/i-18/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102385	TG(15/i-18/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102388	TG(i-15/i-18/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102389	TG(i-15/18/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102391	TG(i-15/18/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102390	TG(i-15/i-18/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102392	TG(15/18/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102393	TG(15/18/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102394	TG(15/18/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102535	TG(15/i-19/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102539	TG(a-15/i-19/12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102537	TG(a-15/19/i-12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102536	TG(a-15/19/12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102538	TG(a-15/i-19/i-12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102542	TG(i-15/i-19/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102541	TG(15/i-19/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102543	TG(i-15/i-19/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102540	TG(i-15/19/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102545	TG(15/19/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102544	TG(i-15/19/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102546	TG(15/19/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102877	TG(i-15/a-21/)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102876	TG(15/a-21/)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102879	TG(15/i-21/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102881	TG(a-15/i-21/)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102878	TG(a-15/a-21/)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102880	TG(a-15/21/)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102882	TG(i-15/i-21/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102883	TG(i-15/21/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0102884	TG(15/21/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103524	TG(i-16/8/i-22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103525	TG(i-16/8/22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103527	TG(16/8/i-22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103526	TG(16/8/22)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103575	TG(i-16//)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103574	TG(i-16//i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103576	TG(16//)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103577	TG(16//i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103660	TG(16/i-12/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103661	TG(i-16/12/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103662	TG(16/i-12/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103664	TG(i-16/i-12/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103663	TG(i-16/i-12/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103667	TG(16/12/i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103665	TG(i-16/12/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103666	TG(16/12/18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103797	TG(i-16/a-13/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103796	TG(16/a-13/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1

HMDB0103801	TG(16/a-13/i-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103799	TG(16/a-13/17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103798	TG(i-16/a-13/i-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103800	TG(i-16/a-13/17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103802	TG(16/i-13/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103803	TG(i-16/13/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103805	TG(16/i-13/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103804	TG(i-16/i-13/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103808	TG(i-16/13/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103806	TG(16/i-13/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103809	TG(i-16/i-13/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103807	TG(i-16/i-13/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103812	TG(16/13/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103813	TG(16/13/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103810	TG(i-16/13/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103811	TG(16/13/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103940	TG(16/16/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103941	TG(i-16/i-16/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103942	TG(16/i-14/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103946	TG(16/14/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103943	TG(i-16/i-14/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103944	TG(i-16/i-16/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0103945	TG(i-16/14/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104062	TG(16/a-15/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104065	TG(16/a-15/15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104063	TG(i-16/a-15/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104066	TG(i-16/a-15/15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104064	TG(i-16/a-15/i-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104068	TG(16/i-15/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104069	TG(i-16/15/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104070	TG(i-16/i-15/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104067	TG(16/a-15/i-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104073	TG(i-16/i-15/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104074	TG(i-16/15/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104071	TG(16/i-15/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104072	TG(16/i-15/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104077	TG(16/15/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104078	TG(16/15/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104075	TG(i-16/i-15/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104076	TG(i-16/15/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104079	TG(16/15/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104202	TG(i-16/16/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104199	TG(16/i-16/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104200	TG(i-16/16/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104201	TG(16/i-16/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104301	TG(i-16/a-17/i-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104300	TG(i-16/a-17/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104302	TG(16/a-17/13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104299	TG(16/a-17/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104303	TG(i-16/a-17/13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104305	TG(16/i-17/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104304	TG(16/a-17/i-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104306	TG(i-16/17/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104308	TG(16/i-17/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104310	TG(i-16/i-17/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104307	TG(i-16/i-17/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104309	TG(16/i-17/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104311	TG(i-16/17/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104312	TG(i-16/i-17/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104313	TG(i-16/17/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104314	TG(16/17/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104315	TG(16/17/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104316	TG(16/17/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104458	TG(i-16/18/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104457	TG(16/i-18/12)	C49H94O6	M+NH4	796.7389	-2.1

HMDB0104461	TG(i-16/i-18/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104459	TG(16/i-18/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104460	TG(i-16/i-18/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104462	TG(i-16/18/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104463	TG(16/18/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104464	TG(16/18/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104682	TG(16/i-/-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104685	TG(16/-/-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104683	TG(i-16/i-/-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104684	TG(i-16/-/-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104966	TG(i-16/i-22/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104965	TG(16/i-22/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104967	TG(i-16/22/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0104968	TG(16/22/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105263	TG(a-17/8/a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105266	TG(i-17/8/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105265	TG(a-17/8/i-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105264	TG(a-17/8/21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105269	TG(17/8/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105270	TG(17/8/i-21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105268	TG(i-17/8/21)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105267	TG(i-17/8/a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105271	TG(17/8/a-21)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105342	TG(a-17/i-19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105341	TG(a-17//19)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105346	TG(17//i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105345	TG(17//19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105343	TG(i-17//i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105344	TG(i-17//19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105458	TG(a-17/a-17/12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105459	TG(17/17/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105461	TG(a-17/12/i-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105460	TG(a-17/12/17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105462	TG(a-17/i-12/i-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105464	TG(i-17/i-17/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105466	TG(17/i-12/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105465	TG(i-17/i-12/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105463	TG(a-17/i-12/17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105469	TG(i-17/i-12/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105468	TG(17/i-12/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105467	TG(a-17/a-17/i-12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105470	TG(i-17/12/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105473	TG(17/17/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105472	TG(i-17/12/17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105471	TG(i-17/i-17/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105474	TG(17/12/i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105475	TG(17/12/a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105662	TG(i-17/a-13/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105664	TG(i-17/a-13/16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105666	TG(17/a-13/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105665	TG(a-17/a-13/16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105663	TG(17/a-13/16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105668	TG(17/i-13/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105667	TG(a-17/a-13/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105670	TG(a-17/13/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105669	TG(a-17/13/16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105673	TG(i-17/13/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105672	TG(a-17/i-13/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105671	TG(a-17/i-13/i-16)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105674	TG(17/i-13/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105675	TG(i-17/i-13/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105677	TG(i-17/13/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105678	TG(17/13/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105676	TG(i-17/i-13/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105679	TG(17/13/i-16)	C49H94O6	M+NH4	796.7389	-2.1

HMDB0105878	TG(a-17/14/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105882	TG(a-17/i-14/i-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105879	TG(17/i-14/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105881	TG(a-17/14/i-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105880	TG(a-17/14/15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105886	TG(17/i-14/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105883	TG(a-17/i-14/15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105885	TG(i-17/i-14/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105884	TG(i-17/14/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105887	TG(a-17/i-14/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105889	TG(i-17/i-14/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105890	TG(i-17/14/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105888	TG(17/i-14/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105892	TG(i-17/14/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105894	TG(17/14/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105893	TG(17/14/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105891	TG(i-17/i-14/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0105895	TG(17/14/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106068	TG(17/a-15/14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106067	TG(i-17/a-15/i-14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106070	TG(a-17/a-15/14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106069	TG(i-17/a-15/14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106074	TG(a-17/15/14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106073	TG(17/i-15/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106072	TG(a-17/a-15/i-14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106071	TG(17/a-15/i-14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106077	TG(a-17/i-15/14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106075	TG(a-17/15/i-14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106076	TG(a-17/i-15/i-14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106078	TG(i-17/15/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106081	TG(i-17/i-15/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106082	TG(i-17/15/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106079	TG(17/i-15/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106080	TG(i-17/i-15/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106083	TG(17/15/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106084	TG(17/15/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106298	TG(a-17/16/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106299	TG(17/i-16/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106301	TG(a-17/16/i-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106302	TG(a-17/i-16/i-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106300	TG(a-17/16/13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106305	TG(i-17/i-16/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106306	TG(17/i-16/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106303	TG(a-17/i-16/13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106304	TG(i-17/16/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106310	TG(i-17/16/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106308	TG(17/i-16/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106307	TG(a-17/i-16/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106309	TG(i-17/i-16/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106311	TG(i-17/i-16/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106313	TG(17/16/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106314	TG(17/16/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106312	TG(i-17/16/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106315	TG(17/16/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106466	TG(i-17/a-17/i-12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106468	TG(i-17/a-17/12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106467	TG(17/a-17/12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106470	TG(17/i-17/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106469	TG(17/a-17/i-12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106471	TG(a-17/17/12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106473	TG(a-17/i-17/i-12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106472	TG(a-17/17/i-12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106474	TG(a-17/i-17/12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106475	TG(i-17/17/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106477	TG(i-17/17/12)	C49H94O6	M+NH4	796.7389	-2.1

HMDB0106476	TG(17/i-17/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106856	TG(a-17/19/)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106855	TG(17/i-19/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106858	TG(i-17/i-19/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106857	TG(a-17/i-19/)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106860	TG(17/19/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0106859	TG(i-17/19/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107198	TG(i-17/a-21/8)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107197	TG(17/a-21/8)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107201	TG(a-17/21/8)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107199	TG(a-17/a-21/8)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107200	TG(17/i-21/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107202	TG(a-17/i-21/8)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107203	TG(i-17/i-21/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107204	TG(i-17/21/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107205	TG(17/21/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107848	TG(i-18/8/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107850	TG(18/8/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107849	TG(i-18/8/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107851	TG(18/8/i-)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107901	TG(i-18//18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107900	TG(i-18/i-18/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107902	TG(18/18/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107903	TG(18//i-18)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107974	TG(18/i-12/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107975	TG(i-18/12/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107977	TG(i-18/i-12/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107978	TG(i-18/i-12/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107976	TG(18/i-12/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107981	TG(18/12/i-16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107980	TG(18/12/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0107979	TG(i-18/12/16)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108100	TG(18/a-13/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108101	TG(i-18/a-13/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108102	TG(i-18/a-13/i-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108104	TG(i-18/a-13/15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108103	TG(18/a-13/15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108105	TG(18/a-13/i-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108106	TG(18/i-13/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108107	TG(i-18/13/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108109	TG(18/i-13/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108108	TG(i-18/i-13/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108110	TG(18/i-13/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108111	TG(i-18/i-13/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108112	TG(i-18/13/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108114	TG(i-18/13/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108113	TG(i-18/i-13/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108117	TG(18/13/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108116	TG(18/13/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108115	TG(18/13/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108254	TG(18/i-14/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108257	TG(i-18/i-14/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108255	TG(i-18/14/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108256	TG(18/i-14/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108261	TG(18/14/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108258	TG(i-18/i-14/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108259	TG(i-18/14/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108260	TG(18/14/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108368	TG(18/a-15/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108369	TG(i-18/a-15/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108370	TG(i-18/a-15/i-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108371	TG(18/a-15/13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108373	TG(18/a-15/i-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108372	TG(i-18/a-15/13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108374	TG(18/i-15/13)	C49H94O6	M+NH4	796.7389	-2.1

HMDB0108375	TG(i-18/15/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108376	TG(i-18/i-15/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108377	TG(18/i-15/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108381	TG(i-18/i-15/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108380	TG(i-18/15/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108378	TG(18/i-15/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108379	TG(i-18/i-15/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108383	TG(18/15/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108385	TG(18/15/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108382	TG(i-18/15/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108384	TG(18/15/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108530	TG(18/i-16/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108533	TG(i-18/i-16/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108532	TG(18/i-16/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108531	TG(i-18/16/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108535	TG(i-18/16/12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108534	TG(i-18/i-16/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108537	TG(18/16/i-12)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108823	TG(i-18/18/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0108822	TG(18/i-18/)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109019	TG(i-18//8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109020	TG(18//8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109018	TG(i-18/i-8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109017	TG(18/i-8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109574	TG(i-19/8/19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109573	TG(i-19/i-19/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109575	TG(19/19/8)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109576	TG(19/8/i-19)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109623	TG(i-19//i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109625	TG(i-19//17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109626	TG(19//17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109624	TG(i-19//a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109628	TG(19//a-17)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109627	TG(19//i-17)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109693	TG(i-19/i-12/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109691	TG(19/i-12/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109694	TG(19/i-12/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109692	TG(i-19/12/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109696	TG(i-19/i-12/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109697	TG(i-19/12/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109695	TG(19/i-12/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109698	TG(i-19/i-12/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109701	TG(19/12/i-15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109699	TG(i-19/12/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109700	TG(19/12/15)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109702	TG(19/12/a-15)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109818	TG(19/a-13/14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109817	TG(i-19/a-13/i-14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109822	TG(i-19/13/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109821	TG(19/i-13/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109819	TG(i-19/a-13/14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109820	TG(19/a-13/i-14)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109823	TG(19/i-13/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109826	TG(i-19/13/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109824	TG(i-19/i-13/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109825	TG(i-19/i-13/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109828	TG(19/13/i-14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109827	TG(19/13/14)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109973	TG(i-19/i-14/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109971	TG(19/i-14/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109972	TG(i-19/14/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109974	TG(19/i-14/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109978	TG(i-19/i-14/i-13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109976	TG(i-19/i-14/13)	C49H94O6	M+NH4	796.7389	-2.1
HMDB0109975	TG(19/i-14/i-13)	C49H94O6	M+NH4	796.7389	-2.1

	HMDB0109977	TG(i-19/14/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0109979	TG(i-19/14/13)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0109982	TG(19/14/a-13)[rac]	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0109981	TG(19/14/i-13)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0109980	TG(19/14/13)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110088	TG(19/a-15/12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110089	TG(i-19/a-15/12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110090	TG(19/a-15/i-12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110087	TG(i-19/a-15/i-12)[rac]	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110093	TG(19/i-15/i-12)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110091	TG(19/i-15/12)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110092	TG(i-19/15/i-12)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110094	TG(i-19/i-15/12)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110097	TG(19/15/12)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110098	TG(19/15/i-12)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110096	TG(i-19/15/12)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110095	TG(i-19/i-15/i-12)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110381	TG(19/a-17/)[rac]	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110382	TG(i-19/a-17/)[rac]	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110383	TG(19/i-17/)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110386	TG(19/17/)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110384	TG(i-19/i-17/)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110385	TG(i-19/17/)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110676	TG(i-19/19/8)	C49H94O6	M+NH4	796.7389	-2.1
	HMDB0110675	TG(19/i-19/8)	C49H94O6	M+NH4	796.7389	-2.1
797.1000	HMDB0136602	{4-[(5,7-dihydroxy-2-[3,4,6-trihydroxy-5-oxo-8-(3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-2-yl)-5H-benzo[7]annulen-1-yl]-3,4-dihydro-2H-1-benzopyran-3-yl}oxy)carbonyl]-2,6-dihydroxyphenyl}oxidanesulfonic acid	C36H28O19S	M+H	797.1018	-2.3
	HMDB0136603	(2-{1-[5,7-dihydroxy-3-(3,4,5-trihydroxybenzoyloxy)-3,4-dihydro-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-5H-benzo[7]annulen-8-yl}-5,7-dihydroxy-3,4-dihydro-2H-1-benzopyran-3-yl)oxidanesulfonic acid	C36H28O19S	M+H	797.1018	-2.3
	HMDB0136622	{4-[(5,7-dihydroxy-2-[3,4,6-trihydroxy-5-oxo-1-(3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-2-yl)-5H-benzo[7]annulen-8-yl]-3,4-dihydro-2H-1-benzopyran-3-yl}oxy)carbonyl]-2,6-dihydroxyphenyl}oxidanesulfonic acid	C36H28O19S	M+H	797.1018	-2.3
	HMDB0136623	(2-{8-[5,7-dihydroxy-3-(3,4,5-trihydroxybenzoyloxy)-3,4-dihydro-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-5H-benzo[7]annulen-1-yl}-5,7-dihydroxy-3,4-dihydro-2H-1-benzopyran-3-yl)oxidanesulfonic acid	C36H28O19S	M+H	797.1018	-2.3
	HMDB0141889	{4-[(5,7-dihydroxy-2-[3,4,5-trihydroxy-6-oxo-8-(3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-2-yl)-6H-benzo[7]annulen-2-yl]-3,4-dihydro-2H-1-benzopyran-3-yl}oxy)carbonyl]-2,6-dihydroxyphenyl}oxidanesulfonic acid	C36H28O19S	M+H	797.1018	-2.3
	HMDB0141890	(2-{2-[5,7-dihydroxy-3-(3,4,5-trihydroxybenzoyloxy)-3,4-dihydro-2H-1-benzopyran-2-yl]-3,4,5-trihydroxy-6-oxo-6H-benzo[7]annulen-8-yl}-5,7-dihydroxy-3,4-dihydro-2H-1-benzopyran-3-yl)oxidanesulfonic acid	C36H28O19S	M+H	797.1018	-2.3
797.3950	HMDB0001038	Angiotensin IV	C40H54N8O8	M+Na	797.3957	-0.9
797.5282	HMDB0010605	PG(18/18:2(9Z,12Z))	C42H79O10P	M+Na	797.5303	-2.6
	HMDB0010647	PG(18:2(9Z,12Z)/18)	C42H79O10P	M+Na	797.5303	-2.6
	HMDB0010633	PG(18:1(9Z)/18:1(11Z))	C42H79O10P	M+Na	797.5303	-2.6
	HMDB0010619	PG(18:1(11Z)/18:1(9Z))	C42H79O10P	M+Na	797.5303	-2.6
	HMDB0010618	PG(18:1(11Z)/18:1(11Z))	C42H79O10P	M+Na	797.5303	-2.6

	HMDB0010634	PG(18:1(9Z)/18:1(9Z))	C42H79O10P	M+Na	797.5303	-2.6
798.5407	HMDB0009644	PE(22:5(4Z,7Z,Z,13Z,16Z)/P-18:1(11Z))	C45H78NO7P	M+Na	798.5408	-0.1
	HMDB0011458	PE(P-18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C45H78NO7P	M+Na	798.5408	-0.1
	HMDB0009645	PE(22:5(4Z,7Z,Z,13Z,16Z)/P-18:1(9Z))	C45H78NO7P	M+Na	798.5408	-0.1
	HMDB0009678	PE(22:5(7Z,Z,13Z,16Z,19Z)/P-18:1(9Z))	C45H78NO7P	M+Na	798.5408	-0.1
	HMDB0009677	PE(22:5(7Z,Z,13Z,16Z,19Z)/P-18:1(11Z))	C45H78NO7P	M+Na	798.5408	-0.1
	HMDB0009709	PE(22:6(4Z,7Z,Z,13Z,16Z,19Z)/P-18)	C45H78NO7P	M+Na	798.5408	-0.1
	HMDB0011394	PE(P-18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C45H78NO7P	M+Na	798.5408	-0.1
	HMDB0011426	PE(P-18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C45H78NO7P	M+Na	798.5408	-0.1
	HMDB0011425	PE(P-18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C45H78NO7P	M+Na	798.5408	-0.1
	HMDB0011459	PE(P-18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C45H78NO7P	M+Na	798.5408	-0.1
799.1531	HMDB0134883	{2-[(2-{4-[3-(2,4-dihydroxyphenyl)-3-oxoprop-1-en-1-yl]phenoxy}-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl)oxy]-4-hydroxy-4-({[(2E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxy}methyl)oxolan-3-yl]oxidanesulfonic acid	C35H36O18S	M+Na	799.1515	2.1
	HMDB0134882	{4-[(1E)-3-({5-[(2-{4-[3-(2,4-dihydroxyphenyl)-3-oxoprop-1-en-1-yl]phenoxy}-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl)oxy]-3,4-dihydroxyoxolan-3-yl}methoxy)-3-oxoprop-1-en-1-yl]phenyl]oxidanesulfonic acid	C35H36O18S	M+Na	799.1515	2.1
	HMDB0134930	[2-({4,5-dihydroxy-2-[4-(7-hydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)phenoxy]-6-(hydroxymethyl)oxan-3-yl}oxy)-4-hydroxy-4-({[(2E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxy}methyl)oxolan-3-yl]oxidanesulfonic acid	C35H36O18S	M+Na	799.1515	2.1
	HMDB0134929	{4-[(1E)-3-({5-({4,5-dihydroxy-2-[4-(7-hydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)phenoxy]-6-(hydroxymethyl)oxan-3-yl}oxy)-3,4-dihydroxyoxolan-3-yl]methoxy}-3-oxoprop-1-en-1-yl]phenyl]oxidanesulfonic acid	C35H36O18S	M+Na	799.1515	2.1
799.3913	HMDB0177586	[8-({6-[(acetyloxy)methyl]-3,4,5-trihydroxyoxan-2-yl}oxy)-16-hydroxy-14-[5-(2-hydroxypropan-2-yl)-2-methyloxolan-2-yl]-2,6,6,,11-pentamethyltetracyclo[8.7,,heptadecan-5-yl]oxidanesulfonic acid	C38H64O14S	M+Na	799.3909	0.5
	HMDB0177587	[8-({6-[(acetyloxy)methyl]-3,4,5-trihydroxyoxan-2-yl}oxy)-5-hydroxy-14-[5-(2-hydroxypropan-2-yl)-2-methyloxolan-2-yl]-2,6,6,,11-pentamethyltetracyclo[8.7,,heptadecan-16-yl]oxidanesulfonic acid	C38H64O14S	M+Na	799.3909	0.5
799.4856	HMDB0040655	Mabioside D	C42H70O14	M+H	799.4838	2.2
	HMDB0173530	6-(16-hydroxy-2,6,6,,11-pentamethyl-5-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}tetracyclo[8.7,,heptadecan-14-yl]-2-methyl-6-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}hept-1-en-3-one	C42H70O14	M+H	799.4838	2.2
	HMDB0173531	6-(5-{[4,5-dihydroxy-6-(hydroxymethyl)-3-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}oxan-2-yl]oxy}-16-hydroxy-2,6,6,,11-pentamethyltetracyclo[8.7,,heptadecan-14-yl]-6-hydroxy-2-methylhept-1-en-3-one	C42H70O14	M+H	799.4838	2.2
	HMDB0010604	PG(18/18:1(9Z))	C42H81O10P	M+Na	799.5460	-1.8

799.5445	HMDB0010632	PG(18:1(9Z)/18)	C42H81O10P	M+Na	799.5460	-1.8
	HMDB0010617	PG(18:1(11Z)/18)	C42H81O10P	M+Na	799.5460	-1.8
	HMDB0010603	PG(18/18:1(11Z))	C42H81O10P	M+Na	799.5460	-1.8
800.6165	HMDB0113878	PE-NMe2(14:1(9Z)/24:1(15Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0114244	PE-NMe2(:2(11Z,14Z)/18)	C45H86NO8P	M+H	800.6164	0.1
	HMDB0113996	PE-NMe2(18/:2(11Z,14Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0114632	PE-NMe2(24:1(15Z)/14:1(9Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0114469	PE-NMe2(22:2(13Z,16Z)/16)	C45H86NO8P	M+H	800.6164	0.1
	HMDB0114441	PE-NMe2(22:1(13Z)/16:1(9Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0114216	PE-NMe2(:1(11Z)/18:1(11Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0114217	PE-NMe2(:1(11Z)/18:1(9Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0114189	PE-NMe2(/18:2(9Z,12Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0114077	PE-NMe2(18:2(9Z,12Z)/)	C45H86NO8P	M+H	800.6164	0.1
	HMDB0114049	PE-NMe2(18:1(9Z)/:1(11Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0114022	PE-NMe2(18:1(11Z)/:1(11Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0113955	PE-NMe2(16/22:2(13Z,16Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0113977	PE-NMe2(16:1(9Z)/22:1(13Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0009552	PE(22:2(13Z,16Z)/18)	C45H86NO8P	M+H	800.6164	0.1
	HMDB0009521	PE(22:1(13Z)/18:1(9Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0009520	PE(22:1(13Z)/18:1(11Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0009295	PE(:2(11Z,14Z)/)	C45H86NO8P	M+H	800.6164	0.1
	HMDB0009231	PE(/:2(11Z,14Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0009105	PE(18:2(9Z,12Z)/22)	C45H86NO8P	M+H	800.6164	0.1
	HMDB0009073	PE(18:1(9Z)/22:1(13Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0009040	PE(18:1(11Z)/22:1(13Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0009008	PE(18/22:2(13Z,16Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0007954	PC(15/22:2(13Z,16Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0008592	PC(22:2(13Z,16Z)/15)	C45H86NO8P	M+H	800.6164	0.1
	HMDB0008981	PE(16:1(9Z)/24:1(15Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0009489	PE(22/18:2(9Z,12Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0009263	PE(:1(11Z)/:1(11Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0009749	PE(24:1(15Z)/16:1(9Z))	C45H86NO8P	M+H	800.6164	0.1
	HMDB0115552	PA(:2(11Z,14Z)/22:1(13Z))	C45H83O8P	M+NH4	800.6164	0.1

HMDB0115578	PA(:3(8Z,11Z,14Z)/22)	C45H83O8P	M+NH4	800.6164	0.1
HMDB0115590	PA(22/:3(8Z,11Z,14Z))	C45H83O8P	M+NH4	800.6164	0.1
HMDB0115592	PA(22:1(13Z):2(11Z,14Z))	C45H83O8P	M+NH4	800.6164	0.1
HMDB0115437	PA(24/18:3(6Z,9Z,12Z))	C45H83O8P	M+NH4	800.6164	0.1
HMDB0115463	PA(24:1(15Z)/18:2(9Z,12Z))	C45H83O8P	M+NH4	800.6164	0.1
HMDB0115438	PA(24/18:3(9Z,12Z,15Z))	C45H83O8P	M+NH4	800.6164	0.1
HMDB0115309	PA(22:2(13Z,16Z):1(11Z))	C45H83O8P	M+NH4	800.6164	0.1
HMDB0115255	PA(22/:3(5Z,8Z,11Z))	C45H83O8P	M+NH4	800.6164	0.1
HMDB0115136	PA(:3(5Z,8Z,11Z)/22)	C45H83O8P	M+NH4	800.6164	0.1
HMDB0115111	PA(:1(11Z)/22:2(13Z,16Z))	C45H83O8P	M+NH4	800.6164	0.1
HMDB0115025	PA(18:3(9Z,12Z,15Z)/24)	C45H83O8P	M+NH4	800.6164	0.1
HMDB0114998	PA(18:3(6Z,9Z,12Z)/24)	C45H83O8P	M+NH4	800.6164	0.1
HMDB0114972	PA(18:2(9Z,12Z)/24:1(15Z))	C45H83O8P	M+NH4	800.6164	0.1
HMDB0113345	PE-NMe(:2(11Z,14Z)/18:2(9Z,12Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113178	PE-NMe(18:2(9Z,12Z):2(11Z,14Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0114497	PE-NMe2(22:4(7Z,Z,13Z,16Z)/15)	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113290	PE-NMe(/18:4(6Z,9Z,12Z,15Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113234	PE-NMe(18:3(9Z,12Z,15Z):1(11Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113205	PE-NMe(18:3(6Z,9Z,12Z):1(11Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113151	PE-NMe(18:1(9Z):3(8Z,11Z,14Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113150	PE-NMe(18:1(9Z):3(5Z,8Z,11Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113055	PE-NMe(16/22:4(7Z,Z,13Z,16Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113124	PE-NMe(18:1(11Z):3(8Z,11Z,14Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113098	PE-NMe(18/:4(5Z,8Z,11Z,14Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113099	PE-NMe(18/:4(8Z,11Z,14Z,17Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113318	PE-NMe(:1(11Z)/18:3(9Z,12Z,15Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113934	PE-NMe2(15/22:4(7Z,Z,13Z,16Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113427	PE-NMe(:4(5Z,8Z,11Z,14Z)/18)	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113595	PE-NMe(22:4(7Z,Z,13Z,16Z)/16)	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113455	PE-NMe(:4(8Z,11Z,14Z,17Z)/18)	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113262	PE-NMe(18:4(6Z,9Z,12Z,15Z)/)	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113401	PE-NMe(:3(8Z,11Z,14Z)/18:1(9Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113372	PE-NMe(:3(5Z,8Z,11Z)/18:1(11Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113373	PE-NMe(:3(5Z,8Z,11Z)/18:1(9Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113317	PE-NMe(:1(11Z)/18:3(6Z,9Z,12Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113123	PE-NMe(18:1(11Z):3(5Z,8Z,11Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113400	PE-NMe(:3(8Z,11Z,14Z)/18:1(11Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008138	PC(18:2(9Z,12Z)/18:2(9Z,12Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008170	PC(18:3(6Z,9Z,12Z)/18:1(9Z))	C44H80NO8P	M+Na	804.5514	1.9

804.5529

HMDB0008169	PC(18:3(6Z,9Z,12Z)/18:1(11Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008202	PC(18:3(9Z,12Z,15Z)/18:1(11Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008203	PC(18:3(9Z,12Z,15Z)/18:1(9Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008365	PC(:3(5Z,8Z,11Z)/16:1(9Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008398	PC(:3(8Z,11Z,14Z)/16:1(9Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008429	PC(:4(5Z,8Z,11Z,14Z)/16)	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008462	PC(:4(8Z,11Z,14Z,17Z)/16)	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008106	PC(18:1(9Z)/18:3(6Z,9Z,12Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008107	PC(18:1(9Z)/18:3(9Z,12Z,15Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0007889	PC(14/22:4(7Z,Z,13Z,16Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0007982	PC(16/:4(5Z,8Z,11Z,14Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0007983	PC(16/:4(8Z,11Z,14Z,17Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008013	PC(16:1(9Z)/:3(5Z,8Z,11Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008014	PC(16:1(9Z)/:3(8Z,11Z,14Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008042	PC(18/18:4(6Z,9Z,12Z,15Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008073	PC(18:1(11Z)/18:3(6Z,9Z,12Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008074	PC(18:1(11Z)/18:3(9Z,12Z,15Z))	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008623	PC(22:4(7Z,Z,13Z,16Z)/14)	C44H80NO8P	M+Na	804.5514	1.9
HMDB0008234	PC(18:4(6Z,9Z,12Z,15Z)/18)	C44H80NO8P	M+Na	804.5514	1.9
HMDB0113161	PE-NMe(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113188	PE-NMe(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113189	PE-NMe(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113679	PE-NMe(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113680	PE-NMe(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113356	PE-NMe(:2(11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113654	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113627	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113215	PE-NMe(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113244	PE-NMe(18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113383	PE-NMe(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113384	PE-NMe(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113412	PE-NMe(:3(8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C46H78NO8P	M+H	804.5538	-1.1

HMDB0113411	PE-NMe(:3(8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113437	PE-NMe(:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113438	PE-NMe(:4(5Z,8Z,11Z,14Z)/:3(8Z,11Z,14Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113466	PE-NMe(:4(8Z,11Z,14Z,17Z)/:3(8Z,11Z,14Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113465	PE-NMe(:4(8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113601	PE-NMe(22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113602	PE-NMe(22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008726	PC(22:6(4Z,7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008436	PC(:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008023	PC(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008435	PC(:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008405	PC(:3(8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008468	PC(:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008469	PC(:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008500	PC(:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008149	PC(18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008245	PC(18:4(6Z,9Z,12Z,15Z)/:3(8Z,11Z,14Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008213	PC(18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008214	PC(18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113134	PE-NMe(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008244	PC(18:4(6Z,9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008181	PC(18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008372	PC(:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0008180	PC(18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113493	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/:2(11Z,14Z))	C46H78NO8P	M+H	804.5538	-1.1
HMDB0113077	PE-NMe(16:1(9Z)/22:2(13Z,16Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0113096	PE-NMe(18/:3(5Z,8Z,11Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0113097	PE-NMe(18/:3(8Z,11Z,14Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0113177	PE-NMe(18:2(9Z,12Z)/:1(11Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0113204	PE-NMe(18:3(6Z,9Z,12Z)/)	C44H82NO8P	M+Na	806.5670	2.7
HMDB0113233	PE-NMe(18:3(9Z,12Z,15Z)/)	C44H82NO8P	M+Na	806.5670	2.7
HMDB0113344	PE-NMe(:2(11Z,14Z)/18:1(9Z))	C44H82NO8P	M+Na	806.5670	2.7

HMDB0113343	PE-NMe(:2(11Z,14Z)/18:1(11Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0113149	PE-NMe(18:1(9Z):2(11Z,14Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0113122	PE-NMe(18:1(11Z):2(11Z,14Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0113567	PE-NMe(22:2(13Z,16Z)/16:1(9Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0113399	PE-NMe(:3(8Z,11Z,14Z)/18)	C44H82NO8P	M+Na	806.5670	2.7
HMDB0113371	PE-NMe(:3(5Z,8Z,11Z)/18)	C44H82NO8P	M+Na	806.5670	2.7
HMDB0113316	PE-NMe(:1(11Z)/18:2(9Z,12Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0113289	PE-NMe(/18:3(9Z,12Z,15Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0113288	PE-NMe(/18:3(6Z,9Z,12Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0008041	PC(18/18:3(9Z,12Z,15Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0007921	PC(14:1(9Z)/22:2(13Z,16Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0008591	PC(22:2(13Z,16Z)/14:1(9Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0007980	PC(16/:3(5Z,8Z,11Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0007981	PC(16/:3(8Z,11Z,14Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0008012	PC(16:1(9Z):2(11Z,14Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0008040	PC(18/18:3(6Z,9Z,12Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0008072	PC(18:1(11Z)/18:2(9Z,12Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0008105	PC(18:1(9Z)/18:2(9Z,12Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0008136	PC(18:2(9Z,12Z)/18:1(11Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0008137	PC(18:2(9Z,12Z)/18:1(9Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0008168	PC(18:3(6Z,9Z,12Z)/18)	C44H82NO8P	M+Na	806.5670	2.7
HMDB0008201	PC(18:3(9Z,12Z,15Z)/18)	C44H82NO8P	M+Na	806.5670	2.7
HMDB0008332	PC(:2(11Z,14Z)/16:1(9Z))	C44H82NO8P	M+Na	806.5670	2.7
HMDB0008364	PC(:3(5Z,8Z,11Z)/16)	C44H82NO8P	M+Na	806.5670	2.7
HMDB0008397	PC(:3(8Z,11Z,14Z)/16)	C44H82NO8P	M+Na	806.5670	2.7
HMDB0008725	PC(22:6(4Z,7Z,Z,13Z,16Z,19Z)/16)	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008693	PC(22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008660	PC(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008498	PC(:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008499	PC(:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008467	PC(:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008434	PC(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C46H80NO8P	M+H	806.5694	-0.3

806.5692

HMDB0008404	PC(:3(8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008403	PC(:3(8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008179	PC(18:3(6Z,9Z,12Z)/:3(8Z,11Z,14Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008148	PC(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008116	PC(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008211	PC(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008083	PC(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008147	PC(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008024	PC(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008022	PC(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0007991	PC(16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008178	PC(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008243	PC(18:4(6Z,9Z,12Z,15Z)/:2(11Z,14Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008212	PC(18:3(9Z,12Z,15Z)/:3(8Z,11Z,14Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008371	PC(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008339	PC(:2(11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0008370	PC(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0113409	PE-NMe(:3(8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0113132	PE-NMe(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0113410	PE-NMe(:3(8Z,11Z,14Z)/:3(8Z,11Z,14Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0113187	PE-NMe(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0113160	PE-NMe(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0113107	PE-NMe(18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0113327	PE-NMe(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0113133	PE-NMe(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0113159	PE-NMe(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0113381	PE-NMe(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0113272	PE-NMe(18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0113492	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/:1(11Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0113464	PE-NMe(:4(8Z,11Z,14Z,17Z)/:2(11Z,14Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0113436	PE-NMe(:4(5Z,8Z,11Z,14Z)/:2(11Z,14Z))	C46H80NO8P	M+H	806.5694	-0.3
HMDB0113355	PE-NMe(:2(11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C46H80NO8P	M+H	806.5694	-0.3

	HMDB0113574	PE-NMe(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C46H80NO8P	M+H	806.5694	-0.3
	HMDB0113600	PE-NMe(22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C46H80NO8P	M+H	806.5694	-0.3
	HMDB0113625	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z))	C46H80NO8P	M+H	806.5694	-0.3
	HMDB0113626	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z))	C46H80NO8P	M+H	806.5694	-0.3
	HMDB0113653	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C46H80NO8P	M+H	806.5694	-0.3
	HMDB0113652	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C46H80NO8P	M+H	806.5694	-0.3
	HMDB0113678	PE-NMe(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18)	C46H80NO8P	M+H	806.5694	-0.3
	HMDB0113354	PE-NMe(:2(11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C46H80NO8P	M+H	806.5694	-0.3
	HMDB0113382	PE-NMe(:3(5Z,8Z,11Z)/:3(8Z,11Z,14Z))	C46H80NO8P	M+H	806.5694	-0.3
806.7230	HMDB0042512	TG(14/18:2(9Z,12Z)/15)	C50H92O6	M+NH4	806.7232	-0.3
	HMDB0047749	TG(14:1(9Z)/15/18:1(11Z))	C50H92O6	M+NH4	806.7232	-0.3
	HMDB0042106	TG(14/15/18:2(9Z,12Z))	C50H92O6	M+NH4	806.7232	-0.3
	HMDB0043227	TG(15/18:1(11Z)/14:1(9Z))	C50H92O6	M+NH4	806.7232	-0.3
	HMDB0043171	TG(15/14:1(9Z)/18:1(11Z))	C50H92O6	M+NH4	806.7232	-0.3
	HMDB0047750	TG(14:1(9Z)/15/18:1(9Z))	C50H92O6	M+NH4	806.7232	-0.3
	HMDB0043256	TG(15/18:1(9Z)/14:1(9Z))	C50H92O6	M+NH4	806.7232	-0.3
	HMDB0043172	TG(15/14:1(9Z)/18:1(9Z))	C50H92O6	M+NH4	806.7232	-0.3
	HMDB0042974	TG(15/14/18:2(9Z,12Z))	C50H92O6	M+NH4	806.7232	-0.3
	HMDB0043199	TG(15/16:1(9Z)/16:1(9Z))	C50H92O6	M+NH4	806.7232	-0.3
	HMDB0048435	TG(16:1(9Z)/15/16:1(9Z))	C50H92O6	M+NH4	806.7232	-0.3
	HMDB0113148	PE-NMe(18:1(9Z)/:1(11Z))	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0113121	PE-NMe(18:1(11Z)/:1(11Z))	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0113566	PE-NMe(22:2(13Z,16Z)/16)	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0113076	PE-NMe(16:1(9Z)/22:1(13Z))	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0113729	PE-NMe(24:1(15Z)/14:1(9Z))	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0113054	PE-NMe(16/22:2(13Z,16Z))	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0113176	PE-NMe(18:2(9Z,12Z)/)	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0113287	PE-NMe(/18:2(9Z,12Z))	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0113314	PE-NMe(:1(11Z)/18:1(11Z))	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0113315	PE-NMe(:1(11Z)/18:1(9Z))	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0113539	PE-NMe(22:1(13Z)/16:1(9Z))	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0112977	PE-NMe(14:1(9Z)/24:1(15Z))	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0113342	PE-NMe(:2(11Z,14Z)/18)	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0113095	PE-NMe(18/:2(11Z,14Z))	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0114468	PE-NMe2(22:2(13Z,16Z)/15)	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0113933	PE-NMe2(15/22:2(13Z,16Z))	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0062690	1,2-dioleoyl-sn-glycero-3-phosphocholine	C44H84NO8P	M+Na	808.5827	2.1
	HMDB0000593	1,2-dioleoyl-sn-glycero-3-phosphocholine	C44H84NO8P	M+Na	808.5827	2.1

808.5844

HMDB0008590	PC(22:2(13Z,16Z)/14)	C44H84NO8P	M+Na	808.5827	2.1
HMDB0008559	PC(22:1(13Z)/14:1(9Z))	C44H84NO8P	M+Na	808.5827	2.1
HMDB0008331	PC(:2(11Z,14Z)/16)	C44H84NO8P	M+Na	808.5827	2.1
HMDB0008299	PC(:1(11Z)/16:1(9Z))	C44H84NO8P	M+Na	808.5827	2.1
HMDB0008135	PC(18:2(9Z,12Z)/18)	C44H84NO8P	M+Na	808.5827	2.1
HMDB0008103	PC(18:1(9Z)/18:1(11Z))	C44H84NO8P	M+Na	808.5827	2.1
HMDB0008070	PC(18:1(11Z)/18:1(11Z))	C44H84NO8P	M+Na	808.5827	2.1
HMDB0008071	PC(18:1(11Z)/18:1(9Z))	C44H84NO8P	M+Na	808.5827	2.1
HMDB0008039	PC(18/18:2(9Z,12Z))	C44H84NO8P	M+Na	808.5827	2.1
HMDB0008011	PC(16:1(9Z)/:1(11Z))	C44H84NO8P	M+Na	808.5827	2.1
HMDB0007979	PC(16/:2(11Z,14Z))	C44H84NO8P	M+Na	808.5827	2.1
HMDB0007920	PC(14:1(9Z)/22:1(13Z))	C44H84NO8P	M+Na	808.5827	2.1
HMDB0007888	PC(14/22:2(13Z,16Z))	C44H84NO8P	M+Na	808.5827	2.1
HMDB0008692	PC(22:5(7Z,Z,13Z,16Z,19Z)/16)	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008659	PC(22:5(4Z,7Z,Z,13Z,16Z)/16)	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008627	PC(22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008497	PC(:5(5Z,8Z,11Z,14Z,17Z)/18)	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008466	PC(:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008465	PC(:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008242	PC(18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008210	PC(18:3(9Z,12Z,15Z)/:2(11Z,14Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008177	PC(18:3(6Z,9Z,12Z)/:2(11Z,14Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008146	PC(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008139	PC(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008114	PC(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008115	PC(18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008081	PC(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008082	PC(18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008050	PC(18/:5(5Z,8Z,11Z,14Z,17Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008021	PC(16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0007989	PC(16/22:5(4Z,7Z,Z,13Z,16Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0007990	PC(16/22:5(7Z,Z,13Z,16Z,19Z))	C46H82NO8P	M+H	808.5851	-0.8

HMDB0008306	PC(:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008402	PC(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008432	PC(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008338	PC(:2(11Z,14Z)/18:3(9Z,12Z,15Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008433	PC(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008337	PC(:2(11Z,14Z)/18:3(6Z,9Z,12Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0008369	PC(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113158	PE-NMe(18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113214	PE-NMe(18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113271	PE-NMe(18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113298	PE-NMe(/:5(5Z,8Z,11Z,14Z,17Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113326	PE-NMe(:1(11Z)/:4(8Z,11Z,14Z,17Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113325	PE-NMe(:1(11Z)/:4(5Z,8Z,11Z,14Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113131	PE-NMe(18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113105	PE-NMe(18/22:5(4Z,7Z,Z,13Z,16Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113106	PE-NMe(18/22:5(7Z,Z,13Z,16Z,19Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113435	PE-NMe(:4(5Z,8Z,11Z,14Z)/:1(11Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113651	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/18)	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113380	PE-NMe(:3(5Z,8Z,11Z)/:2(11Z,14Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113408	PE-NMe(:3(8Z,11Z,14Z)/:2(11Z,14Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113352	PE-NMe(:2(11Z,14Z)/:3(5Z,8Z,11Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113624	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/18)	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113599	PE-NMe(22:4(7Z,Z,13Z,16Z)/18:1(9Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113463	PE-NMe(:4(8Z,11Z,14Z,17Z)/:1(11Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113491	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/)	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113546	PE-NMe(22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113572	PE-NMe(22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113573	PE-NMe(22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113598	PE-NMe(22:4(7Z,Z,13Z,16Z)/18:1(11Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113353	PE-NMe(:2(11Z,14Z)/:3(8Z,11Z,14Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0113243	PE-NMe(18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C46H82NO8P	M+H	808.5851	-0.8
HMDB0043165	TG(15/14:1(9Z)/18)	C50H94O6	M+NH4	808.7389	-0.1
HMDB0042969	TG(15/14/18:1(9Z))	C50H94O6	M+NH4	808.7389	-0.1
HMDB0043863	TG(16/15/16:1(9Z))	C50H94O6	M+NH4	808.7389	-0.1

808.7388	HMDB0043193	TG(15/16:1(9Z)/16)	C50H94O6	M+NH4	808.7389	-0.1
	HMDB0043025	TG(15/16/16:1(9Z))	C50H94O6	M+NH4	808.7389	-0.1
	HMDB0042362	TG(14/18:1(9Z)/15)	C50H94O6	M+NH4	808.7389	-0.1
	HMDB0042968	TG(15/14/18:1(11Z))	C50H94O6	M+NH4	808.7389	-0.1
	HMDB0043053	TG(15/18/14:1(9Z))	C50H94O6	M+NH4	808.7389	-0.1
	HMDB0044699	TG(18/15/14:1(9Z))	C50H94O6	M+NH4	808.7389	-0.1
	HMDB0042100	TG(14/15/18:1(11Z))	C50H94O6	M+NH4	808.7389	-0.1
	HMDB0042101	TG(14/15/18:1(9Z))	C50H94O6	M+NH4	808.7389	-0.1
	HMDB0042332	TG(14/18:1(11Z)/15)	C50H94O6	M+NH4	808.7389	-0.1
	HMDB0113313	PE-NMe(:1(11Z)/18)	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0113512	PE-NMe(22/16:1(9Z))	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0113538	PE-NMe(22:1(13Z)/16)	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0113702	PE-NMe(24/14:1(9Z))	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0113728	PE-NMe(24:1(15Z)/14)	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0113932	PE-NMe2(15/22:1(13Z))	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0114439	PE-NMe2(22:1(13Z)/15)	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0113285	PE-NMe(/18:1(11Z))	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0113286	PE-NMe(/18:1(9Z))	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0113147	PE-NMe(18:1(9Z)/)	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0113016	PE-NMe(14:1(9Z)/24)	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0112998	PE-NMe(14/24:1(15Z))	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0113053	PE-NMe(16/22:1(13Z))	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0113075	PE-NMe(16:1(9Z)/22)	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0113094	PE-NMe(18/:1(11Z))	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0113120	PE-NMe(18:1(11Z)/)	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0008558	PC(22:1(13Z)/14)	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0008915	PE(15/24:1(15Z))	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0009747	PE(24:1(15Z)/15)	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0007887	PC(14/22:1(13Z))	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0008526	PC(22/14:1(9Z))	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0008298	PC(:1(11Z)/16)	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0008102	PC(18:1(9Z)/18)	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0008069	PC(18:1(11Z)/18)	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0008037	PC(18/18:1(11Z))	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0008038	PC(18/18:1(9Z))	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0008010	PC(16:1(9Z)/)	C44H86NO8P	M+Na	810.5983	2.4
	HMDB0007978	PC(16/:1(11Z))	C44H86NO8P	M+Na	810.5983	2.4

810.6003

HMDB0008266	PC(/16:1(9Z))	C44H86NO8P	M+Na	810.5983	2.4
HMDB0007919	PC(14:1(9Z)/22)	C44H86NO8P	M+Na	810.5983	2.4
HMDB0008626	PC(22:4(7Z,Z,13Z,16Z)/16)	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008464	PC(:4(8Z,11Z,14Z,17Z)/18)	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008431	PC(:4(5Z,8Z,11Z,14Z)/18)	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008401	PC(:3(8Z,11Z,14Z)/18:1(9Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008400	PC(:3(8Z,11Z,14Z)/18:1(11Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008368	PC(:3(5Z,8Z,11Z)/18:1(9Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008367	PC(:3(5Z,8Z,11Z)/18:1(11Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008176	PC(18:3(6Z,9Z,12Z)/:1(11Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008145	PC(18:2(9Z,12Z)/:2(11Z,14Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008113	PC(18:1(9Z)/:3(8Z,11Z,14Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008112	PC(18:1(9Z)/:3(5Z,8Z,11Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008080	PC(18:1(11Z)/:3(8Z,11Z,14Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008079	PC(18:1(11Z)/:3(5Z,8Z,11Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008049	PC(18/:4(8Z,11Z,14Z,17Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008048	PC(18/:4(5Z,8Z,11Z,14Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0007988	PC(16/22:4(7Z,Z,13Z,16Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008209	PC(18:3(9Z,12Z,15Z)/:1(11Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008273	PC(/18:4(6Z,9Z,12Z,15Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008336	PC(:2(11Z,14Z)/18:2(9Z,12Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008305	PC(:1(11Z)/18:3(9Z,12Z,15Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008241	PC(18:4(6Z,9Z,12Z,15Z)/)	C46H84NO8P	M+H	810.6007	-0.5
HMDB0008304	PC(:1(11Z)/18:3(6Z,9Z,12Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113104	PE-NMe(18/22:4(7Z,Z,13Z,16Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113462	PE-NMe(:4(8Z,11Z,14Z,17Z)/)	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113434	PE-NMe(:4(5Z,8Z,11Z,14Z)/)	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113407	PE-NMe(:3(8Z,11Z,14Z)/:1(11Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113544	PE-NMe(22:1(13Z)/18:3(6Z,9Z,12Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113379	PE-NMe(:3(5Z,8Z,11Z)/:1(11Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113545	PE-NMe(22:1(13Z)/18:3(9Z,12Z,15Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113324	PE-NMe(:1(11Z)/:3(8Z,11Z,14Z))	C46H84NO8P	M+H	810.6007	-0.5

HMDB0113323	PE-NMe(:1(11Z)/:3(5Z,8Z,11Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113297	PE-NMe(/:4(8Z,11Z,14Z,17Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113296	PE-NMe(/:4(5Z,8Z,11Z,14Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113270	PE-NMe(18:4(6Z,9Z,12Z,15Z)/22)	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113242	PE-NMe(18:3(9Z,12Z,15Z)/22:1(13Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113571	PE-NMe(22:2(13Z,16Z)/18:2(9Z,12Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113597	PE-NMe(22:4(7Z,Z,13Z,16Z)/18)	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113213	PE-NMe(18:3(6Z,9Z,12Z)/22:1(13Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113186	PE-NMe(18:2(9Z,12Z)/22:2(13Z,16Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113351	PE-NMe(:2(11Z,14Z)/:2(11Z,14Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113519	PE-NMe(22/18:4(6Z,9Z,12Z,15Z))	C46H84NO8P	M+H	810.6007	-0.5
HMDB0113931	PE-NMe2(15/22)	C44H88NO8P	M+Na	812.6140	2.2
HMDB0114412	PE-NMe2(22/15)	C44H88NO8P	M+Na	812.6140	2.2
HMDB0113701	PE-NMe(24/14)	C44H88NO8P	M+Na	812.6140	2.2
HMDB0113284	PE-NMe(/18)	C44H88NO8P	M+Na	812.6140	2.2
HMDB0113093	PE-NMe(18/)	C44H88NO8P	M+Na	812.6140	2.2
HMDB0113052	PE-NMe(16/22)	C44H88NO8P	M+Na	812.6140	2.2
HMDB0112997	PE-NMe(14/24)	C44H88NO8P	M+Na	812.6140	2.2
HMDB0113511	PE-NMe(22/16)	C44H88NO8P	M+Na	812.6140	2.2
HMDB0008265	PC(/16)	C44H88NO8P	M+Na	812.6140	2.2
HMDB0007977	PC(16/)	C44H88NO8P	M+Na	812.6140	2.2
HMDB0008036	PC(18/18)	C44H88NO8P	M+Na	812.6140	2.2
HMDB0008525	PC(22/14)	C44H88NO8P	M+Na	812.6140	2.2
HMDB0008914	PE(15/24)	C44H88NO8P	M+Na	812.6140	2.2
HMDB0009714	PE(24/15)	C44H88NO8P	M+Na	812.6140	2.2
HMDB0007886	PC(14/22)	C44H88NO8P	M+Na	812.6140	2.2
HMDB0008594	PC(22:2(13Z,16Z)/16:1(9Z))	C46H86NO8P	M+H	812.6164	-0.7
HMDB0008366	PC(:3(5Z,8Z,11Z)/18)	C46H86NO8P	M+H	812.6164	-0.7
HMDB0008144	PC(18:2(9Z,12Z)/:1(11Z))	C46H86NO8P	M+H	812.6164	-0.7
HMDB0008047	PC(18/:3(8Z,11Z,14Z))	C46H86NO8P	M+H	812.6164	-0.7
HMDB0008078	PC(18:1(11Z)/:2(11Z,14Z))	C46H86NO8P	M+H	812.6164	-0.7
HMDB0008111	PC(18:1(9Z)/:2(11Z,14Z))	C46H86NO8P	M+H	812.6164	-0.7

812.6158	HMDB0008020	PC(16:1(9Z)/22:2(13Z,16Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0008175	PC(18:3(6Z,9Z,12Z)/)	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0008208	PC(18:3(9Z,12Z,15Z)/)	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0008271	PC(/18:3(6Z,9Z,12Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0008272	PC(/18:3(9Z,12Z,15Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0008303	PC(:1(11Z)/18:2(9Z,12Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0008334	PC(:2(11Z,14Z)/18:1(11Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0008399	PC(:3(8Z,11Z,14Z)/18)	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0008335	PC(:2(11Z,14Z)/18:1(9Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0008046	PC(18/:3(5Z,8Z,11Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113294	PE-NMe(/:3(5Z,8Z,11Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113295	PE-NMe(/:3(8Z,11Z,14Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113378	PE-NMe(:3(5Z,8Z,11Z)/)	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113241	PE-NMe(18:3(9Z,12Z,15Z)/22)	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113322	PE-NMe(:1(11Z)/:2(11Z,14Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113212	PE-NMe(18:3(6Z,9Z,12Z)/22)	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113185	PE-NMe(18:2(9Z,12Z)/22:1(13Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113157	PE-NMe(18:1(9Z)/22:2(13Z,16Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113130	PE-NMe(18:1(11Z)/22:2(13Z,16Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113406	PE-NMe(:3(8Z,11Z,14Z)/)	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113518	PE-NMe(22/18:3(9Z,12Z,15Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113517	PE-NMe(22/18:3(6Z,9Z,12Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113570	PE-NMe(22:2(13Z,16Z)/18:1(9Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113350	PE-NMe(:2(11Z,14Z)/:1(11Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113569	PE-NMe(22:2(13Z,16Z)/18:1(11Z))	C46H86NO8P	M+H	812.6164	-0.7
	HMDB0113543	PE-NMe(22:1(13Z)/18:2(9Z,12Z))	C46H86NO8P	M+H	812.6164	-0.7
813.6834	HMDB0012107	SM(d18:1/24:1(15Z))	C47H93N2O6P	M+H	813.6844	-1.2
	HMDB0240635	Sm(d18:2/24)	C47H93N2O6P	M+H	813.6844	-1.2
	HMDB0008789	PC(24:1(15Z)/14:1(9Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0007927	PC(14:1(9Z)/24:1(15Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0007987	PC(16/22:2(13Z,16Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0008019	PC(16:1(9Z)/22:1(13Z))	C46H88NO8P	M+H	814.6320	-0.5

814.6316	HMDB0008045	PC(18:2(11Z,14Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0008077	PC(18:1(11Z):1(11Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0008110	PC(18:1(9Z):1(11Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0008143	PC(18:2(9Z,12Z)/)	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0008270	PC(/18:2(9Z,12Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0008301	PC(:1(11Z)/18:1(11Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0008302	PC(:1(11Z)/18:1(9Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0008333	PC(:2(11Z,14Z)/18)	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0008562	PC(22:1(13Z)/16:1(9Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0008593	PC(22:2(13Z,16Z)/16)	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0113568	PE-NMe(22:2(13Z,16Z)/18)	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0113541	PE-NMe(22:1(13Z)/18:1(11Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0113542	PE-NMe(22:1(13Z)/18:1(9Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0113516	PE-NMe(22/18:2(9Z,12Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0113321	PE-NMe(:1(11Z):1(11Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0113184	PE-NMe(18:2(9Z,12Z)/22)	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0113732	PE-NMe(24:1(15Z)/16:1(9Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0113293	PE-NMe(/:2(11Z,14Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0113349	PE-NMe(:2(11Z,14Z)/)	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0113156	PE-NMe(18:1(9Z)/22:1(13Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0113129	PE-NMe(18:1(11Z)/22:1(13Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0113103	PE-NMe(18/22:2(13Z,16Z))	C46H88NO8P	M+H	814.6320	-0.5
	HMDB0113083	PE-NMe(16:1(9Z)/24:1(15Z))	C46H88NO8P	M+H	814.6320	-0.5
815.6993	HMDB0012095	SM(d18/24:1(15Z))	C47H95N2O6P	M+H	815.7001	-0.9
	HMDB0011697	N-lignoceroylsphingosine-1-phosphocholine	C47H95N2O6P	M+H	815.7001	-0.9
	HMDB0044046	TG(16/14:1(9Z)/18:3(9Z,12Z,15Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0043851	TG(16/14/18:4(6Z,9Z,12Z,15Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0044478	TG(16/18:3(9Z,12Z,15Z)/14:1(9Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0047779	TG(14:1(9Z)/16/18:3(6Z,9Z,12Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0042759	TG(14/18:3(9Z,12Z,15Z)/16:1(9Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0048421	TG(16:1(9Z)/14/18:3(6Z,9Z,12Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0048574	TG(16:1(9Z)/14:1(9Z)/18:2(9Z,12Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0048428	TG(16:1(9Z)/14/18:3(9Z,12Z,15Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0042086	TG(14/14:4(8Z,11Z,14Z,17Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0042080	TG(14/14:4(5Z,8Z,11Z,14Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0042317	TG(14/16:1(9Z)/18:3(6Z,9Z,12Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0042289	TG(14/14:1(9Z):3n6)	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0042283	TG(14/14:1(9Z):3(5Z,8Z,11Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0044039	TG(16/14:1(9Z)/18:3(6Z,9Z,12Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0043012	TG(15/15/18:4(6Z,9Z,12Z,15Z))	C51H90O6	M+NH4	816.7076	-2.6

816.7054	HMDB0042608	TG(14/:3n6/14:1(9Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0047916	TG(14:1(9Z)/16:1(9Z)/18:2(9Z,12Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0042428	TG(14/:3(5Z,8Z,11Z)/14:1(9Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0048070	TG(14:1(9Z)/18:2(9Z,12Z)/16:1(9Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0044282	TG(16/18:3(6Z,9Z,12Z)/14:1(9Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0042549	TG(14/18:3(6Z,9Z,12Z)/16:1(9Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0042783	TG(14/18:4(6Z,9Z,12Z,15Z)/16)	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0048115	TG(14:1(9Z)/:2n6/14:1(9Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0047729	TG(14:1(9Z)/14/:3(5Z,8Z,11Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0047895	TG(14:1(9Z)/14:1(9Z)/:2n6)	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0047735	TG(14:1(9Z)/14/:3n6)	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0047786	TG(14:1(9Z)/16/18:3(9Z,12Z,15Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0042324	TG(14/16:1(9Z)/18:3(9Z,12Z,15Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0042145	TG(14/16/18:4(6Z,9Z,12Z,15Z))	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0042631	TG(14/:4(5Z,8Z,11Z,14Z)/14)	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0042811	TG(14/:4(8Z,11Z,14Z,17Z)/14)	C51H90O6	M+NH4	816.7076	-2.6
	HMDB0043656	TG(15/18:4(6Z,9Z,12Z,15Z)/15)	C51H90O6	M+NH4	816.7076	-2.6
818.6056	HMDB0011316	PC(P-18:1(9Z)/:2(11Z,14Z))	C46H86NO7P	M+Na	818.6034	2.7
	HMDB0011283	PC(P-18:1(11Z)/:2(11Z,14Z))	C46H86NO7P	M+Na	818.6034	2.7
	HMDB0011252	PC(P-18/:3(8Z,11Z,14Z))	C46H86NO7P	M+Na	818.6034	2.7
	HMDB0008423	PC(:3(8Z,11Z,14Z)/P-18)	C46H86NO7P	M+Na	818.6034	2.7
	HMDB0008391	PC(:3(5Z,8Z,11Z)/P-18)	C46H86NO7P	M+Na	818.6034	2.7
	HMDB0008359	PC(:2(11Z,14Z)/P-18:1(11Z))	C46H86NO7P	M+Na	818.6034	2.7
	HMDB0013420	PC(O-18/:4(8Z,11Z,14Z,17Z))	C46H86NO7P	M+Na	818.6034	2.7
	HMDB0011251	PC(P-18/:3(5Z,8Z,11Z))	C46H86NO7P	M+Na	818.6034	2.7
	HMDB0008360	PC(:2(11Z,14Z)/P-18:1(9Z))	C46H86NO7P	M+Na	818.6034	2.7
	HMDB0008720	PC(22:5(7Z,Z,13Z,16Z,19Z)/P-18:1(11Z))	C48H84NO7P	M+H	818.6058	-0.3
	HMDB0008752	PC(22:6(4Z,7Z,Z,13Z,16Z,19Z)/P-18)	C48H84NO7P	M+H	818.6058	-0.3
	HMDB0011262	PC(P-18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C48H84NO7P	M+H	818.6058	-0.3
	HMDB0008721	PC(22:5(7Z,Z,13Z,16Z,19Z)/P-18:1(9Z))	C48H84NO7P	M+H	818.6058	-0.3
	HMDB0011293	PC(P-18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C48H84NO7P	M+H	818.6058	-0.3
	HMDB0011294	PC(P-18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C48H84NO7P	M+H	818.6058	-0.3
	HMDB0011326	PC(P-18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C48H84NO7P	M+H	818.6058	-0.3
	HMDB0011327	PC(P-18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C48H84NO7P	M+H	818.6058	-0.3
	HMDB0008687	PC(22:5(4Z,7Z,Z,13Z,16Z)/P-18:1(11Z))	C48H84NO7P	M+H	818.6058	-0.3
	HMDB0008688	PC(22:5(4Z,7Z,Z,13Z,16Z)/P-18:1(9Z))	C48H84NO7P	M+H	818.6058	-0.3
	HMDB0042519	TG(14/18:2(9Z,12Z)/16:1(9Z))	C51H92O6	M+NH4	818.7232	-0.9
	HMDB0042753	TG(14/18:3(9Z,12Z,15Z)/16)	C51H92O6	M+NH4	818.7232	-0.9
	HMDB0047955	TG(14:1(9Z)/18:1(9Z)/16:1(9Z))	C51H92O6	M+NH4	818.7232	-0.9
	HMDB0042578	TG(14/:2n6/14:1(9Z))	C51H92O6	M+NH4	818.7232	-0.9
	HMDB0047889	TG(14:1(9Z)/14:1(9Z)/:1(11Z))	C51H92O6	M+NH4	818.7232	-0.9
	HMDB0044038	TG(16/14:1(9Z)/18:2(9Z,12Z))	C51H92O6	M+NH4	818.7232	-0.9
	HMDB0047910	TG(14:1(9Z)/16:1(9Z)/18:1(11Z))	C51H92O6	M+NH4	818.7232	-0.9
	HMDB0047911	TG(14:1(9Z)/16:1(9Z)/18:1(9Z))	C51H92O6	M+NH4	818.7232	-0.9
	HMDB0044254	TG(16/18:2(9Z,12Z)/14:1(9Z))	C51H92O6	M+NH4	818.7232	-0.9
	HMDB0043850	TG(16/14/18:3(9Z,12Z,15Z))	C51H92O6	M+NH4	818.7232	-0.9

818.7225

HMDB0047778	TG(14:1(9Z)/16/18:2(9Z,12Z))	C51H92O6	M+NH4	818.7232	-0.9
HMDB0043843	TG(16/14/18:3(6Z,9Z,12Z))	C51H92O6	M+NH4	818.7232	-0.9
HMDB0042288	TG(14/14:1(9Z):2n6)	C51H92O6	M+NH4	818.7232	-0.9
HMDB0043004	TG(15/15/18:3(6Z,9Z,12Z))	C51H92O6	M+NH4	818.7232	-0.9
HMDB0042316	TG(14/16:1(9Z)/18:2(9Z,12Z))	C51H92O6	M+NH4	818.7232	-0.9
HMDB0047734	TG(14:1(9Z)/14/:2n6)	C51H92O6	M+NH4	818.7232	-0.9
HMDB0005432	TG(16:1(9Z)/16:1(9Z)/16:1(9Z))	C51H92O6	M+NH4	818.7232	-0.9
HMDB0043424	TG(15/18:3(6Z,9Z,12Z)/15)	C51H92O6	M+NH4	818.7232	-0.9
HMDB0043627	TG(15/18:3(9Z,12Z,15Z)/15)	C51H92O6	M+NH4	818.7232	-0.9
HMDB0042601	TG(14/:3n6/14)	C51H92O6	M+NH4	818.7232	-0.9
HMDB0042421	TG(14/:3(5Z,8Z,11Z)/14)	C51H92O6	M+NH4	818.7232	-0.9
HMDB0042079	TG(14/14/:3n6)	C51H92O6	M+NH4	818.7232	-0.9
HMDB0042073	TG(14/14/:3(5Z,8Z,11Z))	C51H92O6	M+NH4	818.7232	-0.9
HMDB0042137	TG(14/16/18:3(6Z,9Z,12Z))	C51H92O6	M+NH4	818.7232	-0.9
HMDB0042144	TG(14/16/18:3(9Z,12Z,15Z))	C51H92O6	M+NH4	818.7232	-0.9
HMDB0048568	TG(16:1(9Z)/14:1(9Z)/18:1(11Z))	C51H92O6	M+NH4	818.7232	-0.9
HMDB0010422	TG(16:1(9Z)/14:1(9Z)/18:1(9Z))	C51H92O6	M+NH4	818.7232	-0.9
HMDB0048569	TG(16:1(9Z)/14:1(9Z)/18:1(9Z))	C51H92O6	M+NH4	818.7232	-0.9
HMDB0043011	TG(15/15/18:3(9Z,12Z,15Z))	C51H92O6	M+NH4	818.7232	-0.9
HMDB0042543	TG(14/18:3(6Z,9Z,12Z)/16)	C51H92O6	M+NH4	818.7232	-0.9
HMDB0047977	TG(14:1(9Z):1(11Z)/14:1(9Z))	C51H92O6	M+NH4	818.7232	-0.9
HMDB0047932	TG(14:1(9Z)/18:1(11Z)/16:1(9Z))	C51H92O6	M+NH4	818.7232	-0.9

819.5166

HMDB0116743	PG(22:5(4Z,7Z,Z,13Z,16Z)/16)	C44H77O10P	M+Na	819.5147	2.4
HMDB0116609	PG(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C44H77O10P	M+Na	819.5147	2.4
HMDB0116581	PG(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C44H77O10P	M+Na	819.5147	2.4
HMDB0116578	PG(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C44H77O10P	M+Na	819.5147	2.4
HMDB0116621	PG(22:5(7Z,Z,13Z,16Z,19Z)/16)	C44H77O10P	M+Na	819.5147	2.4
HMDB0116610	PG(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C44H77O10P	M+Na	819.5147	2.4
HMDB0010582	PG(16/22:5(4Z,7Z,Z,13Z,16Z))	C44H77O10P	M+Na	819.5147	2.4
HMDB0010596	PG(16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C44H77O10P	M+Na	819.5147	2.4
HMDB0010625	PG(18:1(11Z):4(5Z,8Z,11Z,14Z))	C44H77O10P	M+Na	819.5147	2.4
HMDB0010640	PG(18:1(9Z):4(5Z,8Z,11Z,14Z))	C44H77O10P	M+Na	819.5147	2.4
HMDB0010654	PG(18:2(9Z,12Z):3(8Z,11Z,14Z))	C44H77O10P	M+Na	819.5147	2.4
HMDB0010653	PG(18:2(9Z,12Z):3(5Z,8Z,11Z))	C44H77O10P	M+Na	819.5147	2.4
HMDB0010583	PG(16/22:5(7Z,Z,13Z,16Z,19Z))	C44H77O10P	M+Na	819.5147	2.4
HMDB0010687	PG(18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C46H75O10P	M+H	819.5171	-0.6
HMDB0010688	PG(18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C46H75O10P	M+H	819.5171	-0.6
HMDB0010673	[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(7Z,Z,13Z,16Z,19Z)-docosa-7-,13,16,19-pentaenoyloxy]-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphinic acid	C46H75O10P	M+H	819.5171	-0.6
HMDB0010672	PG(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C46H75O10P	M+H	819.5171	-0.6
HMDB0010659	PG(18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C46H75O10P	M+H	819.5171	-0.6
HMDB0116600	PG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C46H75O10P	M+H	819.5171	-0.6
HMDB0116590	PG(:4(5Z,8Z,11Z,14Z):4(8Z,11Z,14Z,17Z))	C46H75O10P	M+H	819.5171	-0.6

	HMDB0116597	PG(:4(8Z,11Z,14Z,17Z):4(8Z,11Z,14Z,17Z))	C46H75O10P	M+H	819.5171	-0.6
	HMDB0116596	PG(:4(8Z,11Z,14Z,17Z):4(5Z,8Z,11Z,14Z))	C46H75O10P	M+H	819.5171	-0.6
	HMDB0116589	PG(:4(5Z,8Z,11Z,14Z):4(5Z,8Z,11Z,14Z))	C46H75O10P	M+H	819.5171	-0.6
820.6205	HMDB0008619	PC(22:2(13Z,16Z)/P-16)	C46H88NO7P	M+Na	820.6191	1.8
	HMDB0008358	PC(:2(11Z,14Z)/P-18)	C46H88NO7P	M+Na	820.6191	1.8
	HMDB0008327	PC(:1(11Z)/P-18:1(9Z))	C46H88NO7P	M+Na	820.6191	1.8
	HMDB0008326	PC(:1(11Z)/P-18:1(11Z))	C46H88NO7P	M+Na	820.6191	1.8
	HMDB0013439	PC(O-/18:3(6Z,9Z,12Z))	C46H88NO7P	M+Na	820.6191	1.8
	HMDB0011315	PC(P-18:1(9Z):1(11Z))	C46H88NO7P	M+Na	820.6191	1.8
	HMDB0011282	PC(P-18:1(11Z):1(11Z))	C46H88NO7P	M+Na	820.6191	1.8
	HMDB0013440	PC(O-/18:3(9Z,12Z,15Z))	C46H88NO7P	M+Na	820.6191	1.8
	HMDB0011250	PC(P-18/:2(11Z,14Z))	C46H88NO7P	M+Na	820.6191	1.8
	HMDB0011225	PC(P-16/22:2(13Z,16Z))	C46H88NO7P	M+Na	820.6191	1.8
	HMDB0013422	PC(O-18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C48H86NO7P	M+H	820.6215	-1.2
	HMDB0008719	PC(22:5(7Z,Z,13Z,16Z,19Z)/P-18)	C48H86NO7P	M+H	820.6215	-1.2
	HMDB0008654	PC(22:4(7Z,Z,13Z,16Z)/P-18:1(11Z))	C48H86NO7P	M+H	820.6215	-1.2
	HMDB0008686	PC(22:5(4Z,7Z,Z,13Z,16Z)/P-18)	C48H86NO7P	M+H	820.6215	-1.2
	HMDB0011261	PC(P-18/22:5(7Z,Z,13Z,16Z,19Z))	C48H86NO7P	M+H	820.6215	-1.2
	HMDB0008655	PC(22:4(7Z,Z,13Z,16Z)/P-18:1(9Z))	C48H86NO7P	M+H	820.6215	-1.2
	HMDB0011260	PC(P-18/22:5(4Z,7Z,Z,13Z,16Z))	C48H86NO7P	M+H	820.6215	-1.2
	HMDB0011292	PC(P-18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C48H86NO7P	M+H	820.6215	-1.2
	HMDB0011325	PC(P-18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C48H86NO7P	M+H	820.6215	-1.2
820.7380	HMDB0045662	TG(/14:1(9Z)/14:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0042136	TG(14/16/18:2(9Z,12Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0042369	TG(14/18:1(9Z)/16:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0010415	TG(16/14/18:2(9Z,12Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0005376	TG(16/16:1(9Z)/16:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0043003	TG(15/15/18:2(9Z,12Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0043395	TG(15/18:2(9Z,12Z)/15)	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0047794	TG(14:1(9Z)/18/16:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0044033	TG(16/14:1(9Z)/18:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0042398	TG(14/:1(11Z)/14:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0042571	TG(14/:2n6/14)	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0047728	TG(14:1(9Z)/14/:1(11Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0010421	TG(16:1(9Z)/14/18:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0044862	TG(18/14:1(9Z)/16:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0044888	TG(18/16:1(9Z)/14:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0010420	TG(16:1(9Z)/14/18:1(11Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0047772	TG(14:1(9Z)/16/18:1(11Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0044114	TG(16/18:1(9Z)/14:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0042078	TG(14/14/:2n6)	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0044086	TG(16/18:1(11Z)/14:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0042513	TG(14/18:2(9Z,12Z)/16)	C51H94O6	M+NH4	820.7389	-1.1

822.6357	HMDB0044032	TG(16/14:1(9Z)/18:1(11Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0047773	TG(14:1(9Z)/16/18:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0036341	15-Palmitoylsolamin	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0042311	TG(14/16:1(9Z)/18:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0042339	TG(14/18:1(11Z)/16:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0042282	TG(14/14:1(9Z)/:1(11Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0048457	TG(16:1(9Z)/16/16:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0047816	TG(14:1(9Z)/14:1(9Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0042310	TG(14/16:1(9Z)/18:1(11Z))	C51H94O6	M+NH4	820.7389	-1.1
	HMDB0008653	PC(22:4(7Z,Z,13Z,16Z)/P-18)	C48H88NO7P	M+H	822.6371	-1.7
	HMDB0011259	PC(P-18/22:4(7Z,Z,13Z,16Z))	C48H88NO7P	M+H	822.6371	-1.7
	HMDB0013444	PC(O-:1(11Z)/:4(8Z,11Z,14Z,17Z))	C48H88NO7P	M+H	822.6371	-1.7
	HMDB0013431	PC(O-18:1(9Z)/:1(11Z))	C46H90NO7P	M+Na	822.6347	1.2
822.7538	HMDB0013436	PC(O-18:2(9Z,12Z)/)	C46H90NO7P	M+Na	822.6347	1.2
	HMDB0011224	[2-({2-[(13Z)-docos-13-enoyloxy]-3-[(1Z)-hexadec-1-en-1-yloxy]propyl phosphonato}oxy)ethyl]trimethylazanium	C46H90NO7P	M+Na	822.6347	1.2
	HMDB0011281	PC(P-18:1(11Z)/)	C46H90NO7P	M+Na	822.6347	1.2
	HMDB0008586	[2-({3-[(13Z)-docos-13-enoyloxy]-2-[(1Z)-hexadec-1-en-1-yloxy]propyl phosphonato}oxy)ethyl]trimethylazanium	C46H90NO7P	M+Na	822.6347	1.2
	HMDB0011314	(2-({2-(icosanoyloxy)-3-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]propyl phosphonato}oxy)ethyl)trimethylazanium	C46H90NO7P	M+Na	822.6347	1.2
	HMDB0008325	PC(:1(11Z)/P-18)	C46H90NO7P	M+Na	822.6347	1.2
	HMDB0008293	(2-({3-(icosanoyloxy)-2-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]propyl phosphonato}oxy)ethyl)trimethylazanium	C46H90NO7P	M+Na	822.6347	1.2
	HMDB0008294	(2-({3-(icosanoyloxy)-2-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]propyl phosphonato}oxy)ethyl)trimethylazanium	C46H90NO7P	M+Na	822.6347	1.2
	HMDB0011249	Pc(p-18/:1(11z))	C46H90NO7P	M+Na	822.6347	1.2
	HMDB0045480	TG(/14/14:1(9Z))	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0042333	TG(14/18:1(11Z)/16)	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0042072	TG(14/14/:1(11Z))	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0042304	TG(14/16:1(9Z)/18)	C51H96O6	M+NH4	822.7545	-0.9
822.7538	HMDB0042159	TG(14/18/16:1(9Z))	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0042131	TG(14/16/18:1(9Z))	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0042130	TG(14/16/18:1(11Z))	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0042275	TG(14/14:1(9Z)/)	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0044726	TG(18/16/14:1(9Z))	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0010426	TG(18/14/16:1(9Z))	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0044026	TG(16/14:1(9Z)/18)	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0042188	TG(14//14:1(9Z))	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0043918	TG(16/18/14:1(9Z))	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0042363	TG(14/18:1(9Z)/16)	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0010414	TG(16/14/18:1(9Z))	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0042997	TG(15/15/18:1(11Z))	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0042998	TG(15/15/18:1(9Z))	C51H96O6	M+NH4	822.7545	-0.9
822.7538	HMDB0043836	TG(16/14/18:1(11Z))	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0005359	TG(16/16/16:1(9Z))	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0044053	TG(16/16:1(9Z)/16)	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0043250	TG(15/18:1(9Z)/15)	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0043221	TG(15/18:1(11Z)/15)	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0042391	TG(14/:1(11Z)/14)	C51H96O6	M+NH4	822.7545	-0.9
	HMDB0114005	PE-NMe2(18/22:4(7Z,Z,13Z,16Z))	C47H86NO8P	M+H	824.6164	0.4
	HMDB0114087	PE-NMe2(18:2(9Z,12Z)/22:2(13Z,16Z))	C47H86NO8P	M+H	824.6164	0.4

824.6167

HMDB0114115	PE-NMe2(18:3(6Z,9Z,12Z)/22:1(13Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0114364	PE-NMe2(:4(8Z,11Z,14Z,17Z)/)	C47H86NO8P	M+H	824.6164	0.4
HMDB0114421	PE-NMe2(22/18:4(6Z,9Z,12Z,15Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0114446	PE-NMe2(22:1(13Z)/18:3(6Z,9Z,12Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0114447	PE-NMe2(22:1(13Z)/18:3(9Z,12Z,15Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0114474	PE-NMe2(22:2(13Z,16Z)/18:2(9Z,12Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0114500	PE-NMe2(22:4(7Z,Z,13Z,16Z)/18)	C47H86NO8P	M+H	824.6164	0.4
HMDB0114253	PE-NMe2(:2(11Z,14Z)/:2(11Z,14Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0114336	PE-NMe2(:4(5Z,8Z,11Z,14Z)/)	C47H86NO8P	M+H	824.6164	0.4
HMDB0114144	PE-NMe2(18:3(9Z,12Z,15Z)/22:1(13Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0114172	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/22)	C47H86NO8P	M+H	824.6164	0.4
HMDB0114198	PE-NMe2(/:4(5Z,8Z,11Z,14Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0114199	PE-NMe2(/:4(8Z,11Z,14Z,17Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0114225	PE-NMe2(:1(11Z)/:3(5Z,8Z,11Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0114226	PE-NMe2(:1(11Z)/:3(8Z,11Z,14Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0114281	PE-NMe2(:3(5Z,8Z,11Z)/:1(11Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0114309	PE-NMe2(:3(8Z,11Z,14Z)/:1(11Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0009530	PE(22:1(13Z)/:3(8Z,11Z,14Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0009146	PE(18:3(6Z,9Z,12Z)/24:1(15Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0009755	PE(24:1(15Z)/18:3(9Z,12Z,15Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0009723	PE(24/18:4(6Z,9Z,12Z,15Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0009592	PE(22:4(7Z,Z,13Z,16Z)/)	C47H86NO8P	M+H	824.6164	0.4
HMDB0009561	PE(22:2(13Z,16Z)/:2(11Z,14Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0009529	PE(22:1(13Z)/:3(5Z,8Z,11Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0009498	PE(22/:4(5Z,8Z,11Z,14Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0009499	PE(22/:4(8Z,11Z,14Z,17Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0009435	PE(:4(8Z,11Z,14Z,17Z)/22)	C47H86NO8P	M+H	824.6164	0.4
HMDB0009402	PE(:4(5Z,8Z,11Z,14Z)/22)	C47H86NO8P	M+H	824.6164	0.4
HMDB0009370	PE(:3(8Z,11Z,14Z)/22:1(13Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0009337	PE(:3(5Z,8Z,11Z)/22:1(13Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0009305	PE(:2(11Z,14Z)/22:2(13Z,16Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0009240	PE(/22:4(7Z,Z,13Z,16Z))	C47H86NO8P	M+H	824.6164	0.4

HMDB0009211	PE(18:4(6Z,9Z,12Z,15Z)/24)	C47H86NO8P	M+H	824.6164	0.4
HMDB0009179	PE(18:3(9Z,12Z,15Z)/24:1(15Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0009754	PE(24:1(15Z)/18:3(6Z,9Z,12Z))	C47H86NO8P	M+H	824.6164	0.4
HMDB0115470	PA(24:1(15Z)/:4(5Z,8Z,11Z,14Z))	C47H83O8P	M+NH4	824.6164	0.4
HMDB0115445	PA(24/:5(5Z,8Z,11Z,14Z,17Z))	C47H83O8P	M+NH4	824.6164	0.4
HMDB0115392	PA(22:5(7Z,Z,13Z,16Z,19Z)/22)	C47H83O8P	M+NH4	824.6164	0.4
HMDB0115367	PA(22:5(4Z,7Z,Z,13Z,16Z)/22)	C47H83O8P	M+NH4	824.6164	0.4
HMDB0115341	PA(22:4(7Z,Z,13Z,16Z)/22:1(13Z))	C47H83O8P	M+NH4	824.6164	0.4
HMDB0115290	PA(22:1(13Z)/22:4(7Z,Z,13Z,16Z))	C47H83O8P	M+NH4	824.6164	0.4
HMDB0115264	PA(22/22:5(4Z,7Z,Z,13Z,16Z))	C47H83O8P	M+NH4	824.6164	0.4
HMDB0115265	PA(22/22:5(7Z,Z,13Z,16Z,19Z))	C47H83O8P	M+NH4	824.6164	0.4
HMDB0115222	PA(:5(5Z,8Z,11Z,14Z,17Z)/24)	C47H83O8P	M+NH4	824.6164	0.4
HMDB0115197	PA(:4(8Z,11Z,14Z,17Z)/24:1(15Z))	C47H83O8P	M+NH4	824.6164	0.4
HMDB0115170	PA(:4(5Z,8Z,11Z,14Z)/24:1(15Z))	C47H83O8P	M+NH4	824.6164	0.4
HMDB0115471	PA(24:1(15Z)/:4(8Z,11Z,14Z,17Z))	C47H83O8P	M+NH4	824.6164	0.4
HMDB0113462	PE-NMe(:4(8Z,11Z,14Z,17Z)/)	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113434	PE-NMe(:4(5Z,8Z,11Z,14Z)/)	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113407	PE-NMe(:3(8Z,11Z,14Z)/:1(11Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113379	PE-NMe(:3(5Z,8Z,11Z)/:1(11Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113324	PE-NMe(:1(11Z)/:3(8Z,11Z,14Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113323	PE-NMe(:1(11Z)/:3(5Z,8Z,11Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113296	PE-NMe(/:4(5Z,8Z,11Z,14Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113545	PE-NMe(22:1(13Z)/18:3(9Z,12Z,15Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113297	PE-NMe(/:4(8Z,11Z,14Z,17Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113519	PE-NMe(22/18:4(6Z,9Z,12Z,15Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113544	PE-NMe(22:1(13Z)/18:3(6Z,9Z,12Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113351	PE-NMe(:2(11Z,14Z)/:2(11Z,14Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113597	PE-NMe(22:4(7Z,Z,13Z,16Z)/18)	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113571	PE-NMe(22:2(13Z,16Z)/18:2(9Z,12Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113270	PE-NMe(18:4(6Z,9Z,12Z,15Z)/22)	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113242	PE-NMe(18:3(9Z,12Z,15Z)/22:1(13Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113213	PE-NMe(18:3(6Z,9Z,12Z)/22:1(13Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113104	PE-NMe(18/22:4(7Z,Z,13Z,16Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0113186	PE-NMe(18:2(9Z,12Z)/22:2(13Z,16Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008305	PC(:1(11Z)/18:3(9Z,12Z,15Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008336	PC(:2(11Z,14Z)/18:2(9Z,12Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008367	PC(:3(5Z,8Z,11Z)/18:1(11Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008400	PC(:3(8Z,11Z,14Z)/18:1(11Z))	C46H84NO8P	M+Na	832.5827	2.6

832.5848

HMDB0008401	PC(:3(8Z,11Z,14Z)/18:1(9Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008431	PC(:4(5Z,8Z,11Z,14Z)/18)	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008464	PC(:4(8Z,11Z,14Z,17Z)/18)	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008626	PC(22:4(7Z,Z,13Z,16Z)/16)	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008304	PC(:1(11Z)/18:3(6Z,9Z,12Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008273	PC(/18:4(6Z,9Z,12Z,15Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008241	PC(18:4(6Z,9Z,12Z,15Z)/)	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008048	PC(18/:4(5Z,8Z,11Z,14Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008049	PC(18/:4(8Z,11Z,14Z,17Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008079	PC(18:1(11Z)/:3(5Z,8Z,11Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008080	PC(18:1(11Z)/:3(8Z,11Z,14Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008112	PC(18:1(9Z)/:3(5Z,8Z,11Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008113	PC(18:1(9Z)/:3(8Z,11Z,14Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008145	PC(18:2(9Z,12Z)/:2(11Z,14Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008176	PC(18:3(6Z,9Z,12Z)/:1(11Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008209	PC(18:3(9Z,12Z,15Z)/:1(11Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0007988	PC(16/22:4(7Z,Z,13Z,16Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008368	PC(:3(5Z,8Z,11Z)/18:1(9Z))	C46H84NO8P	M+Na	832.5827	2.6
HMDB0008632	PC(22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C48H82NO8P	M+H	832.5851	-0.3
HMDB0008475	PC(:4(8Z,11Z,14Z,17Z)/:3(8Z,11Z,14Z))	C48H82NO8P	M+H	832.5851	-0.3
HMDB0008442	PC(:4(5Z,8Z,11Z,14Z)/:3(8Z,11Z,14Z))	C48H82NO8P	M+H	832.5851	-0.3
HMDB0008441	PC(:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C48H82NO8P	M+H	832.5851	-0.3
HMDB0008411	PC(:3(8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C48H82NO8P	M+H	832.5851	-0.3
HMDB0008410	PC(:3(8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C48H82NO8P	M+H	832.5851	-0.3
HMDB0008633	PC(22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C48H82NO8P	M+H	832.5851	-0.3
HMDB0008664	PC(22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C48H82NO8P	M+H	832.5851	-0.3
HMDB0008729	PC(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C48H82NO8P	M+H	832.5851	-0.3
HMDB0008728	PC(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C48H82NO8P	M+H	832.5851	-0.3
HMDB0008697	PC(22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C48H82NO8P	M+H	832.5851	-0.3
HMDB0008379	PC(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C48H82NO8P	M+H	832.5851	-0.3
HMDB0008378	PC(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C48H82NO8P	M+H	832.5851	-0.3
HMDB0008155	PC(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C48H82NO8P	M+H	832.5851	-0.3

	HMDB0008154	PC(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0008123	PC(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0008090	PC(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0008186	PC(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0008347	PC(:2(11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0008474	PC(:4(8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0008219	PC(18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0008506	PC(:5(5Z,8Z,11Z,14Z,17Z)/:2(11Z,14Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0113633	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/:2(11Z,14Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0113660	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/:2(11Z,14Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0113362	PE-NMe(:2(11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0113361	PE-NMe(:2(11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0113334	PE-NMe(:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0113389	PE-NMe(:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0113417	PE-NMe(:3(8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0113501	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0113582	PE-NMe(22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0113608	PE-NMe(22:4(7Z,Z,13Z,16Z)/:3(8Z,11Z,14Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0113686	PE-NMe(22:6(4Z,7Z,Z,13Z,16Z,19Z)/:1(11Z))	C48H82NO8P	M+H	832.5851	-0.3
	HMDB0113607	PE-NMe(22:4(7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C48H82NO8P	M+H	832.5851	-0.3
832.7383	HMDB0047757	TG(14:1(9Z)/15/:2n6)	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0043628	TG(15/18:3(9Z,12Z,15Z)/16)	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0042971	TG(15/14/:3(5Z,8Z,11Z))	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0043040	TG(15/16/18:3(9Z,12Z,15Z))	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0043206	TG(15/16:1(9Z)/18:2(9Z,12Z))	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0042422	TG(14/:3(5Z,8Z,11Z)/15)	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0043033	TG(15/16/18:3(6Z,9Z,12Z))	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0043425	TG(15/18:3(6Z,9Z,12Z)/16)	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0043878	TG(16/15/18:3(9Z,12Z,15Z))	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0043871	TG(16/15/18:3(6Z,9Z,12Z))	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0043179	TG(15/14:1(9Z)/:2n6)	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0043402	TG(15/18:2(9Z,12Z)/16:1(9Z))	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0042977	TG(15/14/:3n6)	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0043459	TG(15/:2n6/14:1(9Z))	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0042602	TG(14/:3n6/15)	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0048442	TG(16:1(9Z)/15/18:2(9Z,12Z))	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0042103	TG(14/15/:3(5Z,8Z,11Z))	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0042109	TG(14/15/:3n6)	C52H94O6	M+NH4	832.7389	-0.7
	HMDB0113517	PE-NMe(22/18:3(6Z,9Z,12Z))	C46H86NO8P	M+Na	834.5983	2.6
	HMDB0113241	PE-NMe(18:3(9Z,12Z,15Z)/22)	C46H86NO8P	M+Na	834.5983	2.6
	HMDB0113157	PE-NMe(18:1(9Z)/22:2(13Z,16Z))	C46H86NO8P	M+Na	834.5983	2.6

HMDB0113185	PE-NMe(18:2(9Z,12Z)/22:1(13Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0113212	PE-NMe(18:3(6Z,9Z,12Z)/22)	C46H86NO8P	M+Na	834.5983	2.6
HMDB0113294	PE-NMe(/:3(5Z,8Z,11Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0113406	PE-NMe(:3(8Z,11Z,14Z)/)	C46H86NO8P	M+Na	834.5983	2.6
HMDB0113378	PE-NMe(:3(5Z,8Z,11Z)/)	C46H86NO8P	M+Na	834.5983	2.6
HMDB0113295	PE-NMe(/:3(8Z,11Z,14Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0113569	PE-NMe(22:2(13Z,16Z)/18:1(11Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0113130	PE-NMe(18:1(11Z)/22:2(13Z,16Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0113350	PE-NMe(:2(11Z,14Z)/:1(11Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0113322	PE-NMe(:1(11Z)/:2(11Z,14Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0113570	PE-NMe(22:2(13Z,16Z)/18:1(9Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0113543	PE-NMe(22:1(13Z)/18:2(9Z,12Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0113518	PE-NMe(22/18:3(9Z,12Z,15Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008020	PC(16:1(9Z)/22:2(13Z,16Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008594	PC(22:2(13Z,16Z)/16:1(9Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008399	PC(:3(8Z,11Z,14Z)/18)	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008366	PC(:3(5Z,8Z,11Z)/18)	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008334	PC(:2(11Z,14Z)/18:1(11Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008303	PC(:1(11Z)/18:2(9Z,12Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008272	PC(/18:3(9Z,12Z,15Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008271	PC(/18:3(6Z,9Z,12Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008208	PC(18:3(9Z,12Z,15Z)/)	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008175	PC(18:3(6Z,9Z,12Z)/)	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008144	PC(18:2(9Z,12Z)/:1(11Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008111	PC(18:1(9Z)/:2(11Z,14Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008078	PC(18:1(11Z)/:2(11Z,14Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008047	PC(18/:3(8Z,11Z,14Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008335	PC(:2(11Z,14Z)/18:1(9Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008046	PC(18/:3(5Z,8Z,11Z))	C46H86NO8P	M+Na	834.5983	2.6
HMDB0008727	PC(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18)	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008696	PC(22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008695	PC(22:5(7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C48H84NO8P	M+H	834.6007	-0.3

HMDB0008663	PC(22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008662	PC(22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008631	PC(22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008601	PC(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008505	PC(:5(5Z,8Z,11Z,14Z,17Z)/:1(11Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008377	PC(:3(5Z,8Z,11Z)/:3(8Z,11Z,14Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008473	PC(:4(8Z,11Z,14Z,17Z)/:2(11Z,14Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008057	PC(18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008089	PC(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008088	PC(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008251	PC(18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008121	PC(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008122	PC(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008153	PC(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008314	PC(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008345	PC(:2(11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008408	PC(:3(8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008409	PC(:3(8Z,11Z,14Z)/:3(8Z,11Z,14Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008346	PC(:2(11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008440	PC(:4(5Z,8Z,11Z,14Z)/:2(11Z,14Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0008376	PC(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0113472	PE-NMe(:4(8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0113659	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/:1(11Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0113685	PE-NMe(22:6(4Z,7Z,Z,13Z,16Z,19Z)/)	C48H84NO8P	M+H	834.6007	-0.3
HMDB0113360	PE-NMe(:2(11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0113606	PE-NMe(22:4(7Z,Z,13Z,16Z)/:2(11Z,14Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0113581	PE-NMe(22:2(13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0113580	PE-NMe(22:2(13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0113305	PE-NMe(/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0113332	PE-NMe(:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0113333	PE-NMe(:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C48H84NO8P	M+H	834.6007	-0.3
HMDB0113443	PE-NMe(:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	C48H84NO8P	M+H	834.6007	-0.3

	HMDB0113500	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/22:1(13Z))	C48H84NO8P	M+H	834.6007	-0.3
	HMDB0113554	PE-NMe(22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z))	C48H84NO8P	M+H	834.6007	-0.3
	HMDB0113632	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/:1(11Z))	C48H84NO8P	M+H	834.6007	-0.3
834.7547	HMDB0047751	TG(14:1(9Z)/15/:1(11Z))	C52H96O6	M+NH4	834.7545	0.2
	HMDB0043200	TG(15/16:1(9Z)/18:1(11Z))	C52H96O6	M+NH4	834.7545	0.2
	HMDB0011706	TG(15/18:1(9Z)/16:1(9Z))	C52H96O6	M+NH4	834.7545	0.2
	HMDB0043201	TG(15/16:1(9Z)/18:1(9Z))	C52H96O6	M+NH4	834.7545	0.2
	HMDB0011710	TG(15/18:2(9Z,12Z)/16)	C52H96O6	M+NH4	834.7545	0.2
	HMDB0042572	TG(14/:2n6/15)	C52H96O6	M+NH4	834.7545	0.2
	HMDB0043285	TG(15/:1(11Z)/14:1(9Z))	C52H96O6	M+NH4	834.7545	0.2
	HMDB0043173	TG(15/14:1(9Z)/:1(11Z))	C52H96O6	M+NH4	834.7545	0.2
	HMDB0043228	TG(15/18:1(11Z)/16:1(9Z))	C52H96O6	M+NH4	834.7545	0.2
	HMDB0043032	TG(15/16/18:2(9Z,12Z))	C52H96O6	M+NH4	834.7545	0.2
	HMDB0042976	TG(15/14/:2n6)	C52H96O6	M+NH4	834.7545	0.2
	HMDB0042108	TG(14/15/:2n6)	C52H96O6	M+NH4	834.7545	0.2
	HMDB0043870	TG(16/15/18:2(9Z,12Z))	C52H96O6	M+NH4	834.7545	0.2
	HMDB0048437	TG(16:1(9Z)/15/18:1(9Z))	C52H96O6	M+NH4	834.7545	0.2
	HMDB0048436	TG(16:1(9Z)/15/18:1(11Z))	C52H96O6	M+NH4	834.7545	0.2
	HMDB0113083	PE-NMe(16:1(9Z)/24:1(15Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0113103	PE-NMe(18/22:2(13Z,16Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0113129	PE-NMe(18:1(11Z)/22:1(13Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0113156	PE-NMe(18:1(9Z)/22:1(13Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0113349	PE-NMe(:2(11Z,14Z)/)	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0113293	PE-NMe(/:2(11Z,14Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0113568	PE-NMe(22:2(13Z,16Z)/18)	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0113541	PE-NMe(22:1(13Z)/18:1(11Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0113542	PE-NMe(22:1(13Z)/18:1(9Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0113516	PE-NMe(22/18:2(9Z,12Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0113321	PE-NMe(:1(11Z)/:1(11Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0113184	PE-NMe(18:2(9Z,12Z)/22)	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0113732	PE-NMe(24:1(15Z)/16:1(9Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0008333	PC(:2(11Z,14Z)/18)	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0007987	PC(16/22:2(13Z,16Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0007927	PC(14:1(9Z)/24:1(15Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0008019	PC(16:1(9Z)/22:1(13Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0008045	PC(18/:2(11Z,14Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0008077	PC(18:1(11Z)/:1(11Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0008110	PC(18:1(9Z)/:1(11Z))	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0008143	PC(18:2(9Z,12Z)/)	C46H88NO8P	M+Na	836.6140	2.8
	HMDB0008270	PC(/18:2(9Z,12Z))	C46H88NO8P	M+Na	836.6140	2.8

836.6163

HMDB0008301	PC(:1(11Z)/18:1(11Z))	C46H88NO8P	M+Na	836.6140	2.8
HMDB0008302	PC(:1(11Z)/18:1(9Z))	C46H88NO8P	M+Na	836.6140	2.8
HMDB0008562	PC(22:1(13Z)/16:1(9Z))	C46H88NO8P	M+Na	836.6140	2.8
HMDB0008593	PC(22:2(13Z,16Z)/16)	C46H88NO8P	M+Na	836.6140	2.8
HMDB0008789	PC(24:1(15Z)/14:1(9Z))	C46H88NO8P	M+Na	836.6140	2.8
HMDB0008694	PC(22:5(7Z,Z,13Z,16Z,19Z)/18)	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008661	PC(22:5(4Z,7Z,Z,13Z,16Z)/18)	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008630	PC(22:4(7Z,Z,13Z,16Z)/18:1(9Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008629	PC(22:4(7Z,Z,13Z,16Z)/18:1(11Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008599	PC(22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008600	PC(22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008568	PC(22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008056	PC(18/22:5(7Z,Z,13Z,16Z,19Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008312	PC(:1(11Z)/:4(5Z,8Z,11Z,14Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008087	PC(18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008281	PC(/:5(5Z,8Z,11Z,14Z,17Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008120	PC(18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008250	PC(18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008218	PC(18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008055	PC(18/22:5(4Z,7Z,Z,13Z,16Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008313	PC(:1(11Z)/:4(8Z,11Z,14Z,17Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008185	PC(18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008504	PC(:5(5Z,8Z,11Z,14Z,17Z)/)	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008472	PC(:4(8Z,11Z,14Z,17Z)/:1(11Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008439	PC(:4(5Z,8Z,11Z,14Z)/:1(11Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008407	PC(:3(8Z,11Z,14Z)/:2(11Z,14Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008375	PC(:3(5Z,8Z,11Z)/:2(11Z,14Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008344	PC(:2(11Z,14Z)/:3(8Z,11Z,14Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0008343	PC(:2(11Z,14Z)/:3(5Z,8Z,11Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0113303	PE-NMe(/22:5(4Z,7Z,Z,13Z,16Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0113278	PE-NMe(18:4(6Z,9Z,12Z,15Z)/24:1(15Z))	C48H86NO8P	M+H	836.6164	-0.1
HMDB0113304	PE-NMe(/22:5(7Z,Z,13Z,16Z,19Z))	C48H86NO8P	M+H	836.6164	-0.1

	HMDB0113739	PE-NMe(24:1(15Z)/18:4(6Z,9Z,12Z,15Z))	C48H86NO8P	M+H	836.6164	-0.1
	HMDB0113658	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/)	C48H86NO8P	M+H	836.6164	-0.1
	HMDB0113605	PE-NMe(22:4(7Z,Z,13Z,16Z)/:1(11Z))	C48H86NO8P	M+H	836.6164	-0.1
	HMDB0113579	PE-NMe(22:2(13Z,16Z)/:3(8Z,11Z,14Z))	C48H86NO8P	M+H	836.6164	-0.1
	HMDB0113578	PE-NMe(22:2(13Z,16Z)/:3(5Z,8Z,11Z))	C48H86NO8P	M+H	836.6164	-0.1
	HMDB0113553	PE-NMe(22:1(13Z)/:4(8Z,11Z,14Z,17Z))	C48H86NO8P	M+H	836.6164	-0.1
	HMDB0113552	PE-NMe(22:1(13Z)/:4(5Z,8Z,11Z,14Z))	C48H86NO8P	M+H	836.6164	-0.1
	HMDB0113527	PE-NMe(22:/:5(5Z,8Z,11Z,14Z,17Z))	C48H86NO8P	M+H	836.6164	-0.1
	HMDB0113499	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/22)	C48H86NO8P	M+H	836.6164	-0.1
	HMDB0113471	PE-NMe(:4(8Z,11Z,14Z,17Z)/22:1(13Z))	C48H86NO8P	M+H	836.6164	-0.1
	HMDB0113442	PE-NMe(:4(5Z,8Z,11Z,14Z)/22:1(13Z))	C48H86NO8P	M+H	836.6164	-0.1
	HMDB0113416	PE-NMe(:3(8Z,11Z,14Z)/22:2(13Z,16Z))	C48H86NO8P	M+H	836.6164	-0.1
	HMDB0113631	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/)	C48H86NO8P	M+H	836.6164	-0.1
	HMDB0113388	PE-NMe(:3(5Z,8Z,11Z)/22:2(13Z,16Z))	C48H86NO8P	M+H	836.6164	-0.1
	HMDB0113331	PE-NMe(:1(11Z)/22:4(7Z,Z,13Z,16Z))	C48H86NO8P	M+H	836.6164	-0.1
836.7702	HMDB0043026	TG(15/16/18:1(11Z))	C52H98O6	M+NH4	836.7702	0.0
	HMDB0042392	TG(14/:1(11Z)/15)	C52H98O6	M+NH4	836.7702	0.0
	HMDB0043027	TG(15/16/18:1(9Z))	C52H98O6	M+NH4	836.7702	0.0
	HMDB0043194	TG(15/16:1(9Z)/18)	C52H98O6	M+NH4	836.7702	0.0
	HMDB0011705	TG(15/18:1(9Z)/16)	C52H98O6	M+NH4	836.7702	0.0
	HMDB0011713	TG(15/:1(11Z)/14)	C52H98O6	M+NH4	836.7702	0.0
	HMDB0043166	TG(15/14:1(9Z)/)	C52H98O6	M+NH4	836.7702	0.0
	HMDB0042970	TG(15/14/:1(11Z))	C52H98O6	M+NH4	836.7702	0.0
	HMDB0043222	TG(15/18:1(11Z)/16)	C52H98O6	M+NH4	836.7702	0.0
	HMDB0043864	TG(16/15/18:1(11Z))	C52H98O6	M+NH4	836.7702	0.0
	HMDB0043865	TG(16/15/18:1(9Z))	C52H98O6	M+NH4	836.7702	0.0
	HMDB0043054	TG(15/18/16:1(9Z))	C52H98O6	M+NH4	836.7702	0.0
	HMDB0011712	TG(15//14:1(9Z))	C52H98O6	M+NH4	836.7702	0.0
	HMDB0044700	TG(18/15/16:1(9Z))	C52H98O6	M+NH4	836.7702	0.0
	HMDB0045506	TG(/15/14:1(9Z))	C52H98O6	M+NH4	836.7702	0.0
	HMDB0042102	TG(14/15/:1(11Z))	C52H98O6	M+NH4	836.7702	0.0
	HMDB0113060	PE-NMe(16/24:1(15Z))	C46H90NO8P	M+Na	838.6296	1.4
	HMDB0114633	PE-NMe2(24:1(15Z)/15)	C46H90NO8P	M+Na	838.6296	1.4
	HMDB0113939	PE-NMe2(15/24:1(15Z))	C46H90NO8P	M+Na	838.6296	1.4
	HMDB0113731	PE-NMe(24:1(15Z)/16)	C46H90NO8P	M+Na	838.6296	1.4
	HMDB0113705	PE-NMe(24/16:1(9Z))	C46H90NO8P	M+Na	838.6296	1.4
	HMDB0113540	PE-NMe(22:1(13Z)/18)	C46H90NO8P	M+Na	838.6296	1.4
	HMDB0113514	PE-NMe(22/18:1(11Z))	C46H90NO8P	M+Na	838.6296	1.4
	HMDB0113515	PE-NMe(22/18:1(9Z))	C46H90NO8P	M+Na	838.6296	1.4
	HMDB0113082	PE-NMe(16:1(9Z)/24)	C46H90NO8P	M+Na	838.6296	1.4

838.6308

HMDB0113102	PE-NMe(18/22:1(13Z))	C46H90NO8P	M+Na	838.6296	1.4
HMDB0113128	PE-NMe(18:1(11Z)/22)	C46H90NO8P	M+Na	838.6296	1.4
HMDB0113155	PE-NMe(18:1(9Z)/22)	C46H90NO8P	M+Na	838.6296	1.4
HMDB0113292	PE-NMe(/:1(11Z))	C46H90NO8P	M+Na	838.6296	1.4
HMDB0113320	PE-NMe(:1(11Z)/)	C46H90NO8P	M+Na	838.6296	1.4
HMDB0008788	PC(24:1(15Z)/14)	C46H90NO8P	M+Na	838.6296	1.4
HMDB0008269	PC(/18:1(9Z))	C46H90NO8P	M+Na	838.6296	1.4
HMDB0008300	PC(:1(11Z)/18)	C46H90NO8P	M+Na	838.6296	1.4
HMDB0008529	PC(22/16:1(9Z))	C46H90NO8P	M+Na	838.6296	1.4
HMDB0008561	PC(22:1(13Z)/16)	C46H90NO8P	M+Na	838.6296	1.4
HMDB0008756	PC(24/14:1(9Z))	C46H90NO8P	M+Na	838.6296	1.4
HMDB0008268	PC(/18:1(11Z))	C46H90NO8P	M+Na	838.6296	1.4
HMDB0007894	PC(14/24:1(15Z))	C46H90NO8P	M+Na	838.6296	1.4
HMDB0007986	PC(16/22:1(13Z))	C46H90NO8P	M+Na	838.6296	1.4
HMDB0008109	PC(18:1(9Z)/)	C46H90NO8P	M+Na	838.6296	1.4
HMDB0007926	PC(14:1(9Z)/24)	C46H90NO8P	M+Na	838.6296	1.4
HMDB0008076	PC(18:1(11Z)/)	C46H90NO8P	M+Na	838.6296	1.4
HMDB0008018	PC(16:1(9Z)/22)	C46H90NO8P	M+Na	838.6296	1.4
HMDB0008044	PC(18/:1(11Z))	C46H90NO8P	M+Na	838.6296	1.4
HMDB0008536	PC(22/18:4(6Z,9Z,12Z,15Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008184	PC(18:3(6Z,9Z,12Z)/22:1(13Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008566	PC(22:1(13Z)/18:3(6Z,9Z,12Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008567	PC(22:1(13Z)/18:3(9Z,12Z,15Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008598	PC(22:2(13Z,16Z)/18:2(9Z,12Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008628	PC(22:4(7Z,Z,13Z,16Z)/18)	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008471	PC(:4(8Z,11Z,14Z,17Z)/)	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008438	PC(:4(5Z,8Z,11Z,14Z)/)	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008217	PC(18:3(9Z,12Z,15Z)/22:1(13Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008152	PC(18:2(9Z,12Z)/22:2(13Z,16Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008279	PC(/:4(5Z,8Z,11Z,14Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008280	PC(/:4(8Z,11Z,14Z,17Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008054	PC(18/22:4(7Z,Z,13Z,16Z))	C48H88NO8P	M+H	838.6320	-1.5

HMDB0008310	PC(:1(11Z)/:3(5Z,8Z,11Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008342	PC(:2(11Z,14Z)/:2(11Z,14Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008374	PC(:3(5Z,8Z,11Z)/:1(11Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008249	PC(18:4(6Z,9Z,12Z,15Z)/22)	C48H88NO8P	M+H	838.6320	-1.5
HMDB0008311	PC(:1(11Z)/:3(8Z,11Z,14Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0011201	PC(:3(8Z,11Z,14Z)/:1(11Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113712	PE-NMe(24/18:4(6Z,9Z,12Z,15Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113302	PE-NMe(/22:4(7Z,Z,13Z,16Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113277	PE-NMe(18:4(6Z,9Z,12Z,15Z)/24)	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113249	PE-NMe(18:3(9Z,12Z,15Z)/24:1(15Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113220	PE-NMe(18:3(6Z,9Z,12Z)/24:1(15Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113387	PE-NMe(:3(5Z,8Z,11Z)/22:1(13Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113415	PE-NMe(:3(8Z,11Z,14Z)/22:1(13Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113577	PE-NMe(22:2(13Z,16Z)/:2(11Z,14Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113359	PE-NMe(:2(11Z,14Z)/22:2(13Z,16Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113738	PE-NMe(24:1(15Z)/18:3(9Z,12Z,15Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113737	PE-NMe(24:1(15Z)/18:3(6Z,9Z,12Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113604	PE-NMe(22:4(7Z,Z,13Z,16Z)/)	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113551	PE-NMe(22:1(13Z)/:3(8Z,11Z,14Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113550	PE-NMe(22:1(13Z)/:3(5Z,8Z,11Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113526	PE-NMe(22/:4(8Z,11Z,14Z,17Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113525	PE-NMe(22/:4(5Z,8Z,11Z,14Z))	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113470	PE-NMe(:4(8Z,11Z,14Z,17Z)/22)	C48H88NO8P	M+H	838.6320	-1.5
HMDB0113441	PE-NMe(:4(5Z,8Z,11Z,14Z)/22)	C48H88NO8P	M+H	838.6320	-1.5
HMDB0047971	TG(14:1(9Z)/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0044562	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/14:1(9Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0049234	TG(18:1(11Z)/14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0048431	TG(16:1(9Z)/14/:5(5Z,8Z,11Z,14Z,17Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0042535	TG(14/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0048261	TG(14:1(9Z)/18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0047899	TG(14:1(9Z)/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0048100	TG(14:1(9Z)/18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0048278	TG(14:1(9Z)/18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0048605	TG(16:1(9Z)/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0048578	TG(16:1(9Z)/14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0042298	TG(14/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0042089	TG(14/14:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0052509	TG(18:2(9Z,12Z)/14:1(9Z)/18:3(9Z,12Z,15Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0052852	TG(18:3(6Z,9Z,12Z)/14/18:3(9Z,12Z,15Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0052405	TG(18:2(9Z,12Z)/14/18:4(6Z,9Z,12Z,15Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0052502	TG(18:2(9Z,12Z)/14:1(9Z)/18:3(6Z,9Z,12Z))	C53H90O6	M+NH4	840.7076	-1.9

840.7060

HMDB0049855	TG(18:1(9Z)/14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0048584	TG(16:1(9Z)/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0047926	TG(14:1(9Z)/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0048078	TG(14:1(9Z)/18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0047789	TG(14:1(9Z)/16/:5(5Z,8Z,11Z,14Z,17Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0047739	TG(14:1(9Z)/14/22:5(4Z,7Z,Z,13Z,16Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0042557	TG(14/18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0042849	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/16:1(9Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0047948	TG(14:1(9Z)/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0048300	TG(14:1(9Z)/:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0042774	TG(14/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0048279	TG(14:1(9Z)/18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0048162	TG(14:1(9Z)/:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0042728	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/14:1(9Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0042878	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/14:1(9Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0042796	TG(14/18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0044049	TG(16/14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0047920	TG(14:1(9Z)/16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0048085	TG(14:1(9Z)/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0042767	TG(14/18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0042564	TG(14/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0047744	TG(14:1(9Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0042327	TG(14/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0042293	TG(14/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0042901	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/14)	C53H90O6	M+NH4	840.7076	-1.9
HMDB0048941	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/16:1(9Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0052845	TG(18:3(6Z,9Z,12Z)/14/18:3(6Z,9Z,12Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0048207	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0010497	TG(18:3(9Z,12Z,15Z)/14/18:3(9Z,12Z,15Z))	C53H90O6	M+NH4	840.7076	-1.9
HMDB0042326	TG(14/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048597	TG(16:1(9Z)/16:1(9Z)/18:3(6Z,9Z,12Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0044878	TG(18/14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048430	TG(16:1(9Z)/14/:4(8Z,11Z,14Z,17Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048604	TG(16:1(9Z)/16:1(9Z)/18:3(9Z,12Z,15Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048571	TG(16:1(9Z)/14:1(9Z)/:3(5Z,8Z,11Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0049226	TG(18:1(11Z)/14:1(9Z)/18:3(6Z,9Z,12Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0045320	TG(18/18:4(6Z,9Z,12Z,15Z)/14:1(9Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0049233	TG(18:1(11Z)/14:1(9Z)/18:3(9Z,12Z,15Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0044534	TG(16/:4(8Z,11Z,14Z,17Z)/14:1(9Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0047963	TG(14:1(9Z)/18:1(9Z)/18:3(6Z,9Z,12Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0047940	TG(14:1(9Z)/18:1(11Z)/18:3(6Z,9Z,12Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042819	TG(14/:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042766	TG(14/18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048577	TG(16:1(9Z)/14:1(9Z)/:3n6)	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048424	TG(16:1(9Z)/14/:4(5Z,8Z,11Z,14Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042088	TG(14/14/22:5(7Z,Z,13Z,16Z,19Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042320	TG(14/16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042355	TG(14/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042147	TG(14/16/:5(5Z,8Z,11Z,14Z,17Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042083	TG(14/14/22:5(4Z,7Z,Z,13Z,16Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0049715	TG(18:1(9Z)/14/18:4(6Z,9Z,12Z,15Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0010471	TG(18:2(9Z,12Z)/14/18:3(9Z,12Z,15Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0052397	TG(18:2(9Z,12Z)/14/18:3(6Z,9Z,12Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0052501	TG(18:2(9Z,12Z)/14:1(9Z)/18:2(9Z,12Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0049854	TG(18:1(9Z)/14:1(9Z)/18:3(9Z,12Z,15Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0049847	TG(18:1(9Z)/14:1(9Z)/18:3(6Z,9Z,12Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0049087	TG(18:1(11Z)/14/18:4(6Z,9Z,12Z,15Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048473	TG(16:1(9Z)/16/18:4(6Z,9Z,12Z,15Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042556	TG(14/18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042698	TG(14/22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0047913	TG(14:1(9Z)/16:1(9Z)/:3(5Z,8Z,11Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0047970	TG(14:1(9Z)/18:1(9Z)/18:3(9Z,12Z,15Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048095	TG(14:1(9Z)/18:3(6Z,9Z,12Z)/18:1(9Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0044507	TG(16/18:4(6Z,9Z,12Z,15Z)/16:1(9Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0047919	TG(14:1(9Z)/16:1(9Z)/:3n6)	C53H92O6	M+NH4	842.7232	-0.7

842.7226

HMDB0042843	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/16)	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048001	TG(14:1(9Z)/:3(5Z,8Z,11Z)/16:1(9Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0047738	TG(14:1(9Z)/14/22:4(7Z,Z,13Z,16Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042527	TG(14/18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0044075	TG(16/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048255	TG(14:1(9Z)/18:3(9Z,12Z,15Z)/18:1(11Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0047782	TG(14:1(9Z)/16/:4(5Z,8Z,11Z,14Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048256	TG(14:1(9Z)/18:3(9Z,12Z,15Z)/18:1(9Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048094	TG(14:1(9Z)/18:3(6Z,9Z,12Z)/18:1(11Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0043014	TG(15/15/:5(5Z,8Z,11Z,14Z,17Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0043853	TG(16/14/:5(5Z,8Z,11Z,14Z,17Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048077	TG(14:1(9Z)/18:2(9Z,12Z)/18:2(9Z,12Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042639	TG(14/:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042790	TG(14/18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0047947	TG(14:1(9Z)/18:1(11Z)/18:3(9Z,12Z,15Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0044042	TG(16/14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048139	TG(14:1(9Z)/:3n6/16:1(9Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0044366	TG(16/:4(5Z,8Z,11Z,14Z)/14:1(9Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0044048	TG(16/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042534	TG(14/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0047810	TG(14:1(9Z)/18/18:4(6Z,9Z,12Z,15Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042791	TG(14/18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0047788	TG(14:1(9Z)/16/:4(8Z,11Z,14Z,17Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042385	TG(14/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042292	TG(14/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042871	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/14)	C53H92O6	M+NH4	842.7232	-0.7
HMDB0043714	TG(15/:5(5Z,8Z,11Z,14Z,17Z)/15)	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042721	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/14)	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048765	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/16:1(9Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0048919	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/16:1(9Z))	C53H92O6	M+NH4	842.7232	-0.7
HMDB0042609	TG(14/:3n6/16:1(9Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0044170	TG(16/:3(5Z,8Z,11Z)/14:1(9Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0043907	TG(16/16/18:4(6Z,9Z,12Z,15Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042784	TG(14/18:4(6Z,9Z,12Z,15Z)/18)	C53H94O6	M+NH4	844.7389	-1.1
HMDB0048116	TG(14:1(9Z)/:2n6/16:1(9Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0047962	TG(14:1(9Z)/18:1(9Z)/18:2(9Z,12Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042760	TG(14/18:3(9Z,12Z,15Z)/18:1(11Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042551	TG(14/18:3(6Z,9Z,12Z)/18:1(9Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0044479	TG(16/18:3(9Z,12Z,15Z)/16:1(9Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042550	TG(14/18:3(6Z,9Z,12Z)/18:1(11Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0047939	TG(14:1(9Z)/18:1(11Z)/18:2(9Z,12Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0044041	TG(16/14:1(9Z)/:3n6)	C53H94O6	M+NH4	844.7389	-1.1
HMDB0044074	TG(16/16:1(9Z)/18:3(9Z,12Z,15Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0043007	TG(15/15/:4(5Z,8Z,11Z,14Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042633	TG(14/:4(5Z,8Z,11Z,14Z)/16)	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042813	TG(14/:4(8Z,11Z,14Z,17Z)/16)	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042429	TG(14/:3(5Z,8Z,11Z)/16:1(9Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0044035	TG(16/14:1(9Z)/:3(5Z,8Z,11Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0043852	TG(16/14/:4(8Z,11Z,14Z,17Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0047775	TG(14:1(9Z)/16/:3(5Z,8Z,11Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042384	TG(14/18:1(9Z)/18:3(9Z,12Z,15Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0048072	TG(14:1(9Z)/18:2(9Z,12Z)/18:1(9Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042526	TG(14/18:2(9Z,12Z)/18:2(9Z,12Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0047781	TG(14:1(9Z)/16/:3n6)	C53H94O6	M+NH4	844.7389	-1.1
HMDB0047809	TG(14:1(9Z)/18/18:3(9Z,12Z,15Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0048423	TG(16:1(9Z)/14/:3n6)	C53H94O6	M+NH4	844.7389	-1.1
HMDB0049086	TG(18:1(11Z)/14/18:3(9Z,12Z,15Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0049225	TG(18:1(11Z)/14:1(9Z)/18:2(9Z,12Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0048465	TG(16:1(9Z)/16/18:3(6Z,9Z,12Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0049079	TG(18:1(11Z)/14/18:3(6Z,9Z,12Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0047898	TG(14:1(9Z)/14:1(9Z)/22:2(13Z,16Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0044067	TG(16/16:1(9Z)/18:3(6Z,9Z,12Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042761	TG(14/18:3(9Z,12Z,15Z)/18:1(9Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0043013	TG(15/15/:4(8Z,11Z,14Z,17Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0048071	TG(14:1(9Z)/18:2(9Z,12Z)/18:1(11Z))	C53H94O6	M+NH4	844.7389	-1.1

HMDB0044283	TG(16/18:3(6Z,9Z,12Z)/16:1(9Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0047802	TG(14:1(9Z)/18/18:3(6Z,9Z,12Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0044338	TG(16/:3n6/14:1(9Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042377	TG(14/18:1(9Z)/18:3(6Z,9Z,12Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0043846	TG(16/14/:4(5Z,8Z,11Z,14Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0048743	TG(16:1(9Z)/18:2(9Z,12Z)/16:1(9Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0047918	TG(14:1(9Z)/16:1(9Z)/:2n6)	C53H94O6	M+NH4	844.7389	-1.1
HMDB0044870	TG(18/14:1(9Z)/18:3(6Z,9Z,12Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0043685	TG(15/:4(8Z,11Z,14Z,17Z)/15)	C53H94O6	M+NH4	844.7389	-1.1
HMDB0043511	TG(15/:4(5Z,8Z,11Z,14Z)/15)	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042691	TG(14/22:4(7Z,Z,13Z,16Z)/14)	C53H94O6	M+NH4	844.7389	-1.1
HMDB0010470	TG(18:2(9Z,12Z)/14/18:2(9Z,12Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0045104	TG(18/18:3(6Z,9Z,12Z)/14:1(9Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042347	TG(14/18:1(11Z)/18:3(6Z,9Z,12Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042146	TG(14/16/:4(8Z,11Z,14Z,17Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042313	TG(14/16:1(9Z)/:3(5Z,8Z,11Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042175	TG(14/18/18:4(6Z,9Z,12Z,15Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042354	TG(14/18:1(11Z)/18:3(9Z,12Z,15Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042140	TG(14/16/:4(5Z,8Z,11Z,14Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042319	TG(14/16:1(9Z)/:3n6)	C53H94O6	M+NH4	844.7389	-1.1
HMDB0042082	TG(14/14/22:4(7Z,Z,13Z,16Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0049707	TG(18:1(9Z)/14/18:3(6Z,9Z,12Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0049846	TG(18:1(9Z)/14:1(9Z)/18:2(9Z,12Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0044689	TG(18/14/18:4(6Z,9Z,12Z,15Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0048417	TG(16:1(9Z)/14/:3(5Z,8Z,11Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0005435	TG(16:1(9Z)/16:1(9Z)/18:2(9Z,12Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0010424	TG(16:1(9Z)/16/18:3(9Z,12Z,15Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0044877	TG(18/14:1(9Z)/18:3(9Z,12Z,15Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0045293	TG(18/18:3(9Z,12Z,15Z)/14:1(9Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0048576	TG(16:1(9Z)/14:1(9Z)/:2n6)	C53H94O6	M+NH4	844.7389	-1.1
HMDB0049714	TG(18:1(9Z)/14/18:3(9Z,12Z,15Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0048184	TG(14:1(9Z)/22:2(13Z,16Z)/14:1(9Z))	C53H94O6	M+NH4	844.7389	-1.1
HMDB0044501	TG(16/18:4(6Z,9Z,12Z,15Z)/16)	C53H94O6	M+NH4	844.7389	-1.1
HMDB0005433	TG(16:1(9Z)/16:1(9Z)/18:1(9Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0043845	TG(16/14/:3n6)	C53H96O6	M+NH4	846.7545	-1.2
HMDB0043839	TG(16/14/:3(5Z,8Z,11Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0042520	TG(14/18:2(9Z,12Z)/18:1(11Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0044310	TG(16/:2n6/14:1(9Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0047891	TG(14:1(9Z)/14:1(9Z)/22:1(13Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0044255	TG(16/18:2(9Z,12Z)/16:1(9Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0042603	TG(14/:3n6/16)	C53H96O6	M+NH4	846.7545	-1.2
HMDB0042754	TG(14/18:3(9Z,12Z,15Z)/18)	C53H96O6	M+NH4	846.7545	-1.2
HMDB0047737	TG(14:1(9Z)/14/22:2(13Z,16Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0042668	TG(14/22:2(13Z,16Z)/14:1(9Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0047957	TG(14:1(9Z)/18:1(9Z)/18:1(9Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0043000	TG(15/15/:3(5Z,8Z,11Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0043899	TG(16/16/18:3(6Z,9Z,12Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0044040	TG(16/14:1(9Z)/:2n6)	C53H96O6	M+NH4	846.7545	-1.2
HMDB0047933	TG(14:1(9Z)/18:1(11Z)/18:1(11Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0010417	TG(16/16/18:3(9Z,12Z,15Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0047780	TG(14:1(9Z)/16/:2n6)	C53H96O6	M+NH4	846.7545	-1.2
HMDB0042318	TG(14/16:1(9Z)/:2n6)	C53H96O6	M+NH4	846.7545	-1.2
HMDB0048570	TG(16:1(9Z)/14:1(9Z)/:1(11Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0044681	TG(18/14/18:3(6Z,9Z,12Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0048590	TG(16:1(9Z)/16:1(9Z)/18:1(11Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0043006	TG(15/15/:3n6)	C53H96O6	M+NH4	846.7545	-1.2
HMDB0042544	TG(14/18:3(6Z,9Z,12Z)/18)	C53H96O6	M+NH4	846.7545	-1.2
HMDB0042346	TG(14/18:1(11Z)/18:2(9Z,12Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0042579	TG(14/:2n6/16:1(9Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0042423	TG(14/:3(5Z,8Z,11Z)/16)	C53H96O6	M+NH4	846.7545	-1.2
HMDB0047912	TG(14:1(9Z)/16:1(9Z)/:1(11Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0005379	TG(16/16:1(9Z)/18:2(9Z,12Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0047934	TG(14:1(9Z)/18:1(11Z)/18:1(9Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0042521	TG(14/18:2(9Z,12Z)/18:1(9Z))	C53H96O6	M+NH4	846.7545	-1.2
HMDB0047978	TG(14:1(9Z)/:1(11Z)/16:1(9Z))	C53H96O6	M+NH4	846.7545	-1.2

	HMDB0047801	TG(14:1(9Z)/18/18:2(9Z,12Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0047956	TG(14:1(9Z)/18:1(9Z)/18:1(11Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0042376	TG(14/18:1(9Z)/18:2(9Z,12Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0043308	TG(15/:3(5Z,8Z,11Z)/15)	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0043482	TG(15/:3n6/15)	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0044277	TG(16/18:3(6Z,9Z,12Z)/16)	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0044473	TG(16/18:3(9Z,12Z,15Z)/16)	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0036342	15-Oleoylsolamin	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0042291	TG(14/14:1(9Z)/22:2(13Z,16Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0042139	TG(14/16/:3n6)	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0042174	TG(14/18/18:3(9Z,12Z,15Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0042167	TG(14/18/18:3(6Z,9Z,12Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0042133	TG(14/16/:3(5Z,8Z,11Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0010449	TG(18:1(9Z)/14/18:2(9Z,12Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0048422	TG(16:1(9Z)/14/:2n6)	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0044688	TG(18/14/18:3(9Z,12Z,15Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0048464	TG(16:1(9Z)/16/18:2(9Z,12Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0044869	TG(18/14:1(9Z)/18:2(9Z,12Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0045077	TG(18/18:2(9Z,12Z)/14:1(9Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0049220	TG(18:1(11Z)/14:1(9Z)/18:1(9Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0048023	TG(14:1(9Z)/22:1(13Z)/14:1(9Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0048611	TG(16:1(9Z)/18:1(11Z)/16:1(9Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0048633	TG(16:1(9Z)/18:1(9Z)/16:1(9Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0049219	TG(18:1(11Z)/14:1(9Z)/18:1(11Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0049841	TG(18:1(9Z)/14:1(9Z)/18:1(9Z))	C53H96O6	M+NH4	846.7545	-1.2
	HMDB0010436	TG(18:1(11Z)/14/18:2(9Z,12Z))	C53H96O6	M+NH4	846.7545	-1.2
848.7690	HMDB0042312	TG(14/16:1(9Z)/:1(11Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0044142	TG(16/:1(11Z)/14:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0044087	TG(16/18:1(11Z)/16:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0044249	TG(16/18:2(9Z,12Z)/16)	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0042166	TG(14/18/18:2(9Z,12Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0043005	TG(15/15/:2n6)	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0044115	TG(16/18:1(9Z)/16:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0005377	TG(16/16:1(9Z)/18:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0042371	TG(14/18:1(9Z)/18:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0042370	TG(14/18:1(9Z)/18:1(11Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0042514	TG(14/18:2(9Z,12Z)/18)	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0043453	TG(15/:2n6/15)	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0047795	TG(14:1(9Z)/18/18:1(11Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0047730	TG(14:1(9Z)/14/22:1(13Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0047774	TG(14:1(9Z)/16/:1(11Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0044864	TG(18/14:1(9Z)/18:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0010430	TG(18/14/18:2(9Z,12Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0010423	TG(16:1(9Z)/16/18:1(11Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0042341	TG(14/18:1(11Z)/18:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0042284	TG(14/14:1(9Z)/22:1(13Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0042340	TG(14/18:1(11Z)/18:1(11Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0062639	1-tetradecanoyl-2,3-dioleoyl-sn-glycerol	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0046433	TG(22/14:1(9Z)/14:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0045663	TG(/14:1(9Z)/16:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0045688	TG(/16:1(9Z)/14:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0005430	TG(16:1(9Z)/16:1(9Z)/18)	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0010435	TG(18:1(11Z)/14/18:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0044915	TG(18/18:1(11Z)/14:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0048459	TG(16:1(9Z)/16/18:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0044942	TG(18/18:1(9Z)/14:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0044863	TG(18/14:1(9Z)/18:1(11Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0048416	TG(16:1(9Z)/14/:1(11Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0005362	TG(16/16/18:2(9Z,12Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0044060	TG(16/16:1(9Z)/18:1(11Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0042458	TG(14/22:1(13Z)/14:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0042138	TG(14/16/:2n6)	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0047817	TG(14:1(9Z)//16:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0042573	TG(14/:2n6/16)	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0047796	TG(14:1(9Z)/18/18:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4

	HMDB0044034	TG(16/14:1(9Z):1(11Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0042399	TG(14/:1(11Z)/16:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0043844	TG(16/14/:2n6)	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0042081	TG(14/14/22:2(13Z,16Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0042661	TG(14/22:2(13Z,16Z)/14)	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0044889	TG(18/16:1(9Z)/16:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0010434	TG(18:1(11Z)/14/18:1(11Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0010448	TG(18:1(9Z)/14/18:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0031121	Glycerol 1,2-dihexadecanoate 3-(9Z,12Z-octadecadienoate)	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0031120	Glycerol 1,2-di-(9Z-octadecenoate) 3-tetradecanoate	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0031122	Glycerol 1,3-dihexadecanoate 2-(9Z,12Z-octadecadienoate)	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0047839	TG(14:1(9Z)/22/14:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
	HMDB0048479	TG(16:1(9Z)/18/16:1(9Z))	C53H98O6	M+NH4	848.7702	-1.4
850.7843	HMDB0042161	TG(14/18/18:1(9Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0010416	TG(16/16/18:1(11Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0043946	TG(16//14:1(9Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0005374	TG(16/16:1(9Z)/18)	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0043919	TG(16/18/16:1(9Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0005360	TG(16/16/18:1(9Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0043838	TG(16/14/:1(11Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0042393	TG(14/:1(11Z)/16)	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0042364	TG(14/18:1(9Z)/18)	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0042189	TG(14//16:1(9Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0044027	TG(16/14:1(9Z)/)	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0046258	TG(22/14/14:1(9Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0045481	TG(/14/16:1(9Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0045532	TG(/16/14:1(9Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0010428	TG(18/14/18:1(11Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0044727	TG(18/16/16:1(9Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0010429	TG(18/14/18:1(9Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0044753	TG(18/18/14:1(9Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0042218	TG(14/22/14:1(9Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0042999	TG(15/15/:1(11Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0030969	Glycerol 1,3-dihexadecanoate 2-(9Z-octadecenoate)	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0031119	Glycerol 1,2-dihexadecanoate 3-(9Z-octadecenoate)	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0042451	TG(14/22:1(13Z)/14)	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0042132	TG(14/16/:1(11Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0042074	TG(14/14/22:1(13Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0042276	TG(14/14:1(9Z)/22)	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0042334	TG(14/18:1(11Z)/18)	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0042160	TG(14/18/18:1(11Z))	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0043279	TG(15/:1(11Z)/15)	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0044081	TG(16/18:1(11Z)/16)	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0044109	TG(16/18:1(9Z)/16)	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0044857	TG(18/14:1(9Z)/18)	C53H100O6	M+NH4	850.7858	-1.8
	HMDB0042305	TG(14/16:1(9Z)/)	C53H100O6	M+NH4	850.7858	-1.8
858.7542	HMDB0043686	TG(15/:4(8Z,11Z,14Z,17Z)/16)	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0043880	TG(16/15/:4(8Z,11Z,14Z,17Z))	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0042692	TG(14/22:4(7Z,Z,13Z,16Z)/15)	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0043874	TG(16/15/:4(5Z,8Z,11Z,14Z))	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0043512	TG(15/:4(5Z,8Z,11Z,14Z)/16)	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0043489	TG(15/:3n6/16:1(9Z))	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0042980	TG(15/14/22:4(7Z,Z,13Z,16Z))	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0043209	TG(15/16:1(9Z)/:3n6)	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0043265	TG(15/18:1(9Z)/18:3(6Z,9Z,12Z))	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0043243	TG(15/18:1(11Z)/18:3(9Z,12Z,15Z))	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0049100	TG(18:1(11Z)/15/18:3(6Z,9Z,12Z))	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0048439	TG(16:1(9Z)/15/:3(5Z,8Z,11Z))	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0049107	TG(18:1(11Z)/15/18:3(9Z,12Z,15Z))	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0044716	TG(18/15/18:4(6Z,9Z,12Z,15Z))	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0043432	TG(15/18:3(6Z,9Z,12Z)/18:1(11Z))	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0043042	TG(15/16/:4(8Z,11Z,14Z,17Z))	C54H96O6	M+NH4	858.7545	-0.4
	HMDB0043658	TG(15/18:4(6Z,9Z,12Z,15Z)/18)	C54H96O6	M+NH4	858.7545	-0.4

HMDB0043635	TG(15/18:3(9Z,12Z,15Z)/18:1(11Z))	C54H96O6	M+NH4	858.7545	-0.4
HMDB0043236	TG(15/18:1(11Z)/18:3(6Z,9Z,12Z))	C54H96O6	M+NH4	858.7545	-0.4
HMDB0043203	TG(15/16:1(9Z)/:3(5Z,8Z,11Z))	C54H96O6	M+NH4	858.7545	-0.4
HMDB0043636	TG(15/18:3(9Z,12Z,15Z)/18:1(9Z))	C54H96O6	M+NH4	858.7545	-0.4
HMDB0011709	TG(15/18:1(9Z)/18:3(9Z,12Z,15Z))	C54H96O6	M+NH4	858.7545	-0.4
HMDB0011702	TG(15/16/:4(5Z,8Z,11Z,14Z))	C54H96O6	M+NH4	858.7545	-0.4
HMDB0011711	TG(15/18:2(9Z,12Z)/18:2(9Z,12Z))	C54H96O6	M+NH4	858.7545	-0.4
HMDB0043070	TG(15/18/18:4(6Z,9Z,12Z,15Z))	C54H96O6	M+NH4	858.7545	-0.4
HMDB0043315	TG(15/:3(5Z,8Z,11Z)/16:1(9Z))	C54H96O6	M+NH4	858.7545	-0.4
HMDB0048445	TG(16:1(9Z)/15/:3n6)	C54H96O6	M+NH4	858.7545	-0.4
HMDB0052411	TG(18:2(9Z,12Z)/15/18:2(9Z,12Z))	C54H96O6	M+NH4	858.7545	-0.4
HMDB0049734	TG(18:1(9Z)/15/18:3(9Z,12Z,15Z))	C54H96O6	M+NH4	858.7545	-0.4
HMDB0042112	TG(14/15/22:4(7Z,Z,13Z,16Z))	C54H96O6	M+NH4	858.7545	-0.4
HMDB0049727	TG(18:1(9Z)/15/18:3(6Z,9Z,12Z))	C54H96O6	M+NH4	858.7545	-0.4
HMDB0043433	TG(15/18:3(6Z,9Z,12Z)/18:1(9Z))	C54H96O6	M+NH4	858.7545	-0.4
HMDB0113220	PE-NMe(18:3(6Z,9Z,12Z)/24:1(15Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113441	PE-NMe(:4(5Z,8Z,11Z,14Z)/22)	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113470	PE-NMe(:4(8Z,11Z,14Z,17Z)/22)	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113525	PE-NMe(22/:4(5Z,8Z,11Z,14Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113526	PE-NMe(22/:4(8Z,11Z,14Z,17Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113550	PE-NMe(22:1(13Z)/:3(5Z,8Z,11Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113551	PE-NMe(22:1(13Z)/:3(8Z,11Z,14Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113604	PE-NMe(22:4(7Z,Z,13Z,16Z)/)	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113712	PE-NMe(24/18:4(6Z,9Z,12Z,15Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113737	PE-NMe(24:1(15Z)/18:3(6Z,9Z,12Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113738	PE-NMe(24:1(15Z)/18:3(9Z,12Z,15Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113359	PE-NMe(:2(11Z,14Z)/22:2(13Z,16Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113577	PE-NMe(22:2(13Z,16Z)/:2(11Z,14Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113387	PE-NMe(:3(5Z,8Z,11Z)/22:1(13Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113302	PE-NMe(/22:4(7Z,Z,13Z,16Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113277	PE-NMe(18:4(6Z,9Z,12Z,15Z)/24)	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113249	PE-NMe(18:3(9Z,12Z,15Z)/24:1(15Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0113415	PE-NMe(:3(8Z,11Z,14Z)/22:1(13Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0008471	PC(:4(8Z,11Z,14Z,17Z)/)	C48H88NO8P	M+Na	860.6140	1.8
HMDB0008536	PC(22/18:4(6Z,9Z,12Z,15Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0008566	PC(22:1(13Z)/18:3(6Z,9Z,12Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0008567	PC(22:1(13Z)/18:3(9Z,12Z,15Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0008598	PC(22:2(13Z,16Z)/18:2(9Z,12Z))	C48H88NO8P	M+Na	860.6140	1.8
HMDB0008438	PC(:4(5Z,8Z,11Z,14Z)/)	C48H88NO8P	M+Na	860.6140	1.8
HMDB0008628	PC(22:4(7Z,Z,13Z,16Z)/18)	C48H88NO8P	M+Na	860.6140	1.8

860.6155	HMDB0008374	PC(:3(5Z,8Z,11Z)/:1(11Z))	C48H88NO8P	M+Na	860.6140	1.8
	HMDB0008342	PC(:2(11Z,14Z)/:2(11Z,14Z))	C48H88NO8P	M+Na	860.6140	1.8
	HMDB0008310	PC(:1(11Z)/:3(5Z,8Z,11Z))	C48H88NO8P	M+Na	860.6140	1.8
	HMDB0008311	PC(:1(11Z)/:3(8Z,11Z,14Z))	C48H88NO8P	M+Na	860.6140	1.8
	HMDB0008280	PC(/:4(8Z,11Z,14Z,17Z))	C48H88NO8P	M+Na	860.6140	1.8
	HMDB0008279	PC(/:4(5Z,8Z,11Z,14Z))	C48H88NO8P	M+Na	860.6140	1.8
	HMDB0008249	PC(18:4(6Z,9Z,12Z,15Z)/22)	C48H88NO8P	M+Na	860.6140	1.8
	HMDB0008217	PC(18:3(9Z,12Z,15Z)/22:1(13Z))	C48H88NO8P	M+Na	860.6140	1.8
	HMDB0008184	PC(18:3(6Z,9Z,12Z)/22:1(13Z))	C48H88NO8P	M+Na	860.6140	1.8
	HMDB0008152	PC(18:2(9Z,12Z)/22:2(13Z,16Z))	C48H88NO8P	M+Na	860.6140	1.8
	HMDB0011201	PC(:3(8Z,11Z,14Z)/:1(11Z))	C48H88NO8P	M+Na	860.6140	1.8
	HMDB0008054	PC(18/22:4(7Z,Z,13Z,16Z))	C48H88NO8P	M+Na	860.6140	1.8
	HMDB0008609	PC(22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0008638	PC(22:4(7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0008639	PC(22:4(7Z,Z,13Z,16Z)/:3(8Z,11Z,14Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0008670	PC(22:5(4Z,7Z,Z,13Z,16Z)/:2(11Z,14Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0008703	PC(22:5(7Z,Z,13Z,16Z,19Z)/:2(11Z,14Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0008735	PC(22:6(4Z,7Z,Z,13Z,16Z,19Z)/:1(11Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0008514	PC(:5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0008352	PC(:2(11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0008384	PC(:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0008416	PC(:3(8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0008321	PC(:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0008353	PC(:2(11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0113693	PE-NMe(22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:1(13Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0113667	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/22:2(13Z,16Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0113588	PE-NMe(22:2(13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0113639	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/22:2(13Z,16Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0116731	PE-NMe(22:1(13Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0113587	PE-NMe(22:2(13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C50H86NO8P	M+H	860.6164	-1.0
	HMDB0043029	TG(15/16/:3(5Z,8Z,11Z))	C54H98O6	M+NH4	860.7702	-0.9
	HMDB0043426	TG(15/18:3(6Z,9Z,12Z)/18)	C54H98O6	M+NH4	860.7702	-0.9
	HMDB0011701	TG(15/16/:3(8Z,11Z,14Z))	C54H98O6	M+NH4	860.7702	-0.9
	HMDB0043035	TG(15/16/:3(8Z,11Z,14Z))	C54H98O6	M+NH4	860.7702	-0.9
	HMDB0043062	TG(15/18/18:3(6Z,9Z,12Z))	C54H98O6	M+NH4	860.7702	-0.9

860.7694

HMDB0043546	TG(15/22:2(13Z,16Z)/14:1(9Z))	C54H98O6	M+NH4	860.7702	-0.9
HMDB0043403	TG(15/18:2(9Z,12Z)/18:1(11Z))	C54H98O6	M+NH4	860.7702	-0.9
HMDB0011704	TG(15/18/18:3(9Z,12Z,15Z))	C54H98O6	M+NH4	860.7702	-0.9
HMDB0043460	TG(15/:2n6/16:1(9Z))	C54H98O6	M+NH4	860.7702	-0.9
HMDB0044708	TG(18/15/18:3(6Z,9Z,12Z))	C54H98O6	M+NH4	860.7702	-0.9
HMDB0044715	TG(18/15/18:3(9Z,12Z,15Z))	C54H98O6	M+NH4	860.7702	-0.9
HMDB0048444	TG(16:1(9Z)/15/:2n6)	C54H98O6	M+NH4	860.7702	-0.9
HMDB0043208	TG(15/16:1(9Z)/:2n6)	C54H98O6	M+NH4	860.7702	-0.9
HMDB0043483	TG(15/:3n6/16)	C54H98O6	M+NH4	860.7702	-0.9
HMDB0043235	TG(15/18:1(11Z)/18:2(9Z,12Z))	C54H98O6	M+NH4	860.7702	-0.9
HMDB0043182	TG(15/14:1(9Z)/22:2(13Z,16Z))	C54H98O6	M+NH4	860.7702	-0.9
HMDB0043629	TG(15/18:3(9Z,12Z,15Z)/18)	C54H98O6	M+NH4	860.7702	-0.9
HMDB0043867	TG(16/15/:3(5Z,8Z,11Z))	C54H98O6	M+NH4	860.7702	-0.9
HMDB0011708	TG(15/18:1(9Z)/18:2(9Z,12Z))	C54H98O6	M+NH4	860.7702	-0.9
HMDB0043309	TG(15/:3(5Z,8Z,11Z)/16)	C54H98O6	M+NH4	860.7702	-0.9
HMDB0043404	TG(15/18:2(9Z,12Z)/18:1(9Z))	C54H98O6	M+NH4	860.7702	-0.9
HMDB0047760	TG(14:1(9Z)/15/22:2(13Z,16Z))	C54H98O6	M+NH4	860.7702	-0.9
HMDB0049099	TG(18:1(11Z)/15/18:2(9Z,12Z))	C54H98O6	M+NH4	860.7702	-0.9
HMDB0049726	TG(18:1(9Z)/15/18:2(9Z,12Z))	C54H98O6	M+NH4	860.7702	-0.9
HMDB0043873	TG(16/15/:3n6)	C54H98O6	M+NH4	860.7702	-0.9
HMDB0113736	PE-NMe(24:1(15Z)/18:2(9Z,12Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0113386	PE-NMe(:3(5Z,8Z,11Z)/22)	C48H90NO8P	M+Na	862.6296	2.9
HMDB0113414	PE-NMe(:3(8Z,11Z,14Z)/22)	C48H90NO8P	M+Na	862.6296	2.9
HMDB0113524	PE-NMe(22/:3(8Z,11Z,14Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0113523	PE-NMe(22/:3(5Z,8Z,11Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0113576	PE-NMe(22:2(13Z,16Z)/:1(11Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0113710	PE-NMe(24/18:3(6Z,9Z,12Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0113711	PE-NMe(24/18:3(9Z,12Z,15Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0113358	PE-NMe(:2(11Z,14Z)/22:1(13Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0113549	PE-NMe(22:1(13Z)/:2(11Z,14Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0113248	PE-NMe(18:3(9Z,12Z,15Z)/24)	C48H90NO8P	M+Na	862.6296	2.9
HMDB0113219	PE-NMe(18:3(6Z,9Z,12Z)/24)	C48H90NO8P	M+Na	862.6296	2.9
HMDB0113192	PE-NMe(18:2(9Z,12Z)/24:1(15Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0113330	PE-NMe(:1(11Z)/22:2(13Z,16Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0008086	PC(18:1(11Z)/22:2(13Z,16Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0008597	PC(22:2(13Z,16Z)/18:1(9Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0008596	PC(22:2(13Z,16Z)/18:1(11Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0008565	PC(22:1(13Z)/18:2(9Z,12Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0008535	PC(22/18:3(9Z,12Z,15Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0008534	PC(22/18:3(6Z,9Z,12Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0008406	PC(:3(8Z,11Z,14Z)/)	C48H90NO8P	M+Na	862.6296	2.9
HMDB0008373	PC(:3(5Z,8Z,11Z)/)	C48H90NO8P	M+Na	862.6296	2.9

862.6321

HMDB0008341	PC(:2(11Z,14Z)/:1(11Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0008309	PC(:1(11Z)/:2(11Z,14Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0008278	PC(/:3(8Z,11Z,14Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0008277	PC(/:3(5Z,8Z,11Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0008216	PC(18:3(9Z,12Z,15Z)/22)	C48H90NO8P	M+Na	862.6296	2.9
HMDB0008183	PC(18:3(6Z,9Z,12Z)/22)	C48H90NO8P	M+Na	862.6296	2.9
HMDB0008151	PC(18:2(9Z,12Z)/22:1(13Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0008119	PC(18:1(9Z)/22:2(13Z,16Z))	C48H90NO8P	M+Na	862.6296	2.9
HMDB0113586	PE-NMe(22:2(13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0113559	PE-NMe(22:1(13Z)/22:5(4Z,7Z,Z,13Z,16Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0116730	PE-NMe(22/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0113507	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/24:1(15Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0113560	PE-NMe(22:1(13Z)/22:5(7Z,Z,13Z,16Z,19Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0113638	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/22:1(13Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0113666	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/22:1(13Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0113614	PE-NMe(22:4(7Z,Z,13Z,16Z)/22:2(13Z,16Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0113747	PE-NMe(24:1(15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0113692	PE-NMe(22:6(4Z,7Z,Z,13Z,16Z,19Z)/22)	C50H88NO8P	M+H	862.6320	0.1
HMDB0008288	PC(/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0008576	PC(22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0008481	PC(:4(8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0008607	PC(22:2(13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0008637	PC(22:4(7Z,Z,13Z,16Z)/:2(11Z,14Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0008669	PC(22:5(4Z,7Z,Z,13Z,16Z)/:1(11Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0008702	PC(22:5(7Z,Z,13Z,16Z,19Z)/:1(11Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0008734	PC(22:6(4Z,7Z,Z,13Z,16Z,19Z)/)	C50H88NO8P	M+H	862.6320	0.1
HMDB0008448	PC(:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0008351	PC(:2(11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0008319	PC(:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0008320	PC(:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0008608	PC(22:2(13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0008513	PC(:5(5Z,8Z,11Z,14Z,17Z)/22:1(13Z))	C50H88NO8P	M+H	862.6320	0.1
HMDB0043202	TG(15/16:1(9Z)/:1(11Z))	C54H100O6	M+NH4	862.7858	-0.6

862.7853

HMDB0043397	TG(15/18:2(9Z,12Z)/18)	C54H100O6	M+NH4	862.7858	-0.6
HMDB0042662	TG(14/22:2(13Z,16Z)/15)	C54H100O6	M+NH4	862.7858	-0.6
HMDB0043258	TG(15/18:1(9Z)/18:1(11Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0042979	TG(15/14/22:2(13Z,16Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0043454	TG(15/:2n6/16)	C54H100O6	M+NH4	862.7858	-0.6
HMDB0043286	TG(15/:1(11Z)/16:1(9Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0011703	TG(15/18/18:2(9Z,12Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0049094	TG(18:1(11Z)/15/18:1(9Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0048438	TG(16:1(9Z)/15/:1(11Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0043343	TG(15/22:1(13Z)/14:1(9Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0011700	TG(15/16/:2(11Z,14Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0043034	TG(15/16/:2(11Z,14Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0047753	TG(14:1(9Z)/15/22:1(13Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0043230	TG(15/18:1(11Z)/18:1(9Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0011707	TG(15/18:1(9Z)/18:1(9Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0043229	TG(15/18:1(11Z)/18:1(11Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0043175	TG(15/14:1(9Z)/22:1(13Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0044707	TG(18/15/18:2(9Z,12Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0042111	TG(14/15/22:2(13Z,16Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0049093	TG(18:1(11Z)/15/18:1(11Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0049721	TG(18:1(9Z)/15/18:1(9Z))	C54H100O6	M+NH4	862.7858	-0.6
HMDB0043872	TG(16/15/:2n6)	C54H100O6	M+NH4	862.7858	-0.6
HMDB0113191	PE-NMe(18:2(9Z,12Z)/24)	C48H92NO8P	M+Na	864.6453	2.3
HMDB0113709	PE-NMe(24/18:2(9Z,12Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0113301	PE-NMe(/22:2(13Z,16Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0113329	PE-NMe(:1(11Z)/22:1(13Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0113735	PE-NMe(24:1(15Z)/18:1(9Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0113548	PE-NMe(22:1(13Z)/:1(11Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0113575	PE-NMe(22:2(13Z,16Z)/)	C48H92NO8P	M+Na	864.6453	2.3
HMDB0113734	PE-NMe(24:1(15Z)/18:1(11Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0113136	PE-NMe(18:1(11Z)/24:1(15Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0113522	PE-NMe(22/:2(11Z,14Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0113357	PE-NMe(:2(11Z,14Z)/22)	C48H92NO8P	M+Na	864.6453	2.3
HMDB0113163	PE-NMe(18:1(9Z)/24:1(15Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0011202	PC(22:1(13Z)/18:1(11Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0008792	PC(24:1(15Z)/16:1(9Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0008595	PC(22:2(13Z,16Z)/18)	C48H92NO8P	M+Na	864.6453	2.3
HMDB0008564	PC(22:1(13Z)/18:1(9Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0008533	PC(22/18:2(9Z,12Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0008340	PC(:2(11Z,14Z)/)	C48H92NO8P	M+Na	864.6453	2.3
HMDB0008308	PC(:1(11Z)/:1(11Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0008276	PC(/:2(11Z,14Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0008150	PC(18:2(9Z,12Z)/22)	C48H92NO8P	M+Na	864.6453	2.3

864.6473

HMDB0008118	PC(18:1(9Z)/22:1(13Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0008085	PC(18:1(11Z)/22:1(13Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0008026	PC(16:1(9Z)/24:1(15Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0008053	PC(18/22:2(13Z,16Z))	C48H92NO8P	M+Na	864.6453	2.3
HMDB0008799	PC(24:1(15Z)/18:4(6Z,9Z,12Z,15Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008701	PC(22:5(7Z,Z,13Z,16Z,19Z)/)	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008668	PC(22:5(4Z,7Z,Z,13Z,16Z)/)	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008636	PC(22:4(7Z,Z,13Z,16Z)/:1(11Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008606	PC(22:2(13Z,16Z)/:3(8Z,11Z,14Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008605	PC(22:2(13Z,16Z)/:3(5Z,8Z,11Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008544	PC(22/:5(5Z,8Z,11Z,14Z,17Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008447	PC(:4(5Z,8Z,11Z,14Z)/22:1(13Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008383	PC(:3(5Z,8Z,11Z)/22:2(13Z,16Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008257	PC(18:4(6Z,9Z,12Z,15Z)/24:1(15Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008480	PC(:4(8Z,11Z,14Z,17Z)/22:1(13Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008512	PC(:5(5Z,8Z,11Z,14Z,17Z)/22)	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008415	PC(:3(8Z,11Z,14Z)/22:2(13Z,16Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008287	PC(/22:5(7Z,Z,13Z,16Z,19Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008318	PC(:1(11Z)/22:4(7Z,Z,13Z,16Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008286	PC(/22:5(4Z,7Z,Z,13Z,16Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008574	PC(22:1(13Z)/:4(5Z,8Z,11Z,14Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0008575	PC(22:1(13Z)/:4(8Z,11Z,14Z,17Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0113478	PE-NMe(:4(8Z,11Z,14Z,17Z)/24:1(15Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0113746	PE-NMe(24:1(15Z)/:4(8Z,11Z,14Z,17Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0113745	PE-NMe(24:1(15Z)/:4(5Z,8Z,11Z,14Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0113720	PE-NMe(24/:5(5Z,8Z,11Z,14Z,17Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0113665	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/22)	C50H90NO8P	M+H	864.6477	-0.4
HMDB0113613	PE-NMe(22:4(7Z,Z,13Z,16Z)/22:1(13Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0113558	PE-NMe(22:1(13Z)/22:4(7Z,Z,13Z,16Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0113532	PE-NMe(22/22:5(7Z,Z,13Z,16Z,19Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0116729	PE-NMe(22/22:5(4Z,7Z,Z,13Z,16Z))	C50H90NO8P	M+H	864.6477	-0.4
HMDB0113506	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/24)	C50H90NO8P	M+H	864.6477	-0.4

	HMDB0113449	PE-NMe(:4(5Z,8Z,11Z,14Z)/24:1(15Z))	C50H90NO8P	M+H	864.6477	-0.4
	HMDB0116735	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/22)	C50H90NO8P	M+H	864.6477	-0.4
864.7086	HMDB0054017	TG(:4(5Z,8Z,11Z,14Z)/14/18:4(6Z,9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048949	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048956	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048935	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048587	TG(16:1(9Z)/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048781	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048155	TG(14:1(9Z)/:3n6/18:4(6Z,9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048017	TG(14:1(9Z)/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0044523	TG(16/18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0055199	TG(18:3(9Z,12Z,15Z)/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0052965	TG(18:3(6Z,9Z,12Z)/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0052952	TG(18:3(6Z,9Z,12Z)/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0053743	TG(:3n6/14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0051007	TG(:3(5Z,8Z,11Z)/14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0055358	TG(18:4(6Z,9Z,12Z,15Z)/14:4(8Z,11Z,14Z,17Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0052512	TG(18:2(9Z,12Z)/14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0052946	TG(18:3(6Z,9Z,12Z)/14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0052855	TG(18:3(6Z,9Z,12Z)/14/:5(5Z,8Z,11Z,14Z,17Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0055151	TG(18:3(9Z,12Z,15Z)/14/:5(5Z,8Z,11Z,14Z,17Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0055205	TG(18:3(9Z,12Z,15Z)/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048110	TG(14:1(9Z)/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048315	TG(14:1(9Z)/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0042864	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048281	TG(14:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0042800	TG(14/18:4(6Z,9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0042835	TG(14/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048088	TG(14:1(9Z)/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048330	TG(14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048265	TG(14:1(9Z)/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048369	TG(14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048287	TG(14:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:3n6)	C55H90O6	M+NH4	864.7076	1.2
	HMDB0042777	TG(14/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0042567	TG(14/18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048177	TG(14:1(9Z)/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0042655	TG(14/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048170	TG(14:1(9Z)/:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0047929	TG(14:1(9Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0042806	TG(14/18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048271	TG(14:1(9Z)/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048104	TG(14:1(9Z)/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0042857	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0048308	TG(14:1(9Z)/:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0055369	TG(18:4(6Z,9Z,12Z,15Z)/16/18:4(6Z,9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0054093	TG(:4(5Z,8Z,11Z,14Z)/14:1(9Z)/18:3(9Z,12Z,15Z))	C55H90O6	M+NH4	864.7076	1.2
	HMDB0051006	TG(:3(5Z,8Z,11Z)/14:1(9Z)/18:3(9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0048581	TG(16:1(9Z)/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0048433	TG(16:1(9Z)/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0048948	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0048934	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0048607	TG(16:1(9Z)/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0048586	TG(16:1(9Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0044618	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/14:1(9Z))	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0042537	TG(14/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0048009	TG(14:1(9Z)/:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0042776	TG(14/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0042647	TG(14/:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0048016	TG(14:1(9Z)/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0048324	TG(14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0042799	TG(14/18:4(6Z,9Z,12Z,15Z)/:3n6)	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0047973	TG(14:1(9Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C55H92O6	M+NH4	866.7232	-0.6
	HMDB0048927	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C55H92O6	M+NH4	866.7232	-0.6

866.7227

HMDB0048780	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048759	TG(16:1(9Z)/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0050999	TG(:3(5Z,8Z,11Z)/14:1(9Z)/18:3(6Z,9Z,12Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0049857	TG(18:1(9Z)/14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0052407	TG(18:2(9Z,12Z)/14/:5(5Z,8Z,11Z,14Z,17Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0052881	TG(18:3(6Z,9Z,12Z)/16/18:4(6Z,9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0052945	TG(18:3(6Z,9Z,12Z)/14:1(9Z)/:3n6)	C55H92O6	M+NH4	866.7232	-0.6
HMDB0052505	TG(18:2(9Z,12Z)/14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0055150	TG(18:3(9Z,12Z,15Z)/14/:4(8Z,11Z,14Z,17Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0052511	TG(18:2(9Z,12Z)/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0052964	TG(18:3(6Z,9Z,12Z)/16:1(9Z)/18:3(9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0055163	TG(18:3(9Z,12Z,15Z)/16/18:4(6Z,9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0052848	TG(18:3(6Z,9Z,12Z)/14/:4(5Z,8Z,11Z,14Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0052854	TG(18:3(6Z,9Z,12Z)/14/:4(8Z,11Z,14Z,17Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0052525	TG(18:2(9Z,12Z)/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0049236	TG(18:1(11Z)/14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048773	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0044495	TG(16/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0044299	TG(16/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0047950	TG(14:1(9Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0042834	TG(14/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048147	TG(14:1(9Z)/:3n6/18:3(6Z,9Z,12Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0042566	TG(14/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048097	TG(14:1(9Z)/18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048087	TG(14:1(9Z)/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0042827	TG(14/:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0044515	TG(16/18:4(6Z,9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048258	TG(14:1(9Z)/18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0042445	TG(14/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048081	TG(14:1(9Z)/18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0042654	TG(14/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048103	TG(14:1(9Z)/18:3(6Z,9Z,12Z)/:3n6)	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048132	TG(14:1(9Z)/:2n6/18:4(6Z,9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0047928	TG(14:1(9Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048231	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048264	TG(14:1(9Z)/18:3(9Z,12Z,15Z)/:3n6)	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048286	TG(14:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:2n6)	C55H92O6	M+NH4	866.7232	-0.6
HMDB0044522	TG(16/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0042793	TG(14/18:4(6Z,9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048325	TG(14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0042856	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0042560	TG(14/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0047791	TG(14:1(9Z)/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0044051	TG(16/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0042770	TG(14/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048169	TG(14:1(9Z)/:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0042909	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048346	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0042625	TG(14/:3n6/18:4(6Z,9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0047923	TG(14:1(9Z)/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048307	TG(14:1(9Z)/:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048154	TG(14:1(9Z)/:3n6/18:3(9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0053742	TG(:3n6/14:1(9Z)/18:3(9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0052957	TG(18:3(6Z,9Z,12Z)/16:1(9Z)/18:3(6Z,9Z,12Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0055204	TG(18:3(9Z,12Z,15Z)/16:1(9Z)/18:3(9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0042329	TG(14/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0010517	TG(:4(5Z,8Z,11Z,14Z)/14/18:3(9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0053659	TG(:3n6/14/18:4(6Z,9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0050881	TG(:3(5Z,8Z,11Z)/14/18:4(6Z,9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0048985	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/16:1(9Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0053362	TG(:2n6/14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C55H92O6	M+NH4	866.7232	-0.6
HMDB0042536	TG(14/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0044450	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/14:1(9Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048772	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048758	TG(16:1(9Z)/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2

HMDB0048475	TG(16:1(9Z)/16:5(5Z,8Z,11Z,14Z,17Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0044880	TG(18/14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0044590	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/14:1(9Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048942	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0049235	TG(18:1(11Z)/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0049255	TG(18:1(11Z)/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0005436	TG(16:1(9Z)/16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042553	TG(14/18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042646	TG(14/:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042530	TG(14/18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048131	TG(14:1(9Z)/:2n6/18:3(9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042851	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0047922	TG(14:1(9Z)/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042729	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0044271	TG(16/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042444	TG(14/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042826	TG(14/:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0044514	TG(16/18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048163	TG(14:1(9Z)/:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042903	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/16)	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048649	TG(16:1(9Z)/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0049229	TG(18:1(11Z)/14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0049875	TG(18:1(9Z)/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0052847	TG(18:3(6Z,9Z,12Z)/14/:3n6)	C55H94O6	M+NH4	868.7389	-1.2
HMDB0052880	TG(18:3(6Z,9Z,12Z)/16/18:3(9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0049856	TG(18:1(9Z)/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0052517	TG(18:2(9Z,12Z)/16:1(9Z)/18:3(6Z,9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0052435	TG(18:2(9Z,12Z)/16/18:4(6Z,9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0049717	TG(18:1(9Z)/14/:5(5Z,8Z,11Z,14Z,17Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0010472	TG(18:2(9Z,12Z)/14/:4(5Z,8Z,11Z,14Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0052524	TG(18:2(9Z,12Z)/16:1(9Z)/18:3(9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0052406	TG(18:2(9Z,12Z)/14/:4(8Z,11Z,14Z,17Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0052944	TG(18:3(6Z,9Z,12Z)/14:1(9Z)/:2n6)	C55H94O6	M+NH4	868.7389	-1.2
HMDB0052504	TG(18:2(9Z,12Z)/14:1(9Z)/:3n6)	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048427	TG(16:1(9Z)/14/22:5(4Z,7Z,Z,13Z,16Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048943	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0045374	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/14:1(9Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048606	TG(16:1(9Z)/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0049089	TG(18:1(11Z)/14/:5(5Z,8Z,11Z,14Z,17Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048580	TG(16:1(9Z)/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048627	TG(16:1(9Z)/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0044563	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/16:1(9Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048926	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048751	TG(16:1(9Z)/18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048432	TG(16:1(9Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0049850	TG(18:1(9Z)/14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0044298	TG(16/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048280	TG(14:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048080	TG(14:1(9Z)/18:2(9Z,12Z)/:3n6)	C55H94O6	M+NH4	868.7389	-1.2
HMDB0044494	TG(16/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042769	TG(14/18:3(9Z,12Z,15Z)/:3n6)	C55H94O6	M+NH4	868.7389	-1.2
HMDB0047943	TG(14:1(9Z)/18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0044487	TG(16/18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048302	TG(14:1(9Z)/:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042850	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0043855	TG(16/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042624	TG(14/:3n6/18:3(9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0047790	TG(14:1(9Z)/16/22:5(7Z,Z,13Z,16Z,19Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048008	TG(14:1(9Z)/:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042437	TG(14/:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048146	TG(14:1(9Z)/:3n6/18:2(9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0043016	TG(15/15/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048102	TG(14:1(9Z)/18:3(6Z,9Z,12Z)/:2n6)	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042763	TG(14/18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0047972	TG(14:1(9Z)/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C55H94O6	M+NH4	868.7389	-1.2

HMDB0044291	TG(16/18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042559	TG(14/18:3(6Z,9Z,12Z)/:3n6)	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048124	TG(14:1(9Z)/:2n6/18:3(6Z,9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0044050	TG(16/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048208	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042617	TG(14/:3n6/18:3(6Z,9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048074	TG(14:1(9Z)/18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048164	TG(14:1(9Z)/:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042798	TG(14/18:4(6Z,9Z,12Z,15Z)/:2n6)	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042387	TG(14/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0047966	TG(14:1(9Z)/18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042879	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0044077	TG(16/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0047949	TG(14:1(9Z)/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042595	TG(14/:2n6/18:4(6Z,9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0047785	TG(14:1(9Z)/16/22:5(4Z,7Z,Z,13Z,16Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0044045	TG(16/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0047812	TG(14:1(9Z)/18/:5(5Z,8Z,11Z,14Z,17Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048301	TG(14:1(9Z)/:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048263	TG(14:1(9Z)/18:3(9Z,12Z,15Z)/:2n6)	C55H94O6	M+NH4	868.7389	-1.2
HMDB0047994	TG(14:1(9Z)/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0043772	TG(15/22:6(4Z,7Z,Z,13Z,16Z,19Z)/15)	C55H94O6	M+NH4	868.7389	-1.2
HMDB0010499	TG(18:3(9Z,12Z,15Z)/16/18:3(9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0050446	TG(:1(11Z)/14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0052873	TG(18:3(6Z,9Z,12Z)/16/18:3(6Z,9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0050998	TG(:3(5Z,8Z,11Z)/14:1(9Z)/18:2(9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0050873	TG(:3(5Z,8Z,11Z)/14/18:3(6Z,9Z,12Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0053361	TG(:2n6/14:1(9Z)/18:3(9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0050880	TG(:3(5Z,8Z,11Z)/14/18:3(9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0053271	TG(:2n6/14/18:4(6Z,9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0053658	TG(:3n6/14/18:3(9Z,12Z,15Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042328	TG(14/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042149	TG(14/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042357	TG(14/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0042323	TG(14/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048963	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0048831	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C55H94O6	M+NH4	868.7389	-1.2
HMDB0044103	TG(16/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042792	TG(14/18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042699	TG(14/22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042529	TG(14/18:2(9Z,12Z)/:3n6)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042558	TG(14/18:3(6Z,9Z,12Z)/:2n6)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042723	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/16)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044263	TG(16/18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044486	TG(16/18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042844	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/18)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042640	TG(14/:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042820	TG(14/:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042873	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/16)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042616	TG(14/:3n6/18:2(9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0047959	TG(14:1(9Z)/18:1(9Z)/:3(5Z,8Z,11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0043854	TG(16/14/22:5(7Z,Z,13Z,16Z,19Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0043010	TG(15/15/22:5(4Z,7Z,Z,13Z,16Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044367	TG(16/:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048079	TG(14:1(9Z)/18:2(9Z,12Z)/:2n6)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042523	TG(14/18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048002	TG(14:1(9Z)/:3(5Z,8Z,11Z)/18:1(11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0043849	TG(16/14/22:5(4Z,7Z,Z,13Z,16Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0047965	TG(14:1(9Z)/18:1(9Z)/:3n6)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042594	TG(14/:2n6/18:3(9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048140	TG(14:1(9Z)/:3n6/18:1(11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0043015	TG(15/15/22:5(7Z,Z,13Z,16Z,19Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044535	TG(16/:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0047936	TG(14:1(9Z)/18:1(11Z)/:3(5Z,8Z,11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0047942	TG(14:1(9Z)/18:1(11Z)/:3n6)	C55H96O6	M+NH4	870.7545	-1.2

HMDB0044270	TG(16/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048096	TG(14:1(9Z)/18:3(6Z,9Z,12Z)/:1(11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042641	TG(14/:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048003	TG(14:1(9Z)/:3(5Z,8Z,11Z)/18:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0047993	TG(14:1(9Z)/:1(11Z)/18:3(9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044290	TG(16/18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0047811	TG(14:1(9Z)/18/:4(8Z,11Z,14Z,17Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048495	TG(16:1(9Z)/18/18:4(6Z,9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044873	TG(18/14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048626	TG(16:1(9Z)/18:1(11Z)/18:3(9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048920	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/18:1(11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0045185	TG(18/:4(5Z,8Z,11Z,14Z)/14:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0005446	TG(16:1(9Z)/18:2(9Z,12Z)/18:2(9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0049129	TG(18:1(11Z)/16/18:4(6Z,9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048921	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/18:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0049082	TG(18:1(11Z)/14/:4(5Z,8Z,11Z,14Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048619	TG(16:1(9Z)/18:1(11Z)/18:3(6Z,9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048593	TG(16:1(9Z)/16:1(9Z)/:3(5Z,8Z,11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044879	TG(18/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0052516	TG(18:2(9Z,12Z)/16:1(9Z)/18:2(9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0049867	TG(18:1(9Z)/16:1(9Z)/18:3(6Z,9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0049716	TG(18:1(9Z)/14/:4(8Z,11Z,14Z,17Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0049843	TG(18:1(9Z)/14:1(9Z)/:3(5Z,8Z,11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0049849	TG(18:1(9Z)/14:1(9Z)/:3n6)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048474	TG(16:1(9Z)/16/:4(8Z,11Z,14Z,17Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048648	TG(16:1(9Z)/18:1(9Z)/18:3(9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0049228	TG(18:1(11Z)/14:1(9Z)/:3n6)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0045347	TG(18/:4(8Z,11Z,14Z,17Z)/14:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044905	TG(18/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048766	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/18:1(11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048767	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/18:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048641	TG(16:1(9Z)/18:1(9Z)/18:3(6Z,9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044691	TG(18/14/:5(5Z,8Z,11Z,14Z,17Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048599	TG(16:1(9Z)/16:1(9Z)/:3n6)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0045321	TG(18/18:4(6Z,9Z,12Z,15Z)/16:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0049222	TG(18:1(11Z)/14:1(9Z)/:3(5Z,8Z,11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0049088	TG(18:1(11Z)/14/:4(8Z,11Z,14Z,17Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048468	TG(16:1(9Z)/16/:4(5Z,8Z,11Z,14Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048426	TG(16:1(9Z)/14/22:4(7Z,Z,13Z,16Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0049254	TG(18:1(11Z)/16:1(9Z)/18:3(9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044422	TG(16/22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0049247	TG(18:1(11Z)/16:1(9Z)/18:3(6Z,9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0049874	TG(18:1(9Z)/16:1(9Z)/18:3(9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042380	TG(14/18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0043909	TG(16/16/:5(5Z,8Z,11Z,14Z,17Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0047784	TG(14:1(9Z)/16/22:4(7Z,Z,13Z,16Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042436	TG(14/:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044508	TG(16/18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048141	TG(14:1(9Z)/:3n6/18:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048257	TG(14:1(9Z)/18:3(9Z,12Z,15Z)/:1(11Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0047833	TG(14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048123	TG(14:1(9Z)/:2n6/18:2(9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0047986	TG(14:1(9Z)/:1(11Z)/18:3(6Z,9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044131	TG(16/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044076	TG(16/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042415	TG(14/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0047805	TG(14:1(9Z)/18/:4(5Z,8Z,11Z,14Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0005380	TG(16/16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042821	TG(14/:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042587	TG(14/:2n6/18:3(6Z,9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044509	TG(16/18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044044	TG(16/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042768	TG(14/18:3(9Z,12Z,15Z)/:2n6)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042386	TG(14/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044557	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/16)	C55H96O6	M+NH4	870.7545	-1.2

HMDB0043743	TG(15/22:5(7Z,Z,13Z,16Z,19Z)/15)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0043598	TG(15/22:5(4Z,7Z,Z,13Z,16Z)/15)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0010473	TG(18:2(9Z,12Z)/16/18:3(9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042322	TG(14/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042148	TG(14/16/22:5(7Z,Z,13Z,16Z,19Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042356	TG(14/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042143	TG(14/16/22:5(4Z,7Z,Z,13Z,16Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0052427	TG(18:2(9Z,12Z)/16/18:3(6Z,9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0052503	TG(18:2(9Z,12Z)/14:1(9Z)/:2n6)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0052846	TG(18:3(6Z,9Z,12Z)/14/:2n6)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0052399	TG(18:2(9Z,12Z)/14/:3n6)	C55H96O6	M+NH4	870.7545	-1.2
HMDB0049755	TG(18:1(9Z)/16/18:4(6Z,9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0010450	TG(18:1(9Z)/14/:4(5Z,8Z,11Z,14Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0045679	TG(/14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0050438	TG(:1(11Z)/14:1(9Z)/18:3(6Z,9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0050313	TG(:1(11Z)/14/18:4(6Z,9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0046104	TG(/18:4(6Z,9Z,12Z,15Z)/14:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0050445	TG(:1(11Z)/14:1(9Z)/18:3(9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0050872	TG(:3(5Z,8Z,11Z)/14/18:2(9Z,12Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0053270	TG(:2n6/14/18:3(9Z,12Z,15Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042177	TG(14/18/:5(5Z,8Z,11Z,14Z,17Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0042350	TG(14/18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048677	TG(16:1(9Z)/:3(5Z,8Z,11Z)/16:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0048809	TG(16:1(9Z)/:3n6/16:1(9Z))	C55H96O6	M+NH4	870.7545	-1.2
HMDB0044285	TG(16/18:3(6Z,9Z,12Z)/18:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044063	TG(16/16:1(9Z)/:3(5Z,8Z,11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042814	TG(14/:4(8Z,11Z,14Z,17Z)/18)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044171	TG(16/:3(5Z,8Z,11Z)/16:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044339	TG(16/:3n6/16:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044130	TG(16/18:1(9Z)/18:3(9Z,12Z,15Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044480	TG(16/18:3(9Z,12Z,15Z)/18:1(11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0048185	TG(14:1(9Z)/22:2(13Z,16Z)/16:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0047921	TG(14:1(9Z)/16:1(9Z)/22:2(13Z,16Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0043009	TG(15/15/22:4(7Z,Z,13Z,16Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042552	TG(14/18:3(6Z,9Z,12Z)/:1(11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0047941	TG(14:1(9Z)/18:1(11Z)/:2n6)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044502	TG(16/18:4(6Z,9Z,12Z,15Z)/18)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044123	TG(16/18:1(9Z)/18:3(6Z,9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0047825	TG(14:1(9Z)/18:3(6Z,9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042586	TG(14/:2n6/18:2(9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0048117	TG(14:1(9Z)/:2n6/18:1(11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0043908	TG(16/16/:4(8Z,11Z,14Z,17Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042634	TG(14/:4(5Z,8Z,11Z,14Z)/18)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042762	TG(14/18:3(9Z,12Z,15Z)/:1(11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042379	TG(14/18:1(9Z)/:3n6)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0047985	TG(14:1(9Z)/:1(11Z)/18:2(9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0005363	TG(16/16/:4(5Z,8Z,11Z,14Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042528	TG(14/18:2(9Z,12Z)/:2n6)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0047832	TG(14:1(9Z)/18:3(9Z,12Z,15Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042611	TG(14/:3n6/18:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0043935	TG(16/18/18:4(6Z,9Z,12Z,15Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042407	TG(14/:1(11Z)/18:3(6Z,9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0047964	TG(14:1(9Z)/18:1(9Z)/:2n6)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042431	TG(14/:3(5Z,8Z,11Z)/18:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042373	TG(14/18:1(9Z)/:3(5Z,8Z,11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042693	TG(14/22:4(7Z,Z,13Z,16Z)/16)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042414	TG(14/:1(11Z)/18:3(9Z,12Z,15Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0048467	TG(16:1(9Z)/16/:3n6)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0048787	TG(16:1(9Z)/:2n6/16:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0045158	TG(18/:3n6/14:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044690	TG(18/14/:4(8Z,11Z,14Z,17Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0048487	TG(16:1(9Z)/18/18:3(6Z,9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044897	TG(18/16:1(9Z)/18:3(6Z,9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0049227	TG(18:1(11Z)/14:1(9Z)/:2n6)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0048618	TG(16:1(9Z)/18:1(11Z)/18:2(9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2

HMDB0049081	TG(18:1(11Z)/14:3n6)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044996	TG(18:3(5Z,8Z,11Z)/14:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0049121	TG(18:1(11Z)/16:18:3(6Z,9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0045105	TG(18/18:3(6Z,9Z,12Z)/16:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0010444	TG(18:1(11Z)/16:1(9Z)/18:2(9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0048745	TG(16:1(9Z)/18:2(9Z,12Z)/18:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0048461	TG(16:1(9Z)/16:3(5Z,8Z,11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044743	TG(18/16:18:4(6Z,9Z,12Z,15Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042785	TG(14/18:4(6Z,9Z,12Z,15Z)/)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042205	TG(14//18:4(6Z,9Z,12Z,15Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044284	TG(16/18:3(6Z,9Z,12Z)/18:1(11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0047804	TG(14:1(9Z)/18:3n6)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0005390	TG(16/18:2(9Z,12Z)/18:2(9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044069	TG(16/16:1(9Z):3n6)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042430	TG(14:3(5Z,8Z,11Z)/18:1(11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044102	TG(16/18:1(11Z)/18:3(9Z,12Z,15Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0010440	TG(18:1(11Z)/16/18:3(9Z,12Z,15Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044904	TG(18/16:1(9Z)/18:3(9Z,12Z,15Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0049075	TG(18:1(11Z)/14:3(5Z,8Z,11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0048744	TG(16:1(9Z)/18:2(9Z,12Z)/18:1(11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0005440	TG(16:1(9Z)/18:1(9Z)/18:2(9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0048598	TG(16:1(9Z)/16:1(9Z):2n6)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0048494	TG(16:1(9Z)/18/18:3(9Z,12Z,15Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044095	TG(16/18:1(11Z)/18:3(6Z,9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0048073	TG(14:1(9Z)/18:2(9Z,12Z)/1(11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042610	TG(14:3n6/18:1(11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0048118	TG(14:1(9Z):2n6/18:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0047798	TG(14:1(9Z)/18:3(5Z,8Z,11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044481	TG(16/18:3(9Z,12Z,15Z)/18:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0043848	TG(16/14/22:4(7Z,Z,13Z,16Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0043569	TG(15/22:4(7Z,Z,13Z,16Z)/15)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044529	TG(16:4(8Z,11Z,14Z,17Z)/16)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044361	TG(16:4(5Z,8Z,11Z,14Z)/16)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0031118	Glycerol 1,3-di-(9Z,12Z-octadecadienoate) 2-hexadecanoate	C55H98O6	M+NH4	872.7702	-1.2
HMDB0031117	Glycerol 1,2-di-(9Z,12Z-octadecadienoate) 3-hexadecanoate	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044866	TG(18/14:1(9Z):3(5Z,8Z,11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0050312	TG(:1(11Z)/14/18:3(9Z,12Z,15Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0046078	TG(/18:3(9Z,12Z,15Z)/14:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0045497	TG(/14/18:4(6Z,9Z,12Z,15Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0045678	TG(/14:1(9Z)/18:3(9Z,12Z,15Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042349	TG(14/18:1(11Z):3n6)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042142	TG(14/16/22:4(7Z,Z,13Z,16Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042343	TG(14/18:1(11Z):3(5Z,8Z,11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042176	TG(14/18:4(8Z,11Z,14Z,17Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042170	TG(14/18:4(5Z,8Z,11Z,14Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0050437	TG(:1(11Z)/14:1(9Z)/18:2(9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0045671	TG(/14:1(9Z)/18:3(6Z,9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044872	TG(18/14:1(9Z):3n6)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0048579	TG(16:1(9Z)/14:1(9Z)/22:2(13Z,16Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0045294	TG(18/18:3(9Z,12Z,15Z)/16:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0044684	TG(18/14:4(5Z,8Z,11Z,14Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0049709	TG(18:1(9Z)/14:3n6)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0049703	TG(18:1(9Z)/14:3(5Z,8Z,11Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0049747	TG(18:1(9Z)/16/18:3(6Z,9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0052398	TG(18:2(9Z,12Z)/14:2n6)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0010451	TG(18:1(9Z)/16/18:3(9Z,12Z,15Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0052426	TG(18:2(9Z,12Z)/16/18:2(9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0049866	TG(18:1(9Z)/16:1(9Z)/18:2(9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0049848	TG(18:1(9Z)/14:1(9Z):2n6)	C55H98O6	M+NH4	872.7702	-1.2
HMDB0050305	TG(:1(11Z)/14/18:3(6Z,9Z,12Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0045896	TG(/18:3(6Z,9Z,12Z)/14:1(9Z))	C55H98O6	M+NH4	872.7702	-1.2
HMDB0042581	TG(14/:2n6/18:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0005384	TG(16/18:1(9Z)/18:2(9Z,12Z))	C55H100O6	M+NH4	874.7858	-1.2

HMDB0047935	TG(14:1(9Z)/18:1(11Z)/:1(11Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0042424	TG(14/:3(5Z,8Z,11Z)/18)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0047803	TG(14:1(9Z)/18/:2n6)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0042545	TG(14/18:3(6Z,9Z,12Z)/)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0047979	TG(14:1(9Z)/:1(11Z)/18:1(11Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0043901	TG(16/16/:3n6)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0042755	TG(14/18:3(9Z,12Z,15Z)/)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0047958	TG(14:1(9Z)/18:1(9Z)/:1(11Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0044278	TG(16/18:3(6Z,9Z,12Z)/18)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0042522	TG(14/18:2(9Z,12Z)/:1(11Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0048024	TG(14:1(9Z)/22:1(13Z)/16:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0047980	TG(14:1(9Z)/:1(11Z)/18:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0042604	TG(14/:3n6/18)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0042669	TG(14/22:2(13Z,16Z)/16:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0047783	TG(14:1(9Z)/16/22:2(13Z,16Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0043927	TG(16/18/18:3(6Z,9Z,12Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0047824	TG(14:1(9Z)/18:2(9Z,12Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0044094	TG(16/18:1(11Z)/18:2(9Z,12Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0044257	TG(16/18:2(9Z,12Z)/18:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0042406	TG(14/:1(11Z)/18:2(9Z,12Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0044043	TG(16/14:1(9Z)/22:2(13Z,16Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0044683	TG(18/14/:3n6)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0048425	TG(16:1(9Z)/14/22:2(13Z,16Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0010443	TG(18:1(11Z)/16:1(9Z)/18:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0048634	TG(16:1(9Z)/18:1(9Z)/18:1(11Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0048572	TG(16:1(9Z)/14:1(9Z)/22:1(13Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0044896	TG(18/16:1(9Z)/18:2(9Z,12Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0010439	TG(18:1(11Z)/16/18:2(9Z,12Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0005438	TG(16:1(9Z)/18:1(9Z)/18:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0044394	TG(16/22:2(13Z,16Z)/14:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0044677	TG(18/14/:3(5Z,8Z,11Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0044311	TG(16/:2n6/16:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0042378	TG(14/18:1(9Z)/:2n6)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0043895	TG(16/16/:3(5Z,8Z,11Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0044256	TG(16/18:2(9Z,12Z)/18:1(11Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0042197	TG(14//18:3(6Z,9Z,12Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0044068	TG(16/16:1(9Z)/:2n6)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0044474	TG(16/18:3(9Z,12Z,15Z)/18)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0047892	TG(14:1(9Z)/14:1(9Z)/24:1(15Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0047914	TG(14:1(9Z)/16:1(9Z)/22:1(13Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0042348	TG(14/18:1(11Z)/:2n6)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0042580	TG(14/:2n6/18:1(11Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0043934	TG(16/18/18:3(9Z,12Z,15Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0042204	TG(14//18:3(9Z,12Z,15Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0048613	TG(16:1(9Z)/18:1(11Z)/18:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0044165	TG(16/:3(5Z,8Z,11Z)/16)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0044333	TG(16/:3n6/16)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0010442	TG(18:1(11Z)/16:1(9Z)/18:1(11Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0049080	TG(18:1(11Z)/14/:2n6)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0045670	TG(/14:1(9Z)/18:2(9Z,12Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0045496	TG(/14/18:3(9Z,12Z,15Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0050304	TG(:1(11Z)/14/18:2(9Z,12Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0045489	TG(/14/18:3(6Z,9Z,12Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0045870	TG(/18:2(9Z,12Z)/14:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0042163	TG(14/18/:3(5Z,8Z,11Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0042321	TG(14/16:1(9Z)/22:2(13Z,16Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0042169	TG(14/18/:3n6)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0049708	TG(18:1(9Z)/14/:2n6)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0049842	TG(18:1(9Z)/14:1(9Z)/:1(11Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0049746	TG(18:1(9Z)/16/18:2(9Z,12Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0048612	TG(16:1(9Z)/18:1(11Z)/18:1(11Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0045078	TG(18/18:2(9Z,12Z)/16:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0005434	TG(16:1(9Z)/16:1(9Z)/:1(11Z))	C55H100O6	M+NH4	874.7858	-1.2
HMDB0044871	TG(18/14:1(9Z)/:2n6)	C55H100O6	M+NH4	874.7858	-1.2
HMDB0049221	TG(18:1(11Z)/14:1(9Z)/:1(11Z))	C55H100O6	M+NH4	874.7858	-1.2

	HMDB0048466	TG(16:1(9Z)/16/:2n6)	C55H100O6	M+NH4	874.7858	-1.2
	HMDB0044735	TG(18/16/18:3(6Z,9Z,12Z))	C55H100O6	M+NH4	874.7858	-1.2
	HMDB0005425	TG(16:1(9Z)/18/18:2(9Z,12Z))	C55H100O6	M+NH4	874.7858	-1.2
	HMDB0010432	TG(18/16/18:3(9Z,12Z,15Z))	C55H100O6	M+NH4	874.7858	-1.2
	HMDB0045131	TG(18/:2n6/14:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
	HMDB0048046	TG(14:1(9Z)/24:1(15Z)/14:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
	HMDB0048655	TG(16:1(9Z)/:1(11Z)/16:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
	HMDB0049861	TG(18:1(9Z)/16:1(9Z)/18:1(9Z))	C55H100O6	M+NH4	874.7858	-1.2
876.8001	HMDB0044036	TG(16/14:1(9Z)/22:1(13Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0044305	TG(16/:2n6/16)	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0005382	TG(16/18:1(9Z)/18:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0044143	TG(16/:1(11Z)/16:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0042401	TG(14/:1(11Z)/18:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0047731	TG(14:1(9Z)/14/24:1(15Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0005369	TG(16/18/18:2(9Z,12Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0044250	TG(16/18:2(9Z,12Z)/18)	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0044089	TG(16/18:1(11Z)/18:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0042168	TG(14/18/:2n6)	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0043847	TG(16/14/22:2(13Z,16Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0042459	TG(14/22:1(13Z)/16:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0042400	TG(14/:1(11Z)/18:1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0047776	TG(14:1(9Z)/16/22:1(13Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0044116	TG(16/18:1(9Z)/18:1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0047819	TG(14:1(9Z)/18:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0047797	TG(14:1(9Z)/18/:1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0047818	TG(14:1(9Z)/18:1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0042515	TG(14/18:2(9Z,12Z)/)	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0043900	TG(16/16/:2n6)	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0010425	TG(16:1(9Z)/18/18:1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0044916	TG(18/18:1(11Z)/16:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0005423	TG(16:1(9Z)/18/18:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0049074	TG(18:1(11Z)/14/:1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0048418	TG(16:1(9Z)/14/22:1(13Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0049702	TG(18:1(9Z)/14/:1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0045488	TG(/14/18:2(9Z,12Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0045664	TG(/14:1(9Z)/18:1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0045714	TG(/18:1(11Z)/14:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0045665	TG(/14:1(9Z)/18:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0044891	TG(18/16:1(9Z)/18:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0048460	TG(16:1(9Z)/16/:1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0044969	TG(18/:1(11Z)/14:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0044943	TG(18/18:1(9Z)/16:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0044890	TG(18/16:1(9Z)/18:1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0044734	TG(18/16/18:2(9Z,12Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0005431	TG(16:1(9Z)/16:1(9Z)/)	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0044865	TG(18/14:1(9Z)/:1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0044682	TG(18/14/:2n6)	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0044198	TG(16/22:1(13Z)/14:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0010438	TG(18:1(11Z)/16/18:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0045740	TG(/18:1(9Z)/14:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0042196	TG(14/18:2(9Z,12Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0047840	TG(14:1(9Z)/22/16:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0042488	TG(14/24:1(15Z)/14:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0005378	TG(16/16:1(9Z)/:1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0043008	TG(15/15/22:2(13Z,16Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0044088	TG(16/18:1(11Z)/18:1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0042574	TG(14/:2n6/18)	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0042663	TG(14/22:2(13Z,16Z)/16)	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0042372	TG(14/18:1(9Z)/:1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0043540	TG(15/22:2(13Z,16Z)/15)	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0031116	Glycerol 2,3-di-(9Z-octadecenoate) 1-hexadecanoate	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0010437	TG(18:1(11Z)/16/18:1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0045689	TG(/16:1(9Z)/16:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0046458	TG(22/16:1(9Z)/14:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0047174	TG(24/14:1(9Z)/14:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6

	HMDB0049741	TG(18:1(9Z)/16:18:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0048501	TG(16:1(9Z)/16:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0046434	TG(22/14:1(9Z)/16:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0042342	TG(14/18:1(11Z)/1(11Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0042141	TG(14/16/22:2(13Z,16Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0042314	TG(14/16:1(9Z)/22:1(13Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0042285	TG(14/14:1(9Z)/24:1(15Z))	C55H102O6	M+NH4	876.8015	-1.6
	HMDB0047862	TG(14:1(9Z)/24/14:1(9Z))	C55H102O6	M+NH4	876.8015	-1.6
880.5908	HMDB0009786	PI(16:2(11Z,14Z))	C45H83O13P	M+NH4	880.5910	-0.2
	HMDB0009875	PI(:2(11Z,14Z)/16)	C45H83O13P	M+NH4	880.5910	-0.2
	HMDB0009809	PI(18/18:2(9Z,12Z))	C45H83O13P	M+NH4	880.5910	-0.2
	HMDB0009824	PI(18:1(11Z)/18:1(11Z))	C45H83O13P	M+NH4	880.5910	-0.2
	HMDB0009825	PI(18:1(11Z)/18:1(9Z))	C45H83O13P	M+NH4	880.5910	-0.2
	HMDB0009836	PI(18:1(9Z)/18:1(11Z))	C45H83O13P	M+NH4	880.5910	-0.2
	HMDB0009837	PI(18:1(9Z)/18:1(9Z))	C45H83O13P	M+NH4	880.5910	-0.2
	HMDB0009847	PI(18:2(9Z,12Z)/18)	C45H83O13P	M+NH4	880.5910	-0.2
886.7850	HMDB0043099	TG(15//18:4(6Z,9Z,12Z,15Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043570	TG(15/22:4(7Z,Z,13Z,16Z)/16)	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043317	TG(15/:3(5Z,8Z,11Z)/18:1(9Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043637	TG(15/18:3(9Z,12Z,15Z)/:1(11Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043434	TG(15/18:3(6Z,9Z,12Z)/:1(11Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043687	TG(15/:4(8Z,11Z,14Z,17Z)/18)	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043261	TG(15/18:1(9Z)/:3(5Z,8Z,11Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043513	TG(15/:4(5Z,8Z,11Z,14Z)/18)	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043038	TG(15/16/22:4(7Z,Z,13Z,16Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043294	TG(15/:1(11Z)/18:3(6Z,9Z,12Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043316	TG(15/:3(5Z,8Z,11Z)/18:1(11Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043491	TG(15/:3n6/18:1(9Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043267	TG(15/18:1(9Z)/:3n6)	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043301	TG(15/:1(11Z)/18:3(9Z,12Z,15Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043232	TG(15/18:1(11Z)/:3(5Z,8Z,11Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043659	TG(15/18:4(6Z,9Z,12Z,15Z)/)	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043071	TG(15/18/:4(8Z,11Z,14Z,17Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043876	TG(16/15/22:4(7Z,Z,13Z,16Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043065	TG(15/18:4(5Z,8Z,11Z,14Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043467	TG(15/:2n6/18:2(9Z,12Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043490	TG(15/:3n6/18:1(11Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043411	TG(15/18:2(9Z,12Z)/:2n6)	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043238	TG(15/18:1(11Z)/:3n6)	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0049096	TG(18:1(11Z)/15/:3(5Z,8Z,11Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0049102	TG(18:1(11Z)/15/:3n6)	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0044711	TG(18/15/:4(5Z,8Z,11Z,14Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0044717	TG(18/15/:4(8Z,11Z,14Z,17Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0052413	TG(18:2(9Z,12Z)/15/:2n6)	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0049729	TG(18:1(9Z)/15/:3n6)	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0049723	TG(18:1(9Z)/15/:3(5Z,8Z,11Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0050331	TG(:1(11Z)/15/18:3(9Z,12Z,15Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0045523	TG(/15/18:4(6Z,9Z,12Z,15Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0050324	TG(:1(11Z)/15/18:3(6Z,9Z,12Z))	C56H100O6	M+NH4	886.7858	-0.9
	HMDB0043461	TG(15/:2n6/18:1(11Z))	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0043293	TG(15/:1(11Z)/18:2(9Z,12Z))	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0043064	TG(15/18/:3n6)	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0043098	TG(15//18:3(9Z,12Z,15Z))	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0043058	TG(15/18/:3(5Z,8Z,11Z))	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0043211	TG(15/16:1(9Z)/22:2(13Z,16Z))	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0043462	TG(15/:2n6/18:1(9Z))	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0043484	TG(15/:3n6/18)	C56H102O6	M+NH4	888.8015	-1.6

888.8000	HMDB0043266	TG(15/18:1(9Z)/:2n6)	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0043237	TG(15/18:1(11Z)/:2n6)	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0043405	TG(15/18:2(9Z,12Z)/:1(11Z))	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0043091	TG(15//18:3(6Z,9Z,12Z))	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0043547	TG(15/22:2(13Z,16Z)/16:1(9Z))	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0043630	TG(15/18:3(9Z,12Z,15Z)/)	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0043427	TG(15/18:3(6Z,9Z,12Z)/)	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0049101	TG(18:1(11Z)/15/:2n6)	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0044710	TG(18/15/:3n6)	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0050323	TG(:1(11Z)/15/18:2(9Z,12Z))	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0045522	TG(/15/18:3(9Z,12Z,15Z))	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0045515	TG(/15/18:3(6Z,9Z,12Z))	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0049728	TG(18:1(9Z)/15/:2n6)	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0044704	TG(18/15/:3(5Z,8Z,11Z))	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0048447	TG(16:1(9Z)/15/22:2(13Z,16Z))	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0043310	TG(15/:3(5Z,8Z,11Z)/18)	C56H102O6	M+NH4	888.8015	-1.6
	HMDB0052967	TG(18:3(6Z,9Z,12Z)/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0053063	TG(18:3(6Z,9Z,12Z)/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0010498	TG(18:3(9Z,12Z,15Z)/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0052954	TG(18:3(6Z,9Z,12Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0055254	TG(18:3(9Z,12Z,15Z)/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0055201	TG(18:3(9Z,12Z,15Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0053174	TG(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0052514	TG(18:2(9Z,12Z)/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0052645	TG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0049591	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0052857	TG(18:3(6Z,9Z,12Z)/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0052750	TG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0048937	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0048783	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0048958	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0048993	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0049000	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0055207	TG(18:3(9Z,12Z,15Z)/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0052757	TG(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0054095	TG(:4(5Z,8Z,11Z,14Z)/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0054706	TG(22:4(7Z,Z,13Z,16Z)/14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0054966	TG(22:5(4Z,7Z,Z,13Z,16Z)/14:1(9Z)/18:3(9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0054911	TG(22:5(4Z,7Z,Z,13Z,16Z)/14/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0054105	TG(:4(5Z,8Z,11Z,14Z)/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0054019	TG(:4(5Z,8Z,11Z,14Z)/14/:5(5Z,8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0055537	TG(:4(8Z,11Z,14Z,17Z)/14/:5(5Z,8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0051009	TG(:3(5Z,8Z,11Z)/14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
	HMDB0053745	TG(:3n6/14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9

890.7249

HMDB0055371	TG(18:4(6Z,9Z,12Z,15Z)/16:5(5Z,8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0055406	TG(18:4(6Z,9Z,12Z,15Z)/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0055360	TG(18:4(6Z,9Z,12Z,15Z)/14:22:5(7Z,Z,13Z,16Z,19Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0052949	TG(18:3(6Z,9Z,12Z)/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0052764	TG(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0050195	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0053076	TG(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048952	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048847	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0042895	TG(14:22:5(7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048246	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0042924	TG(14:22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048354	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048090	TG(14:1(9Z)/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048239	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048376	TG(14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048268	TG(14:1(9Z)/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048327	TG(14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0042917	TG(14:22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0042779	TG(14:18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0044525	TG(16:18:4(6Z,9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048361	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0042860	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048112	TG(14:1(9Z)/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048333	TG(14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/:3n6)	C57H92O6	M+NH4	890.7232	1.9
HMDB0048179	TG(14:1(9Z)/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0042657	TG(14/:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048979	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0044579	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0042837	TG(14/:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048224	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0042808	TG(14:18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0042745	TG(14:22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0042803	TG(14:18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048317	TG(14:1(9Z)/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048311	TG(14:1(9Z)/:4(8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048107	TG(14:1(9Z)/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048290	TG(14:1(9Z)/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048157	TG(14:1(9Z)/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0042569	TG(14:18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H92O6	M+NH4	890.7232	1.9

HMDB0048273	TG(14:1(9Z)/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048173	TG(14:1(9Z)/:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0048019	TG(14:1(9Z)/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0042866	TG(14:/5(5Z,8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0030292	Trielostearin	C57H92O6	M+NH4	890.7232	1.9
HMDB0030491	Glycerol 1,2-di-(9Z,11E,13Z-octadecatrienoate) 3-(8Z,11Z,13E-octadecatrienoate)	C57H92O6	M+NH4	890.7232	1.9
HMDB0055260	TG(18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0055309	TG(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0055411	TG(18:4(6Z,9Z,12Z,15Z)/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0055417	TG(18:4(6Z,9Z,12Z,15Z)/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0055571	TG(:4(8Z,11Z,14Z,17Z)/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0054089	TG(:4(5Z,8Z,11Z,14Z)/14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0053069	TG(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0053167	TG(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C57H92O6	M+NH4	890.7232	1.9
HMDB0044571	TG(16:/5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048971	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0044578	TG(16:/5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052644	TG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052513	TG(18:2(9Z,12Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052966	TG(18:3(6Z,9Z,12Z)/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0055212	TG(18:3(9Z,12Z,15Z)/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0049590	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0055165	TG(18:3(9Z,12Z,15Z)/16:/5(5Z,8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052756	TG(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052630	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0050035	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0055219	TG(18:3(9Z,12Z,15Z)/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0049238	TG(18:1(11Z)/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0045337	TG(18/18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048930	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048825	TG(16:1(9Z)/:3n6/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048992	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0049423	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048609	TG(16:1(9Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048846	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048945	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048936	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048693	TG(16:1(9Z)/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048776	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048978	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048839	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052527	TG(18:2(9Z,12Z)/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052749	TG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052508	TG(18:2(9Z,12Z)/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0050175	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052851	TG(18:3(6Z,9Z,12Z)/14/22:5(4Z,7Z,Z,13Z,16Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0049583	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052742	TG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0050187	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052979	TG(18:3(6Z,9Z,12Z)/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0055370	TG(18:4(6Z,9Z,12Z,15Z)/16:/4(8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0051008	TG(:3(5Z,8Z,11Z)/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0053364	TG(:2n6/14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1

HMDB0050883	TG:(3(5Z,8Z,11Z)/14/:5(5Z,8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0053744	TG(:3n6/14:1(9Z)):4(8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0055206	TG(18:3(9Z,12Z,15Z)/16:1(9Z)):4(8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052993	TG(18:3(6Z,9Z,12Z)/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052409	TG(18:2(9Z,12Z)/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0049859	TG(18:1(9Z)/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0053055	TG(18:3(6Z,9Z,12Z)/18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052948	TG(18:3(6Z,9Z,12Z)/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0049570	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052637	TG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052856	TG(18:3(6Z,9Z,12Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052960	TG(18:3(6Z,9Z,12Z)/16:1(9Z)):4(5Z,8Z,11Z,14Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0052883	TG(18:3(6Z,9Z,12Z)/16/:5(5Z,8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0050194	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0053062	TG(18:3(6Z,9Z,12Z)/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0055152	TG(18:3(9Z,12Z,15Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0053738	TG(:3n6/14:1(9Z)):4(5Z,8Z,11Z,14Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042830	TG(14/:4(8Z,11Z,14Z,17Z)):4(5Z,8Z,11Z,14Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048012	TG(14:1(9Z)):3(5Z,8Z,11Z):4(5Z,8Z,11Z,14Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048084	TG(14:1(9Z)/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0044551	TG(16/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042715	TG(14/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042744	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042447	TG(14/:3(5Z,8Z,11Z)):5(5Z,8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048223	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042773	TG(14/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042627	TG(14/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042568	TG(14/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042916	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048371	TG(14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048018	TG(14:1(9Z)):3(5Z,8Z,11Z):4(8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0047952	TG(14:1(9Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042650	TG(14/:4(5Z,8Z,11Z,14Z)):4(5Z,8Z,11Z,14Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0044383	TG(16/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048370	TG(14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042894	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0047975	TG(14:1(9Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0044301	TG(16/18:3(6Z,9Z,12Z)):5(5Z,8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0044524	TG(16/18:4(6Z,9Z,12Z,15Z)):4(8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048156	TG(14:1(9Z)):3n6/:4(8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048238	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048304	TG(14:1(9Z)):4(8Z,11Z,14Z,17Z):3(5Z,8Z,11Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048134	TG(14:1(9Z)):2n6/:5(5Z,8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048332	TG(14:1(9Z)):5(5Z,8Z,11Z,14Z,17Z):2n6)	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048166	TG(14:1(9Z)):4(5Z,8Z,11Z,14Z):3(5Z,8Z,11Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042539	TG(14/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042853	TG(14/:5(5Z,8Z,11Z,14Z,17Z)):3(5Z,8Z,11Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048089	TG(14:1(9Z)/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042563	TG(14/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042802	TG(14/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048353	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048761	TG(16:1(9Z)/18:2(9Z,12Z)):5(5Z,8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048782	TG(16:1(9Z)/18:3(6Z,9Z,12Z)):4(8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042887	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0044497	TG(16/18:3(9Z,12Z,15Z)):5(5Z,8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048150	TG(14:1(9Z)):3n6/:4(5Z,8Z,11Z,14Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048106	TG(14:1(9Z)/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042859	TG(14/:5(5Z,8Z,11Z,14Z,17Z)):3n6)	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048216	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048310	TG(14:1(9Z)):4(8Z,11Z,14Z,17Z):3n6)	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042737	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042778	TG(14/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048172	TG(14:1(9Z)):4(5Z,8Z,11Z,14Z):3n6)	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042836	TG(14/:4(8Z,11Z,14Z,17Z)):4(8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1

HMDB0048267	TG(14:1(9Z)/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0042656	TG(14:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0044518	TG(16/18:4(6Z,9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0048951	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:3n6)	C57H94O6	M+NH4	892.7389	-1.1
HMDB0053661	TG(:3n6/14:5(5Z,8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0010518	TG(:4(5Z,8Z,11Z,14Z)/14:4(5Z,8Z,11Z,14Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0010507	TG(18:3(9Z,12Z,15Z)/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0051002	TG(:3(5Z,8Z,11Z)/14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0051025	TG(:3(5Z,8Z,11Z)/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0053755	TG(:3n6/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0054104	TG(:4(5Z,8Z,11Z,14Z)/16:1(9Z)/18:3(9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0054643	TG(22:4(7Z,Z,13Z,16Z)/14/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0054705	TG(22:4(7Z,Z,13Z,16Z)/14:1(9Z)/18:3(9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0054039	TG(:4(5Z,8Z,11Z,14Z)/16/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0054018	TG(:4(5Z,8Z,11Z,14Z)/14:4(8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0054910	TG(22:5(4Z,7Z,Z,13Z,16Z)/14/18:3(9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0055536	TG(:4(8Z,11Z,14Z,17Z)/14:4(8Z,11Z,14Z,17Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0055375	TG(18:4(6Z,9Z,12Z,15Z)/18/18:4(6Z,9Z,12Z,15Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0049029	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C57H94O6	M+NH4	892.7389	-1.1
HMDB0049257	TG(18:1(11Z)/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048817	TG(16:1(9Z)/:3n6/18:3(6Z,9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044882	TG(18/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0005447	TG(16:1(9Z)/18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0045310	TG(18/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048803	TG(16:1(9Z)/:2n6/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0049402	TG(18:1(11Z)/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048838	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048929	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/:3n6)	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048608	TG(16:1(9Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044570	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0049091	TG(18:1(11Z)/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0045329	TG(18/18:4(6Z,9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0049237	TG(18:1(11Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048986	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052876	TG(18:3(6Z,9Z,12Z)/16/:4(5Z,8Z,11Z,14Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0055164	TG(18:3(9Z,12Z,15Z)/16:4(8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048987	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048477	TG(16:1(9Z)/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048603	TG(16:1(9Z)/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044619	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0045428	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/14:1(9Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048950	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:2n6)	C57H96O6	M+NH4	894.7545	-1.0
HMDB0049232	TG(18:1(11Z)/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048824	TG(16:1(9Z)/:3n6/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048769	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048692	TG(16:1(9Z)/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048629	TG(16:1(9Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048685	TG(16:1(9Z)/:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048760	TG(16:1(9Z)/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048651	TG(16:1(9Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0049422	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0049415	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048775	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/:3n6)	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048970	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0045121	TG(18/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052636	TG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052959	TG(18:3(6Z,9Z,12Z)/16:1(9Z)/:3n6)	C57H96O6	M+NH4	894.7545	-1.0
HMDB0049582	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052408	TG(18:2(9Z,12Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052526	TG(18:2(9Z,12Z)/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052741	TG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0050174	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052992	TG(18:3(6Z,9Z,12Z)/18:1(9Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052540	TG(18:2(9Z,12Z)/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0

HMDB0052882	TG(18:3(6Z,9Z,12Z)/16:4(8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052403	TG(18:2(9Z,12Z)/14:22:5(4Z,7Z,Z,13Z,16Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052520	TG(18:2(9Z,12Z)/16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0050034	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0050448	TG(:1(11Z)/14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0051024	TG(:3(5Z,8Z,11Z)/16:1(9Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0053273	TG(:2n6/14/:5(5Z,8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0053357	TG(:2n6/14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0053660	TG(:3n6/14/:4(8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0051001	TG(:3(5Z,8Z,11Z)/14:1(9Z)/:3n6)	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052507	TG(18:2(9Z,12Z)/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0049562	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0050027	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0010490	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0049877	TG(18:1(9Z)/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0050186	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0049858	TG(18:1(9Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0050015	TG(18:1(9Z)/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0010475	TG(18:2(9Z,12Z)/16/:5(5Z,8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052850	TG(18:3(6Z,9Z,12Z)/14:22:4(7Z,Z,13Z,16Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0049719	TG(18:1(9Z)/14:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0055170	TG(18:3(9Z,12Z,15Z)/18/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052978	TG(18:3(6Z,9Z,12Z)/18:1(11Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0049569	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052895	TG(18:3(6Z,9Z,12Z)/18/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0010489	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052555	TG(18:2(9Z,12Z)/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0049853	TG(18:1(9Z)/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0050167	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0053363	TG(:2n6/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0045336	TG(18/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044079	TG(16/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044511	TG(16/18:4(6Z,9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048233	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042911	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042562	TG(14/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044294	TG(16/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042858	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/:2n6)	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042597	TG(14/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042626	TG(14/:3n6/:4(8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0047969	TG(14:1(9Z)/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042440	TG(14/:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042772	TG(14/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048289	TG(14:1(9Z)/18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048201	TG(14:1(9Z)/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048127	TG(14:1(9Z)/:2n6/:4(5Z,8Z,11Z,14Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0047946	TG(14:1(9Z)/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0047996	TG(14:1(9Z)/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042910	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048348	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048083	TG(14:1(9Z)/18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048326	TG(14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/:1(11Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048149	TG(14:1(9Z)/:3n6/:3n6)	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042389	TG(14/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044273	TG(16/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048347	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044187	TG(16/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042533	TG(14/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042620	TG(14/:3n6/:4(5Z,8Z,11Z,14Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048232	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044550	TG(16/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044375	TG(16/:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042823	TG(14/:4(8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048171	TG(14:1(9Z)/:4(5Z,8Z,11Z,14Z)/:2n6)	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042714	TG(14/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0

HMDB0048011	TG(14:1(9Z)/:3(5Z,8Z,11Z)/:3n6)	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042886	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0047814	TG(14:1(9Z)/18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048309	TG(14:1(9Z)/:4(8Z,11Z,14Z,17Z)/:2n6)	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042446	TG(14/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0047951	TG(14:1(9Z)/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042707	TG(14/22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044543	TG(16/:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048133	TG(14:1(9Z)/:2n6/:4(8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0047974	TG(14:1(9Z)/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042649	TG(14/:4(5Z,8Z,11Z,14Z)/:3n6)	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044517	TG(16/18:4(6Z,9Z,12Z,15Z)/:3n6)	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044300	TG(16/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048005	TG(14:1(9Z)/:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044355	TG(16/:3n6/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042736	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044490	TG(16/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042643	TG(14/:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042538	TG(14/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044496	TG(16/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042829	TG(14/:4(8Z,11Z,14Z,17Z)/:3n6)	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048143	TG(14:1(9Z)/:3n6/:3(5Z,8Z,11Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0044382	TG(16/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048215	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048923	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0010502	TG(18:3(9Z,12Z,15Z)/18:1(11Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0010503	TG(18:3(9Z,12Z,15Z)/18:1(9Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0051017	TG(:3(5Z,8Z,11Z)/16:1(9Z)/18:3(6Z,9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0053737	TG(:3n6/14:1(9Z)/:3n6)	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052985	TG(18:3(6Z,9Z,12Z)/18:1(9Z)/18:3(6Z,9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0052971	TG(18:3(6Z,9Z,12Z)/18:1(11Z)/18:3(6Z,9Z,12Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0053683	TG(:3n6/16/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0050917	TG(:3(5Z,8Z,11Z)/16/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0053754	TG(:3n6/16:1(9Z)/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0050876	TG(:3(5Z,8Z,11Z)/14/:4(5Z,8Z,11Z,14Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0053375	TG(:2n6/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0053654	TG(:3n6/14/:4(5Z,8Z,11Z,14Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0050882	TG(:3(5Z,8Z,11Z)/14/:4(8Z,11Z,14Z,17Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0010519	TG(:4(5Z,8Z,11Z,14Z)/16/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0054415	TG(22:2(13Z,16Z)/14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0054642	TG(22:4(7Z,Z,13Z,16Z)/14/18:3(9Z,12Z,15Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0042359	TG(14/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0049007	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0048897	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0050995	TG(:3(5Z,8Z,11Z)/14:1(9Z)/:3(5Z,8Z,11Z))	C57H96O6	M+NH4	894.7545	-1.0
HMDB0049297	TG(18:1(11Z)/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044591	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044693	TG(18/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0045094	TG(18/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048832	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048471	TG(16:1(9Z)/16/22:5(4Z,7Z,Z,13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048303	TG(14:1(9Z)/:4(8Z,11Z,14Z,17Z)/:1(11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044105	TG(16/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048105	TG(14:1(9Z)/18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048126	TG(14:1(9Z)/:2n6/:3n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048684	TG(16:1(9Z)/:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049256	TG(18:1(11Z)/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048622	TG(16:1(9Z)/18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0045302	TG(18/18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049414	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0045120	TG(18/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048944	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044876	TG(18/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048497	TG(16:1(9Z)/18/:5(5Z,8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048628	TG(16:1(9Z)/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2

HMDB0049131	TG(18:1(11Z)/16:5(5Z,8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0045113	TG(18/18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048120	TG(14:1(9Z)/:2n6/:3(5Z,8Z,11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048193	TG(14:1(9Z)/22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042383	TG(14/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042417	TG(14/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042730	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044133	TG(16/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0047995	TG(14:1(9Z)/:1(11Z)/:4(8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042388	TG(14/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048200	TG(14:1(9Z)/22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042648	TG(14/:4(5Z,8Z,11Z,14Z)/:2n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044186	TG(16/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042801	TG(14/18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044272	TG(16/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0005391	TG(16/18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044179	TG(16/:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0047945	TG(14:1(9Z)/18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048210	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:1(9Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048040	TG(14:1(9Z)/22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042439	TG(14/:3(5Z,8Z,11Z)/:3n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042596	TG(14/:2n6/:4(8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048165	TG(14:1(9Z)/:4(5Z,8Z,11Z,14Z)/:1(11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042881	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042685	TG(14/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042706	TG(14/22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0050014	TG(18:1(9Z)/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049401	TG(18:1(11Z)/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048602	TG(16:1(9Z)/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0045309	TG(18/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0045375	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/16:1(9Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048795	TG(16:1(9Z)/:2n6/18:3(6Z,9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049250	TG(18:1(11Z)/16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049561	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048928	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/:2n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049231	TG(18:1(11Z)/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049713	TG(18:1(9Z)/14/22:5(4Z,7Z,Z,13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049876	TG(18:1(9Z)/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0052894	TG(18:3(6Z,9Z,12Z)/18/18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0052539	TG(18:2(9Z,12Z)/18:1(11Z)/18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049915	TG(18:1(9Z)/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049870	TG(18:1(9Z)/16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049895	TG(18:1(9Z)/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049577	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049852	TG(18:1(9Z)/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0052532	TG(18:2(9Z,12Z)/18:1(11Z)/18:3(6Z,9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0010482	TG(18:2(9Z,12Z)/18:1(9Z)/18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0052402	TG(18:2(9Z,12Z)/14/22:4(7Z,Z,13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048965	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048476	TG(16:1(9Z)/16/22:5(7Z,Z,13Z,16Z,19Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048671	TG(16:1(9Z)/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048650	TG(16:1(9Z)/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048964	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048747	TG(16:1(9Z)/18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048774	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/:2n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048753	TG(16:1(9Z)/18:2(9Z,12Z)/:3n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0005441	TG(16:1(9Z)/18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049090	TG(18:1(11Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049085	TG(18:1(11Z)/14/22:5(4Z,7Z,Z,13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044451	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049394	TG(18:1(11Z)/18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048816	TG(16:1(9Z)/:3n6/18:2(9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0045328	TG(18/18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049276	TG(18:1(11Z)/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0045401	TG(18/22:5(7Z,Z,13Z,16Z,19Z)/14:1(9Z))	C57H98O6	M+NH4	896.7702	-1.2

HMDB0048802	TG(16:1(9Z)/:2n6/18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044565	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044564	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0045266	TG(18/22:5(4Z,7Z,Z,13Z,16Z)/14:1(9Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044907	TG(18/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048833	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044881	TG(18/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0010418	TG(16/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0047968	TG(14:1(9Z)/18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042880	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044347	TG(16/:3n6/18:3(6Z,9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042852	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/:1(11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044327	TG(16/:2n6/18:4(6Z,9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042828	TG(14/:4(8Z,11Z,14Z,17Z)/:2n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044073	TG(16/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044078	TG(16/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048282	TG(14:1(9Z)/18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044293	TG(16/18:3(6Z,9Z,12Z)/:3n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0047989	TG(14:1(9Z)/:1(11Z)/:4(5Z,8Z,11Z,14Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048266	TG(14:1(9Z)/18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044483	TG(16/18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044516	TG(16/18:4(6Z,9Z,12Z,15Z)/:2n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042590	TG(14/:2n6/:4(5Z,8Z,11Z,14Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042904	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042532	TG(14/18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048010	TG(14:1(9Z)/:3(5Z,8Z,11Z)/:2n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0047835	TG(14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044542	TG(16/:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0047813	TG(14:1(9Z)/18/22:5(7Z,Z,13Z,16Z,19Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042619	TG(14/:3n6/:3n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048148	TG(14:1(9Z)/:3n6/:2n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048209	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:1(11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044287	TG(16/18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0047808	TG(14:1(9Z)/18/22:5(4Z,7Z,Z,13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044374	TG(16/:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042731	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044354	TG(16/:3n6/18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042433	TG(14/:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044489	TG(16/18:3(9Z,12Z,15Z)/:3n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042613	TG(14/:3n6/:3(5Z,8Z,11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0052947	TG(18:3(6Z,9Z,12Z)/14:1(9Z)/22:2(13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0044613	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/16)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0005474	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/18:2(9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0010501	TG(18:3(9Z,12Z,15Z)/18/18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0053653	TG(:3n6/14/:3n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042353	TG(14/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0054414	TG(22:2(13Z,16Z)/14:1(9Z)/18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0054345	TG(22:2(13Z,16Z)/14/18:4(6Z,9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0051538	TG(22:1(13Z)/14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0053272	TG(:2n6/14/:4(8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0053356	TG(:2n6/14:1(9Z)/:3n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0053266	TG(:2n6/14/:4(5Z,8Z,11Z,14Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0050909	TG(:3(5Z,8Z,11Z)/16/18:3(6Z,9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0053682	TG(:3n6/16/18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042358	TG(14/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0042179	TG(14/18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0051000	TG(:3(5Z,8Z,11Z)/14:1(9Z)/:2n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0050875	TG(:3(5Z,8Z,11Z)/14/:3n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0010481	TG(18:2(9Z,12Z)/18:1(9Z)/18:3(6Z,9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0052958	TG(18:3(6Z,9Z,12Z)/16:1(9Z)/:2n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0050007	TG(18:1(9Z)/18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0052519	TG(18:2(9Z,12Z)/16:1(9Z)/:3n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0052430	TG(18:2(9Z,12Z)/16/:4(5Z,8Z,11Z,14Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049718	TG(18:1(9Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0052450	TG(18:2(9Z,12Z)/18/18:4(6Z,9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2

HMDB0050026	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0010453	TG(18:1(9Z)/16:5(5Z,8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0052875	TG(18:3(6Z,9Z,12Z)/16:3n6)	C57H98O6	M+NH4	896.7702	-1.2
HMDB0050166	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0050447	TG(1(11Z)/14:1(9Z)/4(8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0050916	TG(3(5Z,8Z,11Z)/16:18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0053297	TG(2n6/16:18:4(6Z,9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0053374	TG(2n6/16:1(9Z)/18:3(9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0051016	TG(3(5Z,8Z,11Z)/16:1(9Z)/18:2(9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0050441	TG(1(11Z)/14:1(9Z)/4(5Z,8Z,11Z,14Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0050465	TG(1(11Z)/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0045681	TG(14:1(9Z)/5(5Z,8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0050315	TG(1(11Z)/14:5(5Z,8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0046156	TG(5(5Z,8Z,11Z,14Z,17Z)/14:1(9Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0052436	TG(18:2(9Z,12Z)/16:4(8Z,11Z,14Z,17Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0049576	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048875	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0052887	TG(18:3(6Z,9Z,12Z)/18:18:3(6Z,9Z,12Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0050869	TG(3(5Z,8Z,11Z)/14:3(5Z,8Z,11Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0050181	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C57H98O6	M+NH4	896.7702	-1.2
HMDB0048810	TG(16:1(9Z)/3n6/18:1(11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048811	TG(16:1(9Z)/3n6/18:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0045186	TG(18:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049268	TG(18:1(11Z)/18:1(11Z)/18:3(6Z,9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048678	TG(16:1(9Z)/3(5Z,8Z,11Z)/18:1(11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0010441	TG(18:1(11Z)/16:4(5Z,8Z,11Z,14Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048768	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/1(11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048663	TG(16:1(9Z)/1(11Z)/18:3(6Z,9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048637	TG(16:1(9Z)/18:1(9Z)/3(5Z,8Z,11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049296	TG(18:1(11Z)/18:1(9Z)/18:3(9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048125	TG(14:1(9Z)/2n6/2n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049275	TG(18:1(11Z)/18:1(11Z)/18:3(9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049243	TG(18:1(11Z)/16:1(9Z)/3(5Z,8Z,11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044745	TG(18/16:5(5Z,8Z,11Z,14Z,17Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0045093	TG(18/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0005426	TG(16:1(9Z)/18:4(5Z,8Z,11Z,14Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048679	TG(16:1(9Z)/3(5Z,8Z,11Z)/18:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044687	TG(18/14/22:5(4Z,7Z,Z,13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044906	TG(18/16:1(9Z)/4(8Z,11Z,14Z,17Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049409	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/18:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048922	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/1(11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044900	TG(18/16:1(9Z)/4(5Z,8Z,11Z,14Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048621	TG(16:1(9Z)/18:1(11Z)/3n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042822	TG(14:4(8Z,11Z,14Z,17Z)/1(11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042794	TG(14/18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042724	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/18)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0047807	TG(14:1(9Z)/18/22:4(7Z,Z,13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048032	TG(14:1(9Z)/22:1(13Z)/18:3(6Z,9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0005385	TG(16/18:1(9Z)/4(5Z,8Z,11Z,14Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042618	TG(14:3n6/2n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0047828	TG(14:1(9Z)/4(5Z,8Z,11Z,14Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0047856	TG(14:1(9Z)/22/18:4(6Z,9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042684	TG(14/22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042561	TG(14/18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048082	TG(14:1(9Z)/18:2(9Z,12Z)/22:2(13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044292	TG(16/18:3(6Z,9Z,12Z)/2n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048098	TG(14:1(9Z)/18:3(6Z,9Z,12Z)/22:1(13Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044072	TG(16/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044488	TG(16/18:3(9Z,12Z,15Z)/2n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044098	TG(16/18:1(11Z)/4(5Z,8Z,11Z,14Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0047982	TG(14:1(9Z)/1(11Z)/3(5Z,8Z,11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044178	TG(16:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0043937	TG(16/18:5(5Z,8Z,11Z,14Z,17Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048142	TG(14:1(9Z)/3n6/1(11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048192	TG(14:1(9Z)/22:2(13Z,16Z)/18:2(9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6

HMDB0044104	TG(16/18:1(11Z)/4(8Z,11Z,14Z,17Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042701	TG(14/22:4(7Z,Z,13Z,16Z)/18:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042642	TG(14/:4(5Z,8Z,11Z,14Z)/:1(11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0050434	TG(:1(11Z)/14:1(9Z)/:3(5Z,8Z,11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049869	TG(18:1(9Z)/16:1(9Z)/:3n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0052429	TG(18:2(9Z,12Z)/16/:3n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049887	TG(18:1(9Z)/18:1(11Z)/18:3(6Z,9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0052546	TG(18:2(9Z,12Z)/18:1(9Z)/18:2(9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049750	TG(18:1(9Z)/16/:4(5Z,8Z,11Z,14Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0005461	TG(18:1(9Z)/18:2(9Z,12Z)/18:2(9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0052874	TG(18:3(6Z,9Z,12Z)/16/:2n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0045323	TG(18/18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049393	TG(18:1(11Z)/18:2(9Z,12Z)/18:2(9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048752	TG(16:1(9Z)/18:2(9Z,12Z)/:2n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049756	TG(18:1(9Z)/16/:4(8Z,11Z,14Z,17Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0010477	TG(18:2(9Z,12Z)/18/18:3(9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0052518	TG(18:2(9Z,12Z)/16:1(9Z)/:2n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049775	TG(18:1(9Z)/18/18:4(6Z,9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0052506	TG(18:2(9Z,12Z)/14:1(9Z)/22:2(13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049712	TG(18:1(9Z)/14/22:4(7Z,Z,13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049863	TG(18:1(9Z)/16:1(9Z)/:3(5Z,8Z,11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049894	TG(18:1(9Z)/18:1(11Z)/18:3(9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0010459	TG(18:1(9Z)/18:1(9Z)/18:3(6Z,9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0052442	TG(18:2(9Z,12Z)/18/18:3(6Z,9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0052849	TG(18:3(6Z,9Z,12Z)/14/22:2(13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0010460	TG(18:1(9Z)/18:1(9Z)/18:3(9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0045086	TG(18/18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044558	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/18)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049130	TG(18:1(11Z)/16/:4(8Z,11Z,14Z,17Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048496	TG(16:1(9Z)/18/:4(8Z,11Z,14Z,17Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048670	TG(16:1(9Z)/:1(11Z)/18:3(9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0045239	TG(18/22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044875	TG(18/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044932	TG(18/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0045112	TG(18/18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048517	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049289	TG(18:1(11Z)/18:1(9Z)/18:3(6Z,9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049084	TG(18:1(11Z)/14/22:4(7Z,Z,13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048470	TG(16:1(9Z)/16/22:4(7Z,Z,13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0045348	TG(18/:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048794	TG(16:1(9Z)/:2n6/18:2(9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0045322	TG(18/18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044692	TG(18/14/22:5(7Z,Z,13Z,16Z,19Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049150	TG(18:1(11Z)/18/18:4(6Z,9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044959	TG(18/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044423	TG(16/22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048643	TG(16:1(9Z)/18:1(9Z)/:3n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048615	TG(16:1(9Z)/18:1(11Z)/:3(5Z,8Z,11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0045301	TG(18/18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049556	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/18:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049249	TG(18:1(11Z)/16:1(9Z)/:3n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0043905	TG(16/16/22:5(4Z,7Z,Z,13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042677	TG(14/22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042410	TG(14/:1(11Z)/:4(5Z,8Z,11Z,14Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044159	TG(16/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044369	TG(16/:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044132	TG(16/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048004	TG(14:1(9Z)/:3(5Z,8Z,11Z)/:1(11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042416	TG(14/:1(11Z)/:4(8Z,11Z,14Z,17Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044346	TG(16/:3n6/18:2(9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048259	TG(14:1(9Z)/18:3(9Z,12Z,15Z)/22:1(13Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042438	TG(14/:3(5Z,8Z,11Z)/:2n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044368	TG(16/:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042475	TG(14/22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044537	TG(16/:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6

HMDB0042771	TG(14/18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042874	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/18)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0047988	TG(14:1(9Z)/:1(11Z)/:3n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0043910	TG(16/16/22:5(7Z,Z,13Z,16Z,19Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044536	TG(16/:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044259	TG(16/18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042207	TG(14/:5(5Z,8Z,11Z,14Z,17Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044319	TG(16/:2n6/18:3(6Z,9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042700	TG(14/22:4(7Z,Z,13Z,16Z)/18:1(11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042845	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044265	TG(16/18:2(9Z,12Z)/:3n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044326	TG(16/:2n6/18:3(9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042583	TG(14/:2n6/:3(5Z,8Z,11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042589	TG(14/:2n6/:3n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0048039	TG(14:1(9Z)/22:1(13Z)/18:3(9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042382	TG(14/18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0047834	TG(14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044510	TG(16/18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044585	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/16)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044445	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/16)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0045674	TG(/14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0010479	TG(18:2(9Z,12Z)/18:1(11Z)/18:2(9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0034298	Glycerol 1,3-di-(9Z,12Z-octadecadienoate) 2-(9Z-octadecenoate)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0031115	Glycerol 1,2-di-(9Z,12Z-octadecadienoate) 3-(9Z-octadecenoate)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042178	TG(14/18/22:5(7Z,Z,13Z,16Z,19Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042352	TG(14/18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0042173	TG(14/18/22:5(4Z,7Z,Z,13Z,16Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0050457	TG(:1(11Z)/16:1(9Z)/18:3(6Z,9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0045705	TG(/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0050351	TG(:1(11Z)/16/18:4(6Z,9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0045499	TG(/14/:5(5Z,8Z,11Z,14Z,17Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0045680	TG(/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0050308	TG(:1(11Z)/14/:4(5Z,8Z,11Z,14Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0050314	TG(:1(11Z)/14/:4(8Z,11Z,14Z,17Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0046130	TG(/:4(8Z,11Z,14Z,17Z)/14:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0046105	TG(/18:4(6Z,9Z,12Z,15Z)/16:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0050440	TG(:1(11Z)/14:1(9Z)/:3n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0050464	TG(:1(11Z)/16:1(9Z)/18:3(9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0050908	TG(:3(5Z,8Z,11Z)/16/18:2(9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0046450	TG(22/14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0051419	TG(22:1(13Z)/14/18:4(6Z,9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0046858	TG(22/18:4(6Z,9Z,12Z,15Z)/14:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0051537	TG(22:1(13Z)/14:1(9Z)/18:3(9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0051530	TG(22:1(13Z)/14:1(9Z)/18:3(6Z,9Z,12Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0054344	TG(22:2(13Z,16Z)/14/18:3(9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0050874	TG(:3(5Z,8Z,11Z)/14/:2n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0053296	TG(:2n6/16/18:3(9Z,12Z,15Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0053265	TG(:2n6/14/:3n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0053355	TG(:2n6/14:1(9Z)/:2n6)	C57H100O6	M+NH4	898.7858	-1.6
HMDB0045974	TG(/:4(5Z,8Z,11Z,14Z)/14:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0050021	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/18:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0050161	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/18:1(9Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049408	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/18:1(11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0049555	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/18:1(11Z))	C57H100O6	M+NH4	898.7858	-1.6
HMDB0044264	TG(16/18:2(9Z,12Z)/:2n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0047944	TG(14:1(9Z)/18:1(11Z)/22:2(13Z,16Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042764	TG(14/18:3(9Z,12Z,15Z)/22:1(13Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044530	TG(16/:4(8Z,11Z,14Z,17Z)/18)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042409	TG(14/:1(11Z)/:3n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042554	TG(14/18:3(6Z,9Z,12Z)/22:1(13Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044097	TG(16/18:1(11Z)/:3n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0048031	TG(14:1(9Z)/22:1(13Z)/18:2(9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0048119	TG(14:1(9Z)/:2n6/:1(11Z))	C57H102O6	M+NH4	900.8015	-1.4

HMDB0042815	TG(14/4(8Z,11Z,14Z,17Z)/)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0005370	TG(16/18/4(5Z,8Z,11Z,14Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042676	TG(14/22:2(13Z,16Z)/18:2(9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0043936	TG(16/18/4(8Z,11Z,14Z,17Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044172	TG(16/3(5Z,8Z,11Z)/18:1(11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044286	TG(16/18:3(6Z,9Z,12Z)/:1(11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0047987	TG(14:1(9Z)/:1(11Z)/:2n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044158	TG(16/:1(11Z)/18:3(9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0048075	TG(14:1(9Z)/18:2(9Z,12Z)/22:1(13Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0047855	TG(14:1(9Z)/22/18:3(9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042694	TG(14/22:4(7Z,Z,13Z,16Z)/18)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042612	TG(14/:3n6/:1(11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042531	TG(14/18:2(9Z,12Z)/22:2(13Z,16Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044503	TG(16/18:4(6Z,9Z,12Z,15Z)/)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0048187	TG(14:1(9Z)/22:2(13Z,16Z)/18:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0047821	TG(14:1(9Z)/:3(5Z,8Z,11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044151	TG(16/:1(11Z)/18:3(6Z,9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0043963	TG(16/18:4(6Z,9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042786	TG(14/18:4(6Z,9Z,12Z,15Z)/22)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044173	TG(16/3(5Z,8Z,11Z)/18:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0048186	TG(14:1(9Z)/22:2(13Z,16Z)/18:1(11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042474	TG(14/22:1(13Z)/18:3(9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042235	TG(14/22/18:4(6Z,9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042206	TG(14//4(8Z,11Z,14Z,17Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044318	TG(16/:2n6/18:2(9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042467	TG(14/22:1(13Z)/18:3(6Z,9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0047967	TG(14:1(9Z)/18:1(9Z)/22:2(13Z,16Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044125	TG(16/18:1(9Z)/:3n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042588	TG(14/:2n6/:2n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042200	TG(14//4(5Z,8Z,11Z,14Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044362	TG(16/:4(5Z,8Z,11Z,14Z)/18)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042635	TG(14/4(5Z,8Z,11Z,14Z)/)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0049868	TG(18:1(9Z)/16:1(9Z)/:2n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0048662	TG(16:1(9Z)/:1(11Z)/18:2(9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045295	TG(18/18:3(9Z,12Z,15Z)/18:1(11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044686	TG(18/14/22:4(7Z,Z,13Z,16Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045106	TG(18/18:3(6Z,9Z,12Z)/18:1(11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044997	TG(18/:3(5Z,8Z,11Z)/16:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0005445	TG(16:1(9Z)/18:2(9Z,12Z)/:1(11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044924	TG(18/18:1(11Z)/18:3(6Z,9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044744	TG(18/16/4(8Z,11Z,14Z,17Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044958	TG(18/18:1(9Z)/18:3(9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0049388	TG(18:1(11Z)/18:2(9Z,12Z)/18:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0049743	TG(18:1(9Z)/16/:3(5Z,8Z,11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0052401	TG(18:2(9Z,12Z)/14/22:2(13Z,16Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0048516	TG(16:1(9Z)/18:3(9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0005411	TG(18/18:2(9Z,12Z)/18:2(9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0049230	TG(18:1(11Z)/14:1(9Z)/22:2(13Z,16Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0048509	TG(16:1(9Z)/18:3(6Z,9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0049267	TG(18:1(11Z)/18:1(11Z)/18:2(9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044770	TG(18/18/18:4(6Z,9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044931	TG(18/18:1(11Z)/18:3(9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0048642	TG(16:1(9Z)/18:1(9Z)/:2n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0049142	TG(18:1(11Z)/18/18:3(6Z,9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045107	TG(18/18:3(6Z,9Z,12Z)/18:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0049149	TG(18:1(11Z)/18/18:3(9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0049248	TG(18:1(11Z)/16:1(9Z)/:2n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0049288	TG(18:1(11Z)/18:1(9Z)/18:2(9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0049117	TG(18:1(11Z)/16/:3(5Z,8Z,11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0048483	TG(16:1(9Z)/18/:3(5Z,8Z,11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044893	TG(18/16:1(9Z)/:3(5Z,8Z,11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0048620	TG(16:1(9Z)/18:1(11Z)/:2n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0048601	TG(16:1(9Z)/16:1(9Z)/22:2(13Z,16Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0049123	TG(18:1(11Z)/16/:3n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045159	TG(18/:3n6/16:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4

HMDB0048788	TG(16:1(9Z)/:2n6/18:1(11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044738	TG(18/16:4(5Z,8Z,11Z,14Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044951	TG(18/18:1(9Z)/18:3(6Z,9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045296	TG(18/18:3(9Z,12Z,15Z)/18:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044899	TG(18/16:1(9Z)/:3n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0048789	TG(16:1(9Z)/:2n6/18:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0049387	TG(18:1(11Z)/18:2(9Z,12Z)/18:1(11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0048489	TG(16:1(9Z)/18:/:3n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0043904	TG(16/16/22:4(7Z,Z,13Z,16Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042432	TG(14:/3(5Z,8Z,11Z)/:1(11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0047848	TG(14:1(9Z)/22/18:3(6Z,9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0047827	TG(14:1(9Z)/:/:3n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044482	TG(16/18:3(9Z,12Z,15Z)/:1(11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042403	TG(14:/1(11Z)/:3(5Z,8Z,11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044091	TG(16/18:1(11Z)/:3(5Z,8Z,11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044119	TG(16/18:1(9Z)/:3(5Z,8Z,11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044341	TG(16:/3n6/18:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044340	TG(16:/3n6/18:1(11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0010456	TG(18:1(9Z)/18/18:3(9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0044417	TG(16/22:4(7Z,Z,13Z,16Z)/16)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045316	TG(18/18:4(6Z,9Z,12Z,15Z)/18)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0029554	Glycerol 1,2-di-(9Z,12Z-octadecadienoate) 3-octadecanoate	C57H102O6	M+NH4	900.8015	-1.4
HMDB0031114	Glycerol 1,3-di-(9Z,12Z-octadecadienoate) 2-octadecanoate	C57H102O6	M+NH4	900.8015	-1.4
HMDB0031113	Glycerol 1,3-di-(9Z-octadecenoate) 2-(9Z,12Z-octadecadienoate)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0046833	TG(22/18:3(9Z,12Z,15Z)/14:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0046658	TG(22/18:3(6Z,9Z,12Z)/14:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0051529	TG(22:1(13Z)/14:1(9Z)/18:2(9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0046275	TG(22/14/18:4(6Z,9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0053264	TG(:2n6/14:/:2n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045697	TG(/16:1(9Z)/18:3(6Z,9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045897	TG(/18:3(6Z,9Z,12Z)/16:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0050439	TG(:1(11Z)/14:1(9Z)/:2n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0051411	TG(22:1(13Z)/14/18:3(6Z,9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0046449	TG(22/14:1(9Z)/18:3(9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0042172	TG(14/18/22:4(7Z,Z,13Z,16Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0046442	TG(22/14:1(9Z)/18:3(6Z,9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0051418	TG(22:1(13Z)/14/18:3(9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045948	TG(/:3n6/14:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0050343	TG(:1(11Z)/16/18:3(6Z,9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0050301	TG(:1(11Z)/14:/:3(5Z,8Z,11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045704	TG(/16:1(9Z)/18:3(9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0052441	TG(18:2(9Z,12Z)/18/18:2(9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0050001	TG(18:1(9Z)/18:2(9Z,12Z)/18:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0050545	TG(18:1(9Z)/18:1(9Z)/18:2(9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0010474	TG(18:2(9Z,12Z)/16:/:2(11Z,14Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0052428	TG(18:2(9Z,12Z)/16:/:2(11Z,14Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0049749	TG(18:1(9Z)/16:/:3n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0049767	TG(18:1(9Z)/18/18:3(6Z,9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0049851	TG(18:1(9Z)/14:1(9Z)/22:2(13Z,16Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045492	TG(/14:4(5Z,8Z,11Z,14Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0050350	TG(:1(11Z)/16/18:3(9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0046079	TG(/18:3(9Z,12Z,15Z)/16:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045792	TG(/:3(5Z,8Z,11Z)/14:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045673	TG(/14:1(9Z)/:3n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0050456	TG(:1(11Z)/16:1(9Z)/18:2(9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0050307	TG(:1(11Z)/14:/:3n6)	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045667	TG(/14:1(9Z)/:3(5Z,8Z,11Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045549	TG(/16/18:4(6Z,9Z,12Z,15Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0045498	TG(/14:4(8Z,11Z,14Z,17Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0010458	TG(18:1(9Z)/18:1(11Z)/18:2(9Z,12Z))	C57H102O6	M+NH4	900.8015	-1.4
HMDB0048853	TG(16:1(9Z)/22:2(13Z,16Z)/16:1(9Z))	C57H102O6	M+NH4	900.8015	-1.4

902.5752	HMDB0009918	PI(22:5(7Z,Z,13Z,16Z,19Z)/16)	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009795	PI(16/22:5(4Z,7Z,Z,13Z,16Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009796	PI(16/22:5(7Z,Z,13Z,16Z,19Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009804	PI(16:2(9Z,12Z)/22:3(Z,13Z,16Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009832	PI(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009833	PI(18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009845	PI(18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009855	PI(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009854	PI(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009883	PI(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009916	PI(22:5(4Z,7Z,Z,13Z,16Z)/16)	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009908	PI(22:3(Z,13Z,16Z)/16:2(9Z,12Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009902	PI(:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009901	PI(:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009895	PI(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009896	PI(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009890	PI(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0009844	PI(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0062586	[(2R)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]({[(2R,3R,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid	C47H81O13P	M+NH4	902.5753	-0.1
	HMDB0047960	TG(14:1(9Z)/18:1(9Z)/22:1(13Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0044150	TG(16/:1(11Z)/18:2(9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0044096	TG(16/18:1(11Z)/:2n6)	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0044279	TG(16/18:3(6Z,9Z,12Z)/)	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0042756	TG(14/18:3(9Z,12Z,15Z)/22)	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0047981	TG(14:1(9Z)/:1(11Z)/:1(11Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0048026	TG(14:1(9Z)/22:1(13Z)/18:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0044071	TG(16/16:1(9Z)/22:2(13Z,16Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0047915	TG(14:1(9Z)/16:1(9Z)/24:1(15Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0044313	TG(16/:2n6/18:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0043929	TG(16/18/:3n6)	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0042524	TG(14/18:2(9Z,12Z)/22:1(13Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0042199	TG(14//:3n6)	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0048025	TG(14:1(9Z)/22:1(13Z)/18:1(11Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0044312	TG(16/:2n6/18:1(11Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0047806	TG(14:1(9Z)/18/22:2(13Z,16Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0047937	TG(14:1(9Z)/18:1(11Z)/22:1(13Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0042425	TG(14/:3(5Z,8Z,11Z)/)	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0042546	TG(14/18:3(6Z,9Z,12Z)/22)	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0044334	TG(16/:3n6/18)	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0005389	TG(16/18:2(9Z,12Z)/:1(11Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0042582	TG(14/:2n6/:1(11Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0042670	TG(14/22:2(13Z,16Z)/18:1(11Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0043923	TG(16/18/:3(5Z,8Z,11Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0042466	TG(14/22:1(13Z)/18:2(9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3

HMDB0042671	TG(14/22:2(13Z,16Z)/18:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0042408	TG(14/:1(11Z)/:2n6)	C57H104O6	M+NH4	902.8171	-1.3
HMDB0042381	TG(14/18:1(9Z)/22:2(13Z,16Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0044166	TG(16/:3(5Z,8Z,11Z)/18)	C57H104O6	M+NH4	902.8171	-1.3
HMDB0043955	TG(16//18:3(6Z,9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0042605	TG(14/:3n6/)	C57H104O6	M+NH4	902.8171	-1.3
HMDB0048594	TG(16:1(9Z)/16:1(9Z)/22:1(13Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0045079	TG(18/18:2(9Z,12Z)/18:1(11Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0005444	TG(16:1(9Z)/18:2(9Z,12Z)/)	C57H104O6	M+NH4	902.8171	-1.3
HMDB0048656	TG(16:1(9Z)/:1(11Z)/18:1(11Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0048508	TG(16:1(9Z)/18:2(9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0049242	TG(18:1(11Z)/16:1(9Z)/:1(11Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0044898	TG(18/16:1(9Z)/:2n6)	C57H104O6	M+NH4	902.8171	-1.3
HMDB0010447	TG(18:1(11Z)/18/18:2(9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0044395	TG(16/22:2(13Z,16Z)/16:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0048614	TG(16:1(9Z)/18:1(11Z)/:1(11Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0044769	TG(18/18/18:3(9Z,12Z,15Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0005405	TG(18/18:1(9Z)/18:2(9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0049083	TG(18:1(11Z)/14/22:2(13Z,16Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0045132	TG(18/:2n6/16:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0048488	TG(16:1(9Z)/18/:2n6)	C57H104O6	M+NH4	902.8171	-1.3
HMDB0047847	TG(14:1(9Z)/22/18:2(9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0044124	TG(16/18:1(9Z)/:2n6)	C57H104O6	M+NH4	902.8171	-1.3
HMDB0044475	TG(16/18:3(9Z,12Z,15Z)/)	C57H104O6	M+NH4	902.8171	-1.3
HMDB0044874	TG(18/14:1(9Z)/22:2(13Z,16Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0045080	TG(18/18:2(9Z,12Z)/18:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0044923	TG(18/18:1(11Z)/18:2(9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0049122	TG(18:1(11Z)/16/:2n6)	C57H104O6	M+NH4	902.8171	-1.3
HMDB0049283	TG(18:1(11Z)/18:1(9Z)/18:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0049262	TG(18:1(11Z)/18:1(11Z)/18:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0048573	TG(16:1(9Z)/14:1(9Z)/24:1(15Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0048657	TG(16:1(9Z)/:1(11Z)/18:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0044737	TG(18/16/:3n6)	C57H104O6	M+NH4	902.8171	-1.3
HMDB0044731	TG(18/16/:3(5Z,8Z,11Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0005439	TG(16:1(9Z)/18:1(9Z)/:1(11Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0042193	TG(14//:3(5Z,8Z,11Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0042227	TG(14/22/18:3(6Z,9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0042234	TG(14/22/18:3(9Z,12Z,15Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0047826	TG(14:1(9Z)/:2n6)	C57H104O6	M+NH4	902.8171	-1.3
HMDB0048047	TG(14:1(9Z)/24:1(15Z)/16:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0043962	TG(16//18:3(9Z,12Z,15Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0045289	TG(18/18:3(9Z,12Z,15Z)/18)	C57H104O6	M+NH4	902.8171	-1.3
HMDB0045100	TG(18/18:3(6Z,9Z,12Z)/18)	C57H104O6	M+NH4	902.8171	-1.3
HMDB0031108	Tripetroselinin	C57H104O6	M+NH4	902.8171	-1.3
HMDB0010457	TG(18:1(9Z)/18:1(11Z)/18:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0005453	TG(18:1(9Z)/18:1(9Z)/18:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0045871	TG(/18:2(9Z,12Z)/16:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0045212	TG(18/22:2(13Z,16Z)/14:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0050306	TG(:1(11Z)/14/:2n6)	C57H104O6	M+NH4	902.8171	-1.3
HMDB0045922	TG(/:2n6/14:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0051410	TG(22:1(13Z)/14/18:2(9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0046441	TG(22/14:1(9Z)/18:2(9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0046267	TG(22/14/18:3(6Z,9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0046633	TG(22/18:2(9Z,12Z)/14:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0046274	TG(22/14/18:3(9Z,12Z,15Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0042351	TG(14/18:1(11Z)/22:2(13Z,16Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0045672	TG(14:1(9Z)/:2n6)	C57H104O6	M+NH4	902.8171	-1.3
HMDB0045548	TG(/16/18:3(9Z,12Z,15Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0049223	TG(18:1(11Z)/14:1(9Z)/22:1(13Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0044762	TG(18/18/18:3(6Z,9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0048469	TG(16:1(9Z)/16/22:2(13Z,16Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0049711	TG(18:1(9Z)/14/22:2(13Z,16Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0049844	TG(18:1(9Z)/14:1(9Z)/22:1(13Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0049862	TG(18:1(9Z)/16:1(9Z)/:1(11Z))	C57H104O6	M+NH4	902.8171	-1.3
HMDB0049766	TG(18:1(9Z)/18/18:2(9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3

	HMDB0010452	TG(18:1(9Z)/16:2(11Z,14Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0049748	TG(18:1(9Z)/16:2(11Z,14Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0045491	TG(/14:3n6)	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0050342	TG(:1(11Z)/16/18:2(9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0045541	TG(/16/18:3(6Z,9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0045696	TG(/16:1(9Z)/18:2(9Z,12Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0045485	TG(/14:3(5Z,8Z,11Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0048699	TG(16:1(9Z)/22:1(13Z)/16:1(9Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0049261	TG(18:1(11Z)/18:1(11Z)/18:1(11Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0050433	TG(:1(11Z)/14:1(9Z)/:1(11Z))	C57H104O6	M+NH4	902.8171	-1.3
	HMDB0049282	TG(18:1(11Z)/18:1(9Z)/18:1(11Z))	C57H104O6	M+NH4	902.8171	-1.3
904.5903	HMDB0009914	PI(22:4(7Z,Z,13Z,16Z)/16)	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009912	PI(22:4(Z,13Z,16Z,19Z)/16)	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009793	PI(16/22:4(Z,13Z,16Z,19Z))	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009794	PI(16/22:4(7Z,Z,13Z,16Z))	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009816	PI(18/4(8Z,11Z,14Z,17Z))	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009830	PI(18:1(11Z)/:3(5Z,8Z,11Z))	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009831	PI(18:1(11Z)/:3(8Z,11Z,14Z))	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009842	PI(18:1(9Z)/:3(5Z,8Z,11Z))	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009843	PI(18:1(9Z)/:3(8Z,11Z,14Z))	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009853	PI(18:2(9Z,12Z)/:2(11Z,14Z))	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009900	PI(:4(8Z,11Z,14Z,17Z)/18)	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009894	PI(:4(5Z,8Z,11Z,14Z)/18)	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009889	PI(:3(8Z,11Z,14Z)/18:1(9Z))	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009888	PI(:3(8Z,11Z,14Z)/18:1(11Z))	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009882	PI(:3(5Z,8Z,11Z)/18:1(9Z))	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009881	PI(:3(5Z,8Z,11Z)/18:1(11Z))	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009877	PI(:2(11Z,14Z)/18:2(9Z,12Z))	C47H83O13P	M+NH4	904.5910	-0.7
	HMDB0009815	PI(18/4(5Z,8Z,11Z,14Z))	C47H83O13P	M+NH4	904.5910	-0.7
906.7565	HMDB0052424	TG(18:2(9Z,12Z)/15/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043709	TG(15/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043445	TG(15/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043620	TG(15/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043507	TG(15/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043422	TG(15/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043731	TG(15/:5(5Z,8Z,11Z,14Z,17Z)/:3n6)	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043450	TG(15/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0052870	TG(18:3(6Z,9Z,12Z)/15/22:5(7Z,Z,13Z,16Z,19Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0052865	TG(18:3(6Z,9Z,12Z)/15/22:5(4Z,7Z,Z,13Z,16Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043333	TG(15/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043786	TG(15/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043535	TG(15/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043529	TG(15/:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043765	TG(15/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043703	TG(15/:4(8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043592	TG(15/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043725	TG(15/:5(5Z,8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C58H96O6	M+NH4	906.7545	2.2

	HMDB0043758	TG(15/22:5(7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043676	TG(15/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043648	TG(15/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043653	TG(15/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043613	TG(15/22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0055159	TG(18:3(9Z,12Z,15Z)/15/22:5(7Z,Z,13Z,16Z,19Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0054023	TG(4(5Z,8Z,11Z,14Z)/15:4(5Z,8Z,11Z,14Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0055541	TG(4(8Z,11Z,14Z,17Z)/15:4(8Z,11Z,14Z,17Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0054918	TG(22:5(4Z,7Z,Z,13Z,16Z)/15/18:3(9Z,12Z,15Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0054029	TG(4(5Z,8Z,11Z,14Z)/15:4(8Z,11Z,14Z,17Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0054652	TG(22:4(7Z,Z,13Z,16Z)/15/18:4(6Z,9Z,12Z,15Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0050901	TG(3(5Z,8Z,11Z)/15:5(5Z,8Z,11Z,14Z,17Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0053673	TG(3n6/15:5(5Z,8Z,11Z,14Z,17Z))	C58H96O6	M+NH4	906.7545	2.2
	HMDB0043563	TG(15/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C58H100O6	M+NH4	910.7858	2.8
910.7884	HMDB0043415	TG(15/18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043499	TG(15:3n6/3n6)	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043271	TG(15/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043325	TG(15:3(5Z,8Z,11Z)/3n6)	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043276	TG(15/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043774	TG(15/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18)	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043242	TG(15/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043701	TG(15:4(8Z,11Z,14Z,17Z)/2n6)	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043607	TG(15/22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043752	TG(15/22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043471	TG(15:2n6/4(5Z,8Z,11Z,14Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043304	TG(15:1(11Z)/5(5Z,8Z,11Z,14Z,17Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043074	TG(15/18:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043583	TG(15/22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043675	TG(15/18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043724	TG(15:5(5Z,8Z,11Z,14Z,17Z)/1(11Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0050334	TG(1(11Z)/15:5(5Z,8Z,11Z,14Z,17Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0050893	TG(3(5Z,8Z,11Z)/15:3n6)	C58H100O6	M+NH4	910.7858	2.8
	HMDB0053279	TG(2n6/15:4(5Z,8Z,11Z,14Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0053285	TG(2n6/15:4(8Z,11Z,14Z,17Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0054355	TG(22:2(13Z,16Z)/15/18:4(6Z,9Z,12Z,15Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0053665	TG(3n6/15:3n6)	C58H100O6	M+NH4	910.7858	2.8
	HMDB0049738	TG(18:1(9Z)/15/22:5(7Z,Z,13Z,16Z,19Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0049733	TG(18:1(9Z)/15/22:5(4Z,7Z,Z,13Z,16Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043247	TG(15/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043751	TG(15/22:5(7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043319	TG(15:3(5Z,8Z,11Z)/3(5Z,8Z,11Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043493	TG(15:3n6/3(5Z,8Z,11Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043477	TG(15:2n6/4(8Z,11Z,14Z,17Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043606	TG(15/22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0043527	TG(15:4(5Z,8Z,11Z,14Z)/2n6)	C58H100O6	M+NH4	910.7858	2.8
	HMDB0044720	TG(18/15/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0049106	TG(18:1(11Z)/15/22:5(4Z,7Z,Z,13Z,16Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0049111	TG(18:1(11Z)/15/22:5(7Z,Z,13Z,16Z,19Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0052417	TG(18:2(9Z,12Z)/15/22:4(7Z,Z,13Z,16Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0050887	TG(3(5Z,8Z,11Z)/15:3(5Z,8Z,11Z))	C58H100O6	M+NH4	910.7858	2.8
	HMDB0050892	TG(3(5Z,8Z,11Z)/15:2n6)	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043600	TG(15/22:5(4Z,7Z,Z,13Z,16Z)/18)	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043101	TG(15:5(5Z,8Z,11Z,14Z,17Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043577	TG(15/22:4(7Z,Z,13Z,16Z)/18:1(11Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043464	TG(15:2n6/3(5Z,8Z,11Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043578	TG(15/22:4(7Z,Z,13Z,16Z)/18:1(9Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043498	TG(15:3n6/2n6)	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043073	TG(15/18/22:5(7Z,Z,13Z,16Z,19Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043470	TG(15:2n6/3n6)	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043562	TG(15/22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043303	TG(15:1(11Z)/4(8Z,11Z,14Z,17Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043668	TG(15/18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043555	TG(15/22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043521	TG(15:4(5Z,8Z,11Z,14Z)/1(11Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043324	TG(15:3(5Z,8Z,11Z)/2n6)	C58H102O6	M+NH4	912.8015	-1.3

912.8003	HMDB0043068	TG(15/18/22:5(4Z,7Z,Z,13Z,16Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043360	TG(15/22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0050327	TG(:1(11Z)/15:4(5Z,8Z,11Z,14Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0050333	TG(:1(11Z)/15:4(8Z,11Z,14Z,17Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0045525	TG(/15:5(5Z,8Z,11Z,14Z,17Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0049732	TG(18:1(9Z)/15/22:4(7Z,Z,13Z,16Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0052863	TG(18:3(6Z,9Z,12Z)/15/22:2(13Z,16Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0044714	TG(18/15/22:5(4Z,7Z,Z,13Z,16Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0044719	TG(18/15/22:5(7Z,Z,13Z,16Z,19Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0049105	TG(18:1(11Z)/15/22:4(7Z,Z,13Z,16Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043297	TG(15/:1(11Z)/:4(5Z,8Z,11Z,14Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043745	TG(15/22:5(7Z,Z,13Z,16Z,19Z)/18)	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043443	TG(15/18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043270	TG(15/18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043241	TG(15/18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043717	TG(15/:5(5Z,8Z,11Z,14Z,17Z)/)	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043695	TG(15/:4(8Z,11Z,14Z,17Z)/:1(11Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0043646	TG(15/18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0053278	TG(:2n6/15/:3n6)	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0054354	TG(22:2(13Z,16Z)/15/18:3(9Z,12Z,15Z))	C58H102O6	M+NH4	912.8015	-1.3
	HMDB0051436	TG(22:1(13Z)/15/18:4(6Z,9Z,12Z,15Z))	C58H102O6	M+NH4	912.8015	-1.3
914.8145	HMDB0046300	TG(22/15/18:4(6Z,9Z,12Z,15Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043100	TG(15//:4(8Z,11Z,14Z,17Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043128	TG(15/22/18:4(6Z,9Z,12Z,15Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043639	TG(15/18:3(9Z,12Z,15Z)/22:1(13Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043554	TG(15/22:2(13Z,16Z)/18:2(9Z,12Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043688	TG(15/:4(8Z,11Z,14Z,17Z)/)	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043296	TG(15/:1(11Z)/:3n6)	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043571	TG(15/22:4(7Z,Z,13Z,16Z)/18)	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043290	TG(15/:1(11Z)/:3(5Z,8Z,11Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043359	TG(15/22:1(13Z)/18:3(9Z,12Z,15Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043469	TG(15/:2n6/:2n6)	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043067	TG(15/18/22:4(7Z,Z,13Z,16Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043094	TG(15//:4(5Z,8Z,11Z,14Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043492	TG(15/:3n6/:1(11Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0051435	TG(22:1(13Z)/15/18:3(9Z,12Z,15Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0053277	TG(:2n6/15/:2n6)	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0045524	TG(/15:4(8Z,11Z,14Z,17Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0050326	TG(:1(11Z)/15/:3n6)	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0045518	TG(/15:4(5Z,8Z,11Z,14Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0050320	TG(:1(11Z)/15/:3(5Z,8Z,11Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0052416	TG(18:2(9Z,12Z)/15/22:2(13Z,16Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0044713	TG(18/15/22:4(7Z,Z,13Z,16Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043436	TG(15/18:3(6Z,9Z,12Z)/22:1(13Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043352	TG(15/22:1(13Z)/18:3(6Z,9Z,12Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043660	TG(15/18:4(6Z,9Z,12Z,15Z)/22)	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043514	TG(15/:4(5Z,8Z,11Z,14Z)/)	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043318	TG(15/:3(5Z,8Z,11Z)/:1(11Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0043414	TG(15/18:2(9Z,12Z)/22:2(13Z,16Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0051428	TG(22:1(13Z)/15/18:3(6Z,9Z,12Z))	C58H104O6	M+NH4	914.8171	-2.9
	HMDB0052794	TG(18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
	HMDB0050235	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
	HMDB0053072	TG(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C59H94O6	M+NH4	916.7389	1.0
	HMDB0053183	TG(18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/:3n6)	C59H94O6	M+NH4	916.7389	1.0
	HMDB0053176	TG(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
	HMDB0055209	TG(18:3(9Z,12Z,15Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
	HMDB0050197	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
	HMDB0052969	TG(18:3(6Z,9Z,12Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0

HMDB0053170	TG(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055408	TG(18:4(6Z,9Z,12Z,15Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055459	TG(18:4(6Z,9Z,12Z,15Z)/:2n6/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0052752	TG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0052760	TG(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0052647	TG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0052766	TG(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0052780	TG(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055311	TG(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0049633	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0052787	TG(18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0053202	TG(18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0052690	TG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0053021	TG(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0053105	TG(18:3(6Z,9Z,12Z)/:3n6/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055233	TG(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055275	TG(18:3(9Z,12Z,15Z)/:3n6/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055413	TG(18:4(6Z,9Z,12Z,15Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0054021	TG(:4(5Z,8Z,11Z,14Z)/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0054192	TG(:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055573	TG(:4(8Z,11Z,14Z,17Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0054182	TG(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0053946	TG(:3n6/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055539	TG(:4(8Z,11Z,14Z,17Z)/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055686	TG(:5(5Z,8Z,11Z,14Z,17Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0054107	TG(:4(5Z,8Z,11Z,14Z)/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0054968	TG(22:5(4Z,7Z,Z,13Z,16Z)/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0054097	TG(:4(5Z,8Z,11Z,14Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0051305	TG(:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0051169	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055448	TG(18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055373	TG(18:4(6Z,9Z,12Z,15Z)/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055419	TG(18:4(6Z,9Z,12Z,15Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0053851	TG(:3n6/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0051295	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0

916.7398

HMDB0051312	TG(:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0053935	TG(:3n6/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0053747	TG(:3n6/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0053583	TG(:2n6/18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0051011	TG(:3(5Z,8Z,11Z)/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0054708	TG(22:4(7Z,Z,13Z,16Z)/14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0042926	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0042920	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048176	TG(14:1(9Z)/:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0042868	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048226	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048242	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048021	TG(14:1(9Z)/:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048159	TG(14:1(9Z)/:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048248	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0042839	TG(14/:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048336	TG(14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048373	TG(14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3(5Z,8Z,11Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0044527	TG(16/18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0042897	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048363	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048314	TG(14:1(9Z)/:4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048379	TG(14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3n6)	C59H94O6	M+NH4	916.7389	1.0
HMDB0042747	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048319	TG(14:1(9Z)/:4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0042863	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048981	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0049002	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0049044	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048939	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048996	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055262	TG(18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0049593	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0053065	TG(18:3(6Z,9Z,12Z)/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0053118	TG(18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0

HMDB0010508	TG(18:3(9Z,12Z,15Z)/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0049037	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0049023	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048181	TG(14:1(9Z)/:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0042659	TG(14/:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048357	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0044581	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048955	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048960	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048849	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048785	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0048913	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0044635	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0053078	TG(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0010513	TG(18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0054092	TG(:4(5Z,8Z,11Z,14Z)/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055323	TG(18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0054269	TG(:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055577	TG(:4(8Z,11Z,14Z,17Z)/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0054975	TG(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0054913	TG(22:5(4Z,7Z,Z,13Z,16Z)/14/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0055693	TG(:5(5Z,8Z,11Z,14Z,17Z)/16/:5(5Z,8Z,11Z,14Z,17Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0053111	TG(18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0053195	TG(18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C59H94O6	M+NH4	916.7389	1.0
HMDB0053064	TG(18:3(6Z,9Z,12Z)/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0010500	TG(18:3(9Z,12Z,15Z)/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0050177	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053071	TG(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z)/:3n6)	C59H96O6	M+NH4	918.7545	-1.1
HMDB0049572	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0055268	TG(18:3(9Z,12Z,15Z)/:2n6/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0049632	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052751	TG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052779	TG(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1

HMDB0010504	TG(18:3(9Z,12Z,15Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0049486	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052675	TG(18:2(9Z,12Z)/:3n6/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052640	TG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0050095	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052682	TG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0055214	TG(18:3(9Z,12Z,15Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0050234	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053091	TG(18:3(6Z,9Z,12Z)/:2n6/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0049612	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052745	TG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053169	TG(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z)/:3n6)	C59H96O6	M+NH4	918.7545	-1.1
HMDB0010493	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052885	TG(18:3(6Z,9Z,12Z)/16:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053104	TG(18:3(6Z,9Z,12Z)/:3n6/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0050196	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0049592	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053058	TG(18:3(6Z,9Z,12Z)/18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0050227	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052968	TG(18:3(6Z,9Z,12Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052786	TG(18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0050037	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0050190	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053020	TG(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0055208	TG(18:3(9Z,12Z,15Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052981	TG(18:3(6Z,9Z,12Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052585	TG(18:2(9Z,12Z)/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052995	TG(18:3(6Z,9Z,12Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052689	TG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0055255	TG(18:3(9Z,12Z,15Z)/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0051027	TG(:3(5Z,8Z,11Z)/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0050885	TG(:3(5Z,8Z,11Z)/14:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0051151	TG(:3(5Z,8Z,11Z)/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0051168	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053366	TG(:2n6/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0051304	TG(:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053582	TG(:2n6/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1

HMDB0051161	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0051287	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0051294	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0051005	TG(:3(5Z,8Z,11Z)/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0051010	TG(:3(5Z,8Z,11Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053934	TG(:3n6/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0054127	TG(:4(5Z,8Z,11Z,14Z)/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0054091	TG(:4(5Z,8Z,11Z,14Z)/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0010527	TG(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0054116	TG(:4(5Z,8Z,11Z,14Z)/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053741	TG(:3n6/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053479	TG(:2n6/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052646	TG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z)/4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052759	TG(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/:3n6)	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052529	TG(18:2(9Z,12Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053182	TG(18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/:2n6)	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052963	TG(18:3(6Z,9Z,12Z)/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0049586	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/4(5Z,8Z,11Z,14Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0050769	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0055418	TG(18:4(6Z,9Z,12Z,15Z)/18:1(9Z)/4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0055372	TG(18:4(6Z,9Z,12Z,15Z)/16:22:5(7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0055377	TG(18:4(6Z,9Z,12Z,15Z)/18:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0055412	TG(18:4(6Z,9Z,12Z,15Z)/18:1(11Z)/4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053663	TG(:3n6/14:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053839	TG(:3n6/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053746	TG(:3n6/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053757	TG(:3n6/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053570	TG(:2n6/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053850	TG(:3n6/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0054041	TG(:4(5Z,8Z,11Z,14Z)/16:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0042890	TG(14:22:5(7Z,Z,13Z,16Z,19Z)/4(5Z,8Z,11Z,14Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048313	TG(14:1(9Z)/4(8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048378	TG(14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:2n6)	C59H96O6	M+NH4	918.7545	-1.1
HMDB0044385	TG(16:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048235	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0042838	TG(14:4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0042449	TG(14:/3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048225	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048219	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/4(5Z,8Z,11Z,14Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0042629	TG(14:/3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048153	TG(14:1(9Z)/:3n6/22:5(4Z,7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0042913	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3(5Z,8Z,11Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0042658	TG(14:/4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0042833	TG(14:/4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048158	TG(14:1(9Z)/:3n6/22:5(7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048175	TG(14:1(9Z)/4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048350	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:3(5Z,8Z,11Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048241	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:3n6)	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048020	TG(14:1(9Z)/:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048356	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:3n6)	C59H96O6	M+NH4	918.7545	-1.1

HMDB0044553	TG(16/:4(8Z,11Z,14Z,17Z):/5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0042919	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z):/3n6)	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048136	TG(14:1(9Z):/2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0042862	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0042717	TG(14/22:4(7Z,Z,13Z,16Z):/5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0044499	TG(16/18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0042740	TG(14/22:5(4Z,7Z,Z,13Z,16Z):/4(5Z,8Z,11Z,14Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0042653	TG(14/:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0044526	TG(16/18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048905	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048827	TG(16:1(9Z):/3n6/:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0049036	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048779	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0049425	TG(18:1(11Z)/18:3(6Z,9Z,12Z):/5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048933	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048891	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0045339	TG(18/18:4(6Z,9Z,12Z,15Z):/5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048980	TG(16:1(9Z):/4(8Z,11Z,14Z,17Z):/4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048848	TG(16:1(9Z):/4(5Z,8Z,11Z,14Z):/4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048938	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0045391	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0049022	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0044627	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048695	TG(16:1(9Z):/3(5Z,8Z,11Z):/5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0050215	TG(18:1(9Z):/4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0052772	TG(18:2(9Z,12Z):/4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0049015	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048954	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0044303	TG(16/18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0042896	TG(14/22:5(7Z,Z,13Z,16Z,19Z):/4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0042746	TG(14/22:5(4Z,7Z,Z,13Z,16Z):/4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048015	TG(14:1(9Z):/3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0044521	TG(16/18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048989	TG(16:1(9Z):/5(5Z,8Z,11Z,14Z,17Z):/3(5Z,8Z,11Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048912	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048974	TG(16:1(9Z):/4(8Z,11Z,14Z,17Z):/4(5Z,8Z,11Z,14Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0005448	TG(16:1(9Z):/4(5Z,8Z,11Z,14Z):/4(5Z,8Z,11Z,14Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0044574	TG(16/:5(5Z,8Z,11Z,14Z,17Z):/4(5Z,8Z,11Z,14Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0044467	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0044634	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048763	TG(16:1(9Z)/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048995	TG(16:1(9Z):/5(5Z,8Z,11Z,14Z,17Z):/3n6)	C59H96O6	M+NH4	918.7545	-1.1
HMDB0044607	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0048784	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0044580	TG(16/:5(5Z,8Z,11Z,14Z,17Z):/4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1

HMDB0049625	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0055538	TG(:4(8Z,11Z,14Z,17Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0055274	TG(18:3(9Z,12Z,15Z)/:3n6/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0055232	TG(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0055423	TG(18:4(6Z,9Z,12Z,15Z)/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0055547	TG(:4(8Z,11Z,14Z,17Z)/16/:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0054707	TG(22:4(7Z,Z,13Z,16Z)/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0054106	TG(:4(5Z,8Z,11Z,14Z)/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0054974	TG(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z)/18:3(9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0054912	TG(22:5(4Z,7Z,Z,13Z,16Z)/14/:4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0054927	TG(22:5(4Z,7Z,Z,13Z,16Z)/16/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0054715	TG(22:4(7Z,Z,13Z,16Z)/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0054015	TG(:4(5Z,8Z,11Z,14Z)/14/22:5(4Z,7Z,Z,13Z,16Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0054020	TG(:4(5Z,8Z,11Z,14Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0054645	TG(22:4(7Z,Z,13Z,16Z)/14/:5(5Z,8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0055576	TG(:4(8Z,11Z,14Z,17Z)/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0054100	TG(:4(5Z,8Z,11Z,14Z)/16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053097	TG(18:3(6Z,9Z,12Z)/:3n6/18:3(6Z,9Z,12Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0053013	TG(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C59H96O6	M+NH4	918.7545	-1.1
HMDB0049585	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/:3n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049955	TG(18:1(9Z)/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049478	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052523	TG(18:2(9Z,12Z)/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0055213	TG(18:3(9Z,12Z,15Z)/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052681	TG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052667	TG(18:2(9Z,12Z)/:3n6/18:3(6Z,9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050207	TG(18:1(9Z)/:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053083	TG(18:3(6Z,9Z,12Z)/:2n6/18:3(6Z,9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052674	TG(18:2(9Z,12Z)/:3n6/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050189	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:3n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052962	TG(18:3(6Z,9Z,12Z)/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052994	TG(18:3(6Z,9Z,12Z)/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0055166	TG(18:3(9Z,12Z,15Z)/16/22:5(7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049579	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052631	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0010476	TG(18:2(9Z,12Z)/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049465	TG(18:1(11Z)/:3n6/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052758	TG(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/:2n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049604	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052528	TG(18:2(9Z,12Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0055220	TG(18:3(9Z,12Z,15Z)/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0005475	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053057	TG(18:3(6Z,9Z,12Z)/18:2(9Z,12Z)/:3n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050176	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049565	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053090	TG(18:3(6Z,9Z,12Z)/:2n6/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049624	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050075	TG(18:1(9Z)/:3n6/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052980	TG(18:3(6Z,9Z,12Z)/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048805	TG(16:1(9Z)/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048820	TG(16:1(9Z)/:3n6/:4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048653	TG(16:1(9Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052639	TG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z)/:3n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052879	TG(18:3(6Z,9Z,12Z)/16/22:5(4Z,7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049571	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052744	TG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/:3n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052988	TG(18:3(6Z,9Z,12Z)/18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050183	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C59H98O6	M+NH4	920.7702	-1.5

HMDB0050214	TG(18:1(9Z)/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053070	TG(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z)/:2n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049485	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052584	TG(18:2(9Z,12Z)/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0055172	TG(18:3(9Z,12Z,15Z)/18:/:5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0045383	TG(18:/:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0055226	TG(18:3(9Z,12Z,15Z)/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053750	TG(:3n6/16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053466	TG(:2n6/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053365	TG(:2n6/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0051143	TG(:3(5Z,8Z,11Z)/18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0051026	TG(:3(5Z,8Z,11Z)/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053569	TG(:2n6/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053657	TG(:3n6/14/22:5(4Z,7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0055376	TG(18:4(6Z,9Z,12Z,15Z)/18:/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0046121	TG(/18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050761	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053740	TG(:3n6/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053756	TG(:3n6/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050919	TG(:3(5Z,8Z,11Z)/16:/:5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0051286	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053685	TG(:3n6/16:/:5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0051150	TG(:3(5Z,8Z,11Z)/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0051160	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053360	TG(:2n6/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053478	TG(:2n6/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053275	TG(:2n6/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053767	TG(:3n6/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050768	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050450	TG(:1(11Z)/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050617	TG(:1(11Z)/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052660	TG(18:2(9Z,12Z)/:2n6/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050017	TG(18:1(9Z)/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052897	TG(18:3(6Z,9Z,12Z)/18:/:5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050226	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050170	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053007	TG(18:3(6Z,9Z,12Z)/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052771	TG(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049611	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050030	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052542	TG(18:2(9Z,12Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050094	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050750	TG(:1(11Z)/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052577	TG(18:2(9Z,12Z)/:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049879	TG(18:1(9Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052884	TG(18:3(6Z,9Z,12Z)/16/22:5(7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050087	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0052974	TG(18:3(6Z,9Z,12Z)/18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0055267	TG(18:3(9Z,12Z,15Z)/:2n6/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049339	TG(18:1(11Z)/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0010483	TG(18:2(9Z,12Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053168	TG(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z)/:2n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0045123	TG(18/18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044546	TG(16:/:4(8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0042883	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/:3(5Z,8Z,11Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048355	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:2n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048240	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:2n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044493	TG(16/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0042918	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:2n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044357	TG(16:/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048335	TG(14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0005392	TG(16:/:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0042623	TG(14:/:3n6/22:5(4Z,7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044297	TG(16/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044189	TG(16:/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5

HMDB0044275	TG(16/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048212	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048203	TG(14:1(9Z)/22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048218	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/:3n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0042443	TG(14/:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048372	TG(14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:1(11Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0042733	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048152	TG(14:1(9Z)/:3n6/22:4(7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048130	TG(14:1(9Z)/:2n6/22:5(4Z,7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0042448	TG(14/:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0042832	TG(14/:4(8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044384	TG(16/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0042739	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/:3n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0047998	TG(14:1(9Z)/:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048135	TG(14:1(9Z)/:2n6/22:5(7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0042628	TG(14/:3n6/22:5(7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0042652	TG(14/:4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0042599	TG(14/:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048631	TG(16:1(9Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048994	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/:2n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049031	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048694	TG(16:1(9Z)/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048883	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049404	TG(18:1(11Z)/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048904	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0045338	TG(18/18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049030	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044466	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048778	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048932	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048841	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/:3n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0045332	TG(18/18:4(6Z,9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044573	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/:3n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044626	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048762	TG(16:1(9Z)/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049014	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048967	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044459	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049418	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049424	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044567	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048835	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048826	TG(16:1(9Z)/:3n6/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048890	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0042889	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/:3n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044520	TG(16/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048014	TG(14:1(9Z)/:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0042710	TG(14/22:4(7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044498	TG(16/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044552	TG(16/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0042716	TG(14/22:4(7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0045202	TG(18/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0049259	TG(18:1(11Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0045312	TG(18/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048973	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/:3n6)	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044606	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048757	TG(16:1(9Z)/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0045390	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044599	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044439	TG(16/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0048688	TG(16:1(9Z)/:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0045364	TG(18/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0044302	TG(16/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053377	TG(:2n6/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0055381	TG(18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5

HMDB0055546	TG:(4(8Z,11Z,14Z,17Z)/16:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0054034	TG:(4(5Z,8Z,11Z,14Z)/16:4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0010523	TG:(4(5Z,8Z,11Z,14Z)/18:1(9Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050884	TG:(3(5Z,8Z,11Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050879	TG:(3(5Z,8Z,11Z)/14/22:5(4Z,7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0051061	TG:(3(5Z,8Z,11Z)/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053662	TG:(3n6/14/22:5(7Z,Z,13Z,16Z,19Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0051043	TG:(3(5Z,8Z,11Z)/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053779	TG:(3n6/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0051020	TG:(3(5Z,8Z,11Z)/16:1(9Z)/4(5Z,8Z,11Z,14Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0053838	TG:(3n6/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0054714	TG(22:4(7Z,Z,13Z,16Z)/16:1(9Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0054050	TG:(4(5Z,8Z,11Z,14Z)/18/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0054417	TG(22:2(13Z,16Z)/14:1(9Z)/5(5Z,8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0054644	TG(22:4(7Z,Z,13Z,16Z)/14:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0054014	TG:(4(5Z,8Z,11Z,14Z)/14/22:4(7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0054040	TG:(4(5Z,8Z,11Z,14Z)/16:4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0054115	TG:(4(5Z,8Z,11Z,14Z)/18:1(11Z)/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0054661	TG(22:4(7Z,Z,13Z,16Z)/16/18:4(6Z,9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0054926	TG(22:5(4Z,7Z,Z,13Z,16Z)/16/18:3(9Z,12Z,15Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0051004	TG:(3(5Z,8Z,11Z)/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0050036	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/4(8Z,11Z,14Z,17Z))	C59H98O6	M+NH4	920.7702	-1.5
HMDB0005462	TG(18:1(9Z)/18:2(9Z,12Z)/4(5Z,8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050086	TG(18:1(9Z)/4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053006	TG(18:3(6Z,9Z,12Z)/1(11Z)/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050206	TG(18:1(9Z)/4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052666	TG(18:2(9Z,12Z)/3n6/18:2(9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050188	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/2n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052570	TG(18:2(9Z,12Z)/1(11Z)/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049873	TG(18:1(9Z)/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050016	TG(18:1(9Z)/18:2(9Z,12Z)/4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0010455	TG(18:1(9Z)/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0010469	TG(18:2(9Z,12Z)/16/22:5(7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049947	TG(18:1(9Z)/3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049477	TG(18:1(11Z)/4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050163	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/3(5Z,8Z,11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052743	TG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/2n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049619	TG(18:1(11Z)/5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052576	TG(18:2(9Z,12Z)/3(5Z,8Z,11Z)/18:2(9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052909	TG(18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050029	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/3n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053056	TG(18:3(6Z,9Z,12Z)/18:2(9Z,12Z)/2n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050074	TG(18:1(9Z)/3n6/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052890	TG(18:3(6Z,9Z,12Z)/18:4(5Z,8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049464	TG(18:1(11Z)/3n6/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0055177	TG(18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050023	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/3(5Z,8Z,11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049457	TG(18:1(11Z)/3n6/18:3(6Z,9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049878	TG(18:1(9Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049403	TG(18:1(11Z)/18:2(9Z,12Z)/4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049253	TG(18:1(11Z)/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045013	TG(18:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044598	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048756	TG(16:1(9Z)/18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048953	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045194	TG(18:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048630	TG(16:1(9Z)/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048499	TG(16:1(9Z)/18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045356	TG(18:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048652	TG(16:1(9Z)/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044621	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049417	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/3n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049338	TG(18:1(11Z)/3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0010480	TG(18:2(9Z,12Z)/18:1(11Z)/4(5Z,8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049558	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/3(5Z,8Z,11Z))	C59H100O6	M+NH4	922.7858	-1.3

HMDB0048647	TG(16:1(9Z)/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048840	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/:2n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049133	TG(18:1(11Z)/16:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048625	TG(16:1(9Z)/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045311	TG(18/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045382	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045305	TG(18/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048898	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049299	TG(18:1(11Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052659	TG(18:2(9Z,12Z)/:2n6/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0051019	TG(:3(5Z,8Z,11Z)/16:1(9Z)/:3n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050616	TG(:1(11Z)/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050742	TG(:1(11Z)/18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050467	TG(:1(11Z)/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050317	TG(:1(11Z)/14:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0046113	TG(/18:4(6Z,9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0046120	TG(/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050760	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0046095	TG(/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050598	TG(:1(11Z)/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050449	TG(:1(11Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050444	TG(:1(11Z)/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045913	TG(/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0046208	TG(/22:6(4Z,7Z,Z,13Z,16Z,19Z)/14:1(9Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053299	TG(:2n6/16/:5(5Z,8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053684	TG(:3n6/16/:4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050918	TG(:3(5Z,8Z,11Z)/16/:4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053376	TG(:2n6/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050935	TG(:3(5Z,8Z,11Z)/18/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053274	TG(:2n6/14/22:5(7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0051142	TG(:3(5Z,8Z,11Z)/18:2(9Z,12Z)/18:2(9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053656	TG(:3n6/14/22:4(7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0051060	TG(:3(5Z,8Z,11Z)/18:1(9Z)/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053388	TG(:2n6/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050749	TG(:1(11Z)/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045683	TG(/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050609	TG(:1(11Z)/18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052878	TG(18:3(6Z,9Z,12Z)/16:22:4(7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052433	TG(18:2(9Z,12Z)/16:22:5(4Z,7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049444	TG(18:1(11Z)/:2n6/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049603	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049564	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/:3n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050055	TG(18:1(9Z)/:2n6/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052987	TG(18:3(6Z,9Z,12Z)/18:1(9Z)/:3n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052973	TG(18:3(6Z,9Z,12Z)/18:1(11Z)/:3n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049897	TG(18:1(9Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052896	TG(18:3(6Z,9Z,12Z)/18/:4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049954	TG(18:1(9Z)/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0055171	TG(18:3(9Z,12Z,15Z)/18/:4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052652	TG(18:2(9Z,12Z)/:2n6/18:3(6Z,9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052452	TG(18:2(9Z,12Z)/18/:5(5Z,8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052556	TG(18:2(9Z,12Z)/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052550	TG(18:2(9Z,12Z)/18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049584	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/:2n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0010464	TG(18:1(9Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052522	TG(18:2(9Z,12Z)/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0010492	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052624	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052638	TG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z)/:2n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050067	TG(18:1(9Z)/:3n6/18:3(6Z,9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049331	TG(18:1(11Z)/:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052541	TG(18:2(9Z,12Z)/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050169	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/:3n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044539	TG(16/:4(8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044182	TG(16/:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3

HMDB0047997	TG(14:1(9Z)/:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044545	TG(16/:4(8Z,11Z,14Z,17Z)/:3n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044296	TG(16/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044188	TG(16/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0042861	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0042419	TG(14/:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044135	TG(16/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044371	TG(16/:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0042622	TG(14/:3n6/22:4(7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0042888	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/:2n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044350	TG(16/:3n6/:4(5Z,8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044274	TG(16/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048312	TG(14:1(9Z)/:4(8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048196	TG(14:1(9Z)/22:2(13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048042	TG(14:1(9Z)/22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048202	TG(14:1(9Z)/22:2(13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044492	TG(16/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0042738	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/:2n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044377	TG(16/:4(5Z,8Z,11Z,14Z)/:3n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048129	TG(14:1(9Z)/:2n6/22:4(7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044438	TG(16/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049397	TG(18:1(11Z)/18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048972	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/:2n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049009	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045363	TG(18/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048687	TG(16:1(9Z)/:3(5Z,8Z,11Z)/:3n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049278	TG(18:1(11Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048869	TG(16:1(9Z)/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045096	TG(18/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045116	TG(18/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049258	TG(18:1(11Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048899	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045325	TG(18/18:4(6Z,9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048804	TG(16:1(9Z)/:2n6/:4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048882	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044620	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049411	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045175	TG(18/:3n6/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045122	TG(18/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045201	TG(18/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048798	TG(16:1(9Z)/:2n6/:4(5Z,8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044458	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044572	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/:2n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045429	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044909	TG(18/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048681	TG(16:1(9Z)/:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048813	TG(16:1(9Z)/:3n6/:3(5Z,8Z,11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044329	TG(16/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0042442	TG(14/:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0042703	TG(14/22:4(7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0042593	TG(14/:2n6/22:5(4Z,7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044107	TG(16/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048328	TG(14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:1(13Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0047992	TG(14:1(9Z)/:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044356	TG(16/:3n6/:4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0042912	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:1(11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048174	TG(14:1(9Z)/:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0042598	TG(14/:2n6/22:5(7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048217	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/:2n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0047837	TG(14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048673	TG(16:1(9Z)/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048988	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/:1(11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049008	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0045331	TG(18/18:4(6Z,9Z,12Z,15Z)/:3n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048819	TG(16:1(9Z)/:3n6/:3n6)	C59H100O6	M+NH4	922.7858	-1.3

HMDB0044431	TG(16/22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048234	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:1(11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048349	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:1(11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0042709	TG(14/22:4(7Z,Z,13Z,16Z)/:3n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0044269	TG(16/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0042687	TG(14/22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0055225	TG(18:3(9Z,12Z,15Z)/:1(11Z)/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053749	TG(:3n6/16:1(9Z)/:3n6)	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053778	TG(:3n6/18:1(9Z)/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053401	TG(:2n6/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0051053	TG(:3(5Z,8Z,11Z)/18:1(9Z)/18:3(6Z,9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050878	TG(:3(5Z,8Z,11Z)/14/22:4(7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053695	TG(:3n6/18/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053359	TG(:2n6/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050912	TG(:3(5Z,8Z,11Z)/16/:4(5Z,8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053269	TG(:2n6/14/22:5(4Z,7Z,Z,13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053465	TG(:2n6/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0051042	TG(:3(5Z,8Z,11Z)/18:1(11Z)/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053766	TG(:3n6/18:1(11Z)/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053370	TG(:2n6/16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0051035	TG(:3(5Z,8Z,11Z)/18:1(11Z)/18:3(6Z,9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0054090	TG(:4(5Z,8Z,11Z,14Z)/14:1(9Z)/22:2(13Z,16Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0051540	TG(22:1(13Z)/14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0054425	TG(22:2(13Z,16Z)/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0054347	TG(22:2(13Z,16Z)/14:5(5Z,8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0054660	TG(22:4(7Z,Z,13Z,16Z)/16/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0054416	TG(22:2(13Z,16Z)/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0010521	TG(:4(5Z,8Z,11Z,14Z)/18/18:3(9Z,12Z,15Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0053678	TG(:3n6/16/:4(5Z,8Z,11Z,14Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0050221	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0049618	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0052999	TG(18:3(6Z,9Z,12Z)/:1(11Z)/18:3(6Z,9Z,12Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0051013	TG(:3(5Z,8Z,11Z)/16:1(9Z)/:3(5Z,8Z,11Z))	C59H100O6	M+NH4	922.7858	-1.3
HMDB0048818	TG(16:1(9Z)/:3n6/:2n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044903	TG(18/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048686	TG(16:1(9Z)/:3(5Z,8Z,11Z)/:2n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044593	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045298	TG(18/18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045174	TG(18/:3n6/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049396	TG(18:1(11Z)/18:2(9Z,12Z)/:3n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044934	TG(18/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049292	TG(18:1(11Z)/18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044566	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/:1(11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049127	TG(18:1(11Z)/16/22:5(4Z,7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045012	TG(18/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049416	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/:2n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045330	TG(18/18:4(6Z,9Z,12Z,15Z)/:2n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049152	TG(18:1(11Z)/18/:5(5Z,8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045115	TG(18/18:3(6Z,9Z,12Z)/:3n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048791	TG(16:1(9Z)/:2n6/:3(5Z,8Z,11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044411	TG(16/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045267	TG(18/22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048715	TG(16:1(9Z)/22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048493	TG(16:1(9Z)/18/22:5(4Z,7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049390	TG(18:1(11Z)/18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044747	TG(18/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048624	TG(16:1(9Z)/18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044452	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045193	TG(18/:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048834	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/:1(11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048931	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045402	TG(18/22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048797	TG(16:1(9Z)/:2n6/:3n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048498	TG(16:1(9Z)/18/22:5(7Z,Z,13Z,16Z,19Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045376	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C59H102O6	M+NH4	924.8015	-1.9

HMDB0044961	TG(18/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048777	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044592	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048876	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:1(11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045355	TG(18/4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045167	TG(18/3n6/18:3(6Z,9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044908	TG(18/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048861	TG(16:1(9Z)/22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049132	TG(18:1(11Z)/16/22:5(7Z,Z,13Z,16Z,19Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048519	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044614	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048646	TG(16:1(9Z)/18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045304	TG(18/18:3(9Z,12Z,15Z)/:3n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048672	TG(16:1(9Z)/:1(11Z)/:4(8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045005	TG(18/3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045377	TG(18/5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049271	TG(18:1(11Z)/18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048946	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048868	TG(16:1(9Z)/22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044430	TG(16/22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049277	TG(18:1(11Z)/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045148	TG(18/2n6/18:4(6Z,9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045677	TG(/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049890	TG(18:1(9Z)/18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052889	TG(18:3(6Z,9Z,12Z)/18/:3n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052451	TG(18:2(9Z,12Z)/18/:4(8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052651	TG(18:2(9Z,12Z)/:2n6/18:2(9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050168	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/:2n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052562	TG(18:2(9Z,12Z)/:1(11Z)/18:3(6Z,9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049456	TG(18:1(11Z)/:3n6/18:2(9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049330	TG(18:1(11Z)/:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049578	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050009	TG(18:1(9Z)/18:2(9Z,12Z)/:3n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050182	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049436	TG(18:1(11Z)/:2n6/18:3(6Z,9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050003	TG(18:1(9Z)/18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052534	TG(18:2(9Z,12Z)/18:1(11Z)/:3n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050741	TG(:1(11Z)/18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0046094	TG(/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050484	TG(:1(11Z)/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045905	TG(/18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052465	TG(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049443	TG(18:1(11Z)/:2n6/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049916	TG(18:1(9Z)/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049935	TG(18:1(9Z)/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050054	TG(18:1(9Z)/:2n6/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049472	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0010491	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/:2(11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052623	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/:2(11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049946	TG(18:1(9Z)/:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050028	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/:2n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049563	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/:2n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049872	TG(18:1(9Z)/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050066	TG(18:1(9Z)/:3n6/18:2(9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0010454	TG(18:1(9Z)/16/22:5(7Z,Z,13Z,16Z,19Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052908	TG(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048877	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:1(9Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0005443	TG(16:1(9Z)/:1(11Z)/:4(5Z,8Z,11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044453	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049252	TG(18:1(11Z)/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048966	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/:1(11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045095	TG(18/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052569	TG(18:2(9Z,12Z)/:1(11Z)/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052432	TG(18:2(9Z,12Z)/16/22:4(7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0005456	TG(18:1(9Z)/18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9

HMDB0049753	TG(18:1(9Z)/16/22:5(4Z,7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052445	TG(18:2(9Z,12Z)/18:4(5Z,8Z,11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052961	TG(18:3(6Z,9Z,12Z)/16:1(9Z)/22:2(13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049777	TG(18:1(9Z)/18:5(5Z,8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049896	TG(18:1(9Z)/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049598	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052972	TG(18:3(6Z,9Z,12Z)/18:1(11Z)/:2n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052986	TG(18:3(6Z,9Z,12Z)/18:1(9Z)/:2n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050047	TG(18:1(9Z)/:2n6/18:3(6Z,9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0010485	TG(18:2(9Z,12Z)/18:1(9Z)/:3(8Z,11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052549	TG(18:2(9Z,12Z)/18:1(9Z)/:3(8Z,11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049318	TG(18:1(11Z)/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049298	TG(18:1(11Z)/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045109	TG(18/18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0005412	TG(18/18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048151	TG(14:1(9Z)/:3n6/22:2(13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0042854	TG(14/:5(5Z,8Z,11Z,14Z,17Z)/22:1(13Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048189	TG(14:1(9Z)/22:2(13Z,16Z)/:3(5Z,8Z,11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044519	TG(16/18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0043939	TG(16/18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0042413	TG(14/:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044101	TG(16/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044376	TG(16/:4(5Z,8Z,11Z,14Z)/:2n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0047991	TG(14:1(9Z)/:1(11Z)/22:4(7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044106	TG(16/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048063	TG(14:1(9Z)/24:1(15Z)/18:4(6Z,9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044322	TG(16/:2n6/:4(5Z,8Z,11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0042686	TG(14/22:2(13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044343	TG(16/:3n6/:3(5Z,8Z,11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048013	TG(14:1(9Z)/:3(5Z,8Z,11Z)/22:2(13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044134	TG(16/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044161	TG(16/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0042477	TG(14/22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048195	TG(14:1(9Z)/22:2(13Z,16Z)/:3n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0042732	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/:1(11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0042418	TG(14/:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044181	TG(16/:3(5Z,8Z,11Z)/:3n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044268	TG(16/18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0042680	TG(14/22:2(13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048305	TG(14:1(9Z)/:4(8Z,11Z,14Z,17Z)/22:1(13Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044544	TG(16/:4(8Z,11Z,14Z,17Z)/:2n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0042708	TG(14/22:4(7Z,Z,13Z,16Z)/:2n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044175	TG(16/:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0042209	TG(14//22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048167	TG(14:1(9Z)/:4(5Z,8Z,11Z,14Z)/22:1(13Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048211	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/:1(11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0042592	TG(14/:2n6/22:4(7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044349	TG(16/:3n6/:3n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048283	TG(14:1(9Z)/18:4(6Z,9Z,12Z,15Z)/24:1(15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044328	TG(16/:2n6/:4(8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0042831	TG(14/:4(8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048035	TG(14:1(9Z)/22:1(13Z)/:4(5Z,8Z,11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0047831	TG(14:1(9Z)/:22:5(4Z,7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0047836	TG(14:1(9Z)/:22:5(7Z,Z,13Z,16Z,19Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0048041	TG(14:1(9Z)/22:1(13Z)/:4(8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0042651	TG(14/:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0042882	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/:1(11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0042905	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0044129	TG(16/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0047858	TG(14:1(9Z)/22/:5(5Z,8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050590	TG(:1(11Z)/18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0054346	TG(22:2(13Z,16Z)/14/:4(8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0051533	TG(22:1(13Z)/14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052039	TG(24:1(15Z)/14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0046452	TG(22/14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9

HMDB0053739	TG(:3n6/14:1(9Z)/22:2(13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0053387	TG(:2n6/18:1(11Z)/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0051003	TG(:3(5Z,8Z,11Z)/14:1(9Z)/22:2(13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0053400	TG(:2n6/18:1(9Z)/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0053310	TG(:2n6/18/18:4(6Z,9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0053292	TG(:2n6/16:4(5Z,8Z,11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0053268	TG(:2n6/14/22:4(7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0051421	TG(22:1(13Z)/14:5(5Z,8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0054365	TG(22:2(13Z,16Z)/16/18:4(6Z,9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0046908	TG(22:5(5Z,8Z,11Z,14Z,17Z)/14:1(9Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0051555	TG(22:1(13Z)/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0051539	TG(22:1(13Z)/14:1(9Z)/4(8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0054424	TG(22:2(13Z,16Z)/16:1(9Z)/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0054013	TG(:4(5Z,8Z,11Z,14Z)/14/22:2(13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050911	TG(:3(5Z,8Z,11Z)/16:3n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0053694	TG(:3n6/18/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045887	TG(/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045501	TG(/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050311	TG(:1(11Z)/14/22:5(4Z,7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050597	TG(:1(11Z)/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045682	TG(/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0046112	TG(/18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0046087	TG(/18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0046052	TG(/22:5(4Z,7Z,Z,13Z,16Z)/14:1(9Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0046182	TG(/22:5(7Z,Z,13Z,16Z,19Z)/14:1(9Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045707	TG(/16:1(9Z)/5(5Z,8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050316	TG(:1(11Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050353	TG(:1(11Z)/16:5(5Z,8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050608	TG(:1(11Z)/18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0045912	TG(/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050927	TG(:3(5Z,8Z,11Z)/18/18:3(6Z,9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050934	TG(:3(5Z,8Z,11Z)/18/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0051034	TG(:3(5Z,8Z,11Z)/18:1(11Z)/18:2(9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0053298	TG(:2n6/16:4(8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0051052	TG(:3(5Z,8Z,11Z)/18:1(9Z)/18:2(9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0053369	TG(:2n6/16:1(9Z)/:3n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0051018	TG(:3(5Z,8Z,11Z)/16:1(9Z)/:2n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050466	TG(:1(11Z)/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050503	TG(:1(11Z)/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050443	TG(:1(11Z)/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050460	TG(:1(11Z)/16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0046157	TG(/:5(5Z,8Z,11Z,14Z,17Z)/16:1(9Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050081	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050201	TG(18:1(9Z)/:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049471	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049597	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0052901	TG(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0053677	TG(:3n6/16:3n6)	C59H102O6	M+NH4	924.8015	-1.9
HMDB0050905	TG(:3(5Z,8Z,11Z)/16:3(5Z,8Z,11Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0055176	TG(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C59H102O6	M+NH4	924.8015	-1.9
HMDB0049557	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/:1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049285	TG(18:1(11Z)/18:1(9Z)/:3(5Z,8Z,11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048860	TG(16:1(9Z)/22:2(13Z,16Z)/18:2(9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045166	TG(18/:3n6/18:2(9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049395	TG(18:1(11Z)/18:2(9Z,12Z)/:2n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048665	TG(16:1(9Z)/:1(11Z)/:3n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049291	TG(18:1(11Z)/18:1(9Z)/:3n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049410	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/:1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044772	TG(18/18:5(5Z,8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048812	TG(16:1(9Z)/:3n6/:1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049264	TG(18:1(11Z)/18:1(11Z)/:3(5Z,8Z,11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045349	TG(18/:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0005429	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048714	TG(16:1(9Z)/22:1(13Z)/18:3(9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0052877	TG(18:3(6Z,9Z,12Z)/16/22:2(13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5

HMDB0010463	TG(18:1(9Z)/18:1(9Z)/:3(8Z,11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049909	TG(18:1(9Z)/18:1(9Z)/:3(8Z,11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044933	TG(18/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048796	TG(16:1(9Z)/:2n6/:2n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048539	TG(16:1(9Z)/22/18:4(6Z,9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044425	TG(16/22:4(7Z,Z,13Z,16Z)/18:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048659	TG(16:1(9Z)/:1(11Z)/:3(5Z,8Z,11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044424	TG(16/22:4(7Z,Z,13Z,16Z)/18:1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049145	TG(18:1(11Z)/18/:4(5Z,8Z,11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044927	TG(18/18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044902	TG(18/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044986	TG(18/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049270	TG(18:1(11Z)/18:1(11Z)/:3n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045350	TG(18/:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045303	TG(18/18:3(9Z,12Z,15Z)/:2n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045114	TG(18/18:3(6Z,9Z,12Z)/:2n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048707	TG(16:1(9Z)/22:1(13Z)/18:3(6Z,9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044215	TG(16/22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044586	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/18)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045082	TG(18/18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045088	TG(18/18:2(9Z,12Z)/:3n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048755	TG(16:1(9Z)/18:2(9Z,12Z)/22:2(13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045240	TG(18/22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044741	TG(18/16/22:5(4Z,7Z,Z,13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044410	TG(16/22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045147	TG(18/:2n6/18:3(9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044446	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/18)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048924	TG(16:1(9Z)/18:3(9Z,12Z,15Z)/22:1(13Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0005406	TG(18/18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045187	TG(18/:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044746	TG(18/16/22:5(7Z,Z,13Z,16Z,19Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044960	TG(18/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044559	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048492	TG(16:1(9Z)/18/22:4(7Z,Z,13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048518	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049126	TG(18:1(11Z)/16/22:4(7Z,Z,13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048680	TG(16:1(9Z)/:3(5Z,8Z,11Z)/:1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044403	TG(16/22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045188	TG(18/:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049317	TG(18:1(11Z)/:1(11Z)/18:3(9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045879	TG(/18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB00050453	TG(:1(11Z)/16:1(9Z)/:3(5Z,8Z,11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045500	TG(/14/22:5(7Z,Z,13Z,16Z,19Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB00050483	TG(:1(11Z)/18:1(11Z)/18:3(9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB00050310	TG(:1(11Z)/14/22:4(7Z,Z,13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB00050459	TG(:1(11Z)/16:1(9Z)/:3n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB00050346	TG(:1(11Z)/16/:4(5Z,8Z,11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045700	TG(/16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045886	TG(/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045495	TG(/14/22:5(4Z,7Z,Z,13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB00050502	TG(:1(11Z)/18:1(9Z)/18:3(9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB00050495	TG(:1(11Z)/18:1(9Z)/18:3(6Z,9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0046106	TG(/18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045731	TG(/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0046086	TG(/18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045904	TG(/18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045757	TG(/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB00050352	TG(:1(11Z)/16/:4(8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045676	TG(/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0046026	TG(/22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045551	TG(/16/:5(5Z,8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB00050476	TG(:1(11Z)/18:1(11Z)/18:3(6Z,9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045975	TG(/:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB00050370	TG(:1(11Z)/18/18:4(6Z,9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0046107	TG(/18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5

926.8148

HMDB0046131	TG(/:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0005473	TG(18:2(9Z,12Z)/18:2(9Z,12Z):1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0052888	TG(18:3(6Z,9Z,12Z)/18:/:2n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049171	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049934	TG(18:1(9Z)/:1(11Z)/18:3(9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0010462	TG(18:1(9Z)/18:1(9Z):/3(5Z,8Z,11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049889	TG(18:1(9Z)/18:1(11Z):/3n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049770	TG(18:1(9Z)/18:/4(5Z,8Z,11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0050008	TG(18:1(9Z)/18:2(9Z,12Z):/2n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0052464	TG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049435	TG(18:1(11Z):/2n6/18:2(9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049325	TG(18:1(11Z):/3(5Z,8Z,11Z)/18:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049927	TG(18:1(9Z):/1(11Z)/18:3(6Z,9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049451	TG(18:1(11Z):/3n6/18:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0050162	TG(18:1(9Z)/18:3(9Z,12Z,15Z):/1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0052521	TG(18:2(9Z,12Z)/16:1(9Z)/22:2(13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0050046	TG(18:1(9Z):/2n6/18:2(9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0052533	TG(18:2(9Z,12Z)/18:1(11Z):/2n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049752	TG(18:1(9Z)/16/22:4(7Z,Z,13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0050022	TG(18:1(9Z)/18:3(6Z,9Z,12Z):/1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0052457	TG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0052561	TG(18:2(9Z,12Z):/1(11Z)/18:2(9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049883	TG(18:1(9Z)/18:1(11Z):/3(5Z,8Z,11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049795	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049776	TG(18:1(9Z)/18:/4(8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0010484	TG(18:2(9Z,12Z)/18:1(9Z):/2(11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0052548	TG(18:2(9Z,12Z)/18:1(9Z):/2(11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0052444	TG(18:2(9Z,12Z)/18:/3n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049310	TG(18:1(11Z):/1(11Z)/18:3(6Z,9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049151	TG(18:1(11Z)/18:/4(8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045140	TG(18:/:2n6/18:3(6Z,9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048144	TG(14:1(9Z):/3n6/22:1(13Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042203	TG(14/22:5(4Z,7Z,Z,13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048034	TG(14:1(9Z)/22:1(13Z):/3n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042505	TG(14/24:1(15Z)/18:4(6Z,9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044180	TG(16:/3(5Z,8Z,11Z):/2n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0043938	TG(16/18/22:5(7Z,Z,13Z,16Z,19Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042237	TG(14/22:/5(5Z,8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044370	TG(16:/4(5Z,8Z,11Z,14Z):/1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044491	TG(16/18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048194	TG(14:1(9Z)/22:2(13Z,16Z):/2n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044315	TG(16:/2n6:/3(5Z,8Z,11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042875	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042846	TG(14:/5(5Z,8Z,11Z,14Z,17Z)/22)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045004	TG(18:/3(5Z,8Z,11Z)/18:2(9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048770	TG(16:1(9Z)/18:3(6Z,9Z,12Z)/22:1(13Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045324	TG(18/18:4(6Z,9Z,12Z,15Z):/1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044160	TG(16:/1(11Z):/4(8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044128	TG(16/18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042795	TG(14/18:4(6Z,9Z,12Z,15Z)/24:1(15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044512	TG(16/18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0005387	TG(16:/1(11Z):/4(5Z,8Z,11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042621	TG(14:/3n6/22:2(13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0047857	TG(14:1(9Z)/22:/4(8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044538	TG(16:/4(8Z,11Z,14Z,17Z):/1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042824	TG(14:/4(8Z,11Z,14Z,17Z)/22:1(13Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0043965	TG(16//:5(5Z,8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048260	TG(14:1(9Z)/18:3(9Z,12Z,15Z)/24:1(15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042208	TG(14/22:5(7Z,Z,13Z,16Z,19Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042702	TG(14/22:4(7Z,Z,13Z,16Z):/1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042725	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048128	TG(14:1(9Z):/2n6/22:2(13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048099	TG(14:1(9Z)/18:3(6Z,9Z,12Z)/24:1(15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042679	TG(14/22:2(13Z,16Z):/3n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0047851	TG(14:1(9Z)/22:/4(5Z,8Z,11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5

HMDB0047830	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042412	TG(14:1(11Z)/22:4(7Z,Z,13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042441	TG(14:3(5Z,8Z,11Z)/22:2(13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042673	TG(14/22:2(13Z,16Z)/3(5Z,8Z,11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048055	TG(14:1(9Z)/24:1(15Z)/18:3(6Z,9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0043933	TG(16/18/22:5(4Z,7Z,Z,13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042644	TG(14:4(5Z,8Z,11Z,14Z)/22:1(13Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044295	TG(16/18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044100	TG(16/18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048062	TG(14:1(9Z)/24:1(15Z)/18:3(9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044321	TG(16/:2n6/:3n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0047879	TG(14:1(9Z)/24/18:4(6Z,9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048028	TG(14:1(9Z)/22:1(13Z)/3(5Z,8Z,11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042476	TG(14/22:1(13Z)/4(8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0042470	TG(14/22:1(13Z)/4(5Z,8Z,11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0048006	TG(14:1(9Z)/3(5Z,8Z,11Z)/22:1(13Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044348	TG(16/:3n6/:2n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045706	TG(/16:1(9Z)/4(8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0045370	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/18)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0050589	TG(:1(11Z)/18:2(9Z,12Z)/18:2(9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0052038	TG(24:1(15Z)/14:1(9Z)/18:3(9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0047191	TG(24/14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0047582	TG(24/18:4(6Z,9Z,12Z,15Z)/14:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0046859	TG(22/18:4(6Z,9Z,12Z,15Z)/16:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0051547	TG(22:1(13Z)/16:1(9Z)/18:3(6Z,9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0051927	TG(24:1(15Z)/14/18:4(6Z,9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0053655	TG(:3n6/14/22:2(13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0050877	TG(:3(5Z,8Z,11Z)/14/22:2(13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0053368	TG(:2n6/16:1(9Z)/:2n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0050996	TG(:3(5Z,8Z,11Z)/14:1(9Z)/22:1(13Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0053291	TG(:2n6/16/:3n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0053309	TG(:2n6/18/18:3(9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0050926	TG(:3(5Z,8Z,11Z)/18/18:2(9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0050910	TG(:3(5Z,8Z,11Z)/16/:2n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0051414	TG(22:1(13Z)/14/:4(5Z,8Z,11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0046451	TG(22/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0046475	TG(22/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0046277	TG(22/14/:5(5Z,8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0051532	TG(22:1(13Z)/14:1(9Z)/:3n6)	C59H104O6	M+NH4	926.8171	-2.5
HMDB0046733	TG(22/:4(5Z,8Z,11Z,14Z)/14:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0051420	TG(22:1(13Z)/14/:4(8Z,11Z,14Z,17Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0046445	TG(22/14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0046883	TG(22/:4(8Z,11Z,14Z,17Z)/14:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0051554	TG(22:1(13Z)/16:1(9Z)/18:3(9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0054364	TG(22:2(13Z,16Z)/16/18:3(9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0051453	TG(22:1(13Z)/16/18:4(6Z,9Z,12Z,15Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0052031	TG(24:1(15Z)/14:1(9Z)/18:3(6Z,9Z,12Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0053358	TG(:2n6/14:1(9Z)/22:2(13Z,16Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049450	TG(18:1(11Z)/:3n6/18:1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049324	TG(18:1(11Z)/3(5Z,8Z,11Z)/18:1(11Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0049941	TG(18:1(9Z)/3(5Z,8Z,11Z)/18:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0050061	TG(18:1(9Z)/:3n6/18:1(9Z))	C59H104O6	M+NH4	926.8171	-2.5
HMDB0044926	TG(18/18:1(11Z)/:3n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048854	TG(16:1(9Z)/22:2(13Z,16Z)/18:1(11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048855	TG(16:1(9Z)/22:2(13Z,16Z)/18:1(9Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049138	TG(18:1(11Z)/18/:3(5Z,8Z,11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044998	TG(18/:3(5Z,8Z,11Z)/18:1(11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0005398	TG(18/18/:4(5Z,8Z,11Z,14Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048790	TG(16:1(9Z)/:2n6/:1(11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045161	TG(18/:3n6/18:1(9Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045297	TG(18/18:3(9Z,12Z,15Z)/:1(11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044999	TG(18/:3(5Z,8Z,11Z)/18:1(9Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045317	TG(18/18:4(6Z,9Z,12Z,15Z)/)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045087	TG(18/18:2(9Z,12Z)/:2n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049389	TG(18:1(11Z)/18:2(9Z,12Z)/:1(11Z))	C59H106O6	M+NH4	928.8328	-2.7

HMDB0044920	TG(18/18:1(11Z)/:3(5Z,8Z,11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049269	TG(18:1(11Z)/18:1(11Z)/:2n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048511	TG(16:1(9Z)/:3n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048645	TG(16:1(9Z)/18:1(9Z)/22:2(13Z,16Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049144	TG(18:1(11Z)/18/:3n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044214	TG(16/22:1(13Z)/18:3(9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045139	TG(18/:2n6/18:2(9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0043991	TG(16/22/18:4(6Z,9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044418	TG(16/22:4(7Z,Z,13Z,16Z)/18)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044953	TG(18/18:1(9Z)/:3n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048664	TG(16:1(9Z)/:1(11Z)/:2n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044288	TG(16/18:3(6Z,9Z,12Z)/22:1(13Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0047990	TG(14:1(9Z)/:1(11Z)/22:2(13Z,16Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042614	TG(14/:3n6/22:1(13Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042202	TG(14/22:4(7Z,Z,13Z,16Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042463	TG(14/22:1(13Z)/:3(5Z,8Z,11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042816	TG(14/:4(8Z,11Z,14Z,17Z)/22)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044363	TG(16/:4(5Z,8Z,11Z,14Z)/)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042591	TG(14/:2n6/22:2(13Z,16Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042765	TG(14/18:3(9Z,12Z,15Z)/24:1(15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0047871	TG(14:1(9Z)/24/18:3(6Z,9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042678	TG(14/22:2(13Z,16Z)/:2n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044771	TG(18/18/:4(8Z,11Z,14Z,17Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044740	TG(18/16/22:4(7Z,Z,13Z,16Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049290	TG(18:1(11Z)/18:1(9Z)/:2n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042695	TG(14/22:4(7Z,Z,13Z,16Z)/)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042265	TG(14/24/18:4(6Z,9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042434	TG(14/:3(5Z,8Z,11Z)/22:1(13Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044342	TG(16/:3n6/:1(11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042230	TG(14/22/:4(5Z,8Z,11Z,14Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042497	TG(14/24:1(15Z)/18:3(6Z,9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042236	TG(14/22/:4(8Z,11Z,14Z,17Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049251	TG(18:1(11Z)/16:1(9Z)/22:2(13Z,16Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045899	TG(/18:3(6Z,9Z,12Z)/18:1(9Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0050041	TG(18:1(9Z)/:2n6/18:1(9Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049163	TG(18:1(11Z)//18:3(6Z,9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0005460	TG(18:1(9Z)/18:2(9Z,12Z)/:1(11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049430	TG(18:1(11Z)/:2n6/18:1(9Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049871	TG(18:1(9Z)/16:1(9Z)/22:2(13Z,16Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049763	TG(18:1(9Z)/18/:3(5Z,8Z,11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049769	TG(18:1(9Z)/18/:3n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049170	TG(18:1(11Z)//18:3(9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049794	TG(18:1(9Z)//18:3(9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045756	TG(/18:1(9Z)/18:3(9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0046080	TG(/18:3(9Z,12Z,15Z)/18:1(11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0050458	TG(:1(11Z)/16:1(9Z)/:2n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045550	TG(/16/:4(8Z,11Z,14Z,17Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0050369	TG(:1(11Z)/18/18:3(9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045793	TG(/:3(5Z,8Z,11Z)/16:1(9Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0050362	TG(:1(11Z)/18/18:3(6Z,9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0050494	TG(:1(11Z)/18:1(9Z)/18:2(9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045494	TG(/14/22:4(7Z,Z,13Z,16Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0046081	TG(/18:3(9Z,12Z,15Z)/18:1(9Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045949	TG(/:3n6/16:1(9Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0052431	TG(18:2(9Z,12Z)/16/22:2(13Z,16Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049309	TG(18:1(11Z)/:1(11Z)/18:2(9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0005472	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048531	TG(16:1(9Z)/22/18:3(6Z,9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044402	TG(16/22:2(13Z,16Z)/18:2(9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044985	TG(18/:1(11Z)/18:3(9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048748	TG(16:1(9Z)/18:2(9Z,12Z)/22:1(13Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044207	TG(16/22:1(13Z)/18:3(6Z,9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048538	TG(16:1(9Z)/22/18:3(9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048505	TG(16:1(9Z)/:3(5Z,8Z,11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044978	TG(18/:1(11Z)/18:3(6Z,9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7

HMDB0044797	TG(18/18:4(6Z,9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044947	TG(18/18:1(9Z)/:3(5Z,8Z,11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045160	TG(18/:3n6/18:1(11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0010461	TG(18:1(9Z)/18:1(9Z)/:2(11Z,14Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049908	TG(18:1(9Z)/18:1(9Z)/:2(11Z,14Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0052443	TG(18:2(9Z,12Z)/18/:2n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049787	TG(18:1(9Z)/:18:3(6Z,9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049926	TG(18:1(9Z)/:1(11Z)/18:2(9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0052456	TG(18:2(9Z,12Z)/:18:2(9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049888	TG(18:1(9Z)/18:1(11Z)/:2n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0049429	TG(18:1(11Z)/:2n6/18:1(11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048706	TG(16:1(9Z)/22:1(13Z)/18:2(9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048623	TG(16:1(9Z)/18:1(11Z)/22:2(13Z,16Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045108	TG(18/18:3(6Z,9Z,12Z)/:1(11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042504	TG(14/24:1(15Z)/18:3(9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0047844	TG(14:1(9Z)/22/:3(5Z,8Z,11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0005373	TG(16//:4(5Z,8Z,11Z,14Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044153	TG(16/:1(11Z)/:3n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042636	TG(14/:4(5Z,8Z,11Z,14Z)/22)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048054	TG(14:1(9Z)/24:1(15Z)/18:2(9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048076	TG(14:1(9Z)/18:2(9Z,12Z)/24:1(15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044504	TG(16/18:4(6Z,9Z,12Z,15Z)/22)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044531	TG(16/:4(8Z,11Z,14Z,17Z)/)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044147	TG(16/:1(11Z)/:3(5Z,8Z,11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042555	TG(14/18:3(6Z,9Z,12Z)/24:1(15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0047878	TG(14:1(9Z)/24/18:3(9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0047850	TG(14:1(9Z)/22/:3n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048121	TG(14:1(9Z)/:2n6/22:1(13Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044320	TG(16/:2n6/:2n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0043964	TG(16//:4(8Z,11Z,14Z,17Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044174	TG(16/:3(5Z,8Z,11Z)/:1(11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0043932	TG(16/18:22:4(7Z,Z,13Z,16Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044267	TG(16/18:2(9Z,12Z)/22:2(13Z,16Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042469	TG(14/22:1(13Z)/:3n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0044484	TG(16/18:3(9Z,12Z,15Z)/22:1(13Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0042787	TG(14/18:4(6Z,9Z,12Z,15Z)/24)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048188	TG(14:1(9Z)/22:2(13Z,16Z)/:1(11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0048033	TG(14:1(9Z)/22:1(13Z)/:2n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045181	TG(18/:4(5Z,8Z,11Z,14Z)/18)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045343	TG(18/:4(8Z,11Z,14Z,17Z)/18)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045723	TG(/18:1(11Z)/18:3(6Z,9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045878	TG(/18:2(9Z,12Z)/18:2(9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0046558	TG(22/:3(5Z,8Z,11Z)/14:1(9Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0047390	TG(24/18:3(6Z,9Z,12Z)/14:1(9Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0046659	TG(22/18:3(6Z,9Z,12Z)/16:1(9Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0046474	TG(22/16:1(9Z)/18:3(9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0046467	TG(22/16:1(9Z)/18:3(6Z,9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0051919	TG(24:1(15Z)/14/18:3(6Z,9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0051413	TG(22:1(13Z)/14/:3n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0046270	TG(22/14/:4(5Z,8Z,11Z,14Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0052030	TG(24:1(15Z)/14:1(9Z)/18:2(9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0046708	TG(22/:3n6/14:1(9Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0046444	TG(22/14:1(9Z)/:3n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0051531	TG(22:1(13Z)/14:1(9Z)/:2n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0046325	TG(22/16/18:4(6Z,9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0051546	TG(22:1(13Z)/16:1(9Z)/18:2(9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0047023	TG(24/14/18:4(6Z,9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0047183	TG(24/14:1(9Z)/18:3(6Z,9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0050345	TG(:1(11Z)/16/:3n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045544	TG(/16/:4(5Z,8Z,11Z,14Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045898	TG(/18:3(6Z,9Z,12Z)/18:1(11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045730	TG(/18:1(11Z)/18:3(9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045575	TG(/18/18:4(6Z,9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045749	TG(/18:1(9Z)/18:3(6Z,9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0045699	TG(/16:1(9Z)/:3n6)	C59H106O6	M+NH4	928.8328	-2.7

HMDB0045693	TG(/16:1(9Z)/3(5Z,8Z,11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0050442	TG(:1(11Z)/14:1(9Z)/22:2(13Z,16Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0053290	TG(:2n6/16/:2n6)	C59H106O6	M+NH4	928.8328	-2.7
HMDB0050870	TG(:3(5Z,8Z,11Z)/14/22:1(13Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0047190	TG(24/14:1(9Z)/18:3(9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0051926	TG(24:1(15Z)/14/18:3(9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0046438	TG(22/14:1(9Z)/3(5Z,8Z,11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0051452	TG(22:1(13Z)/16/18:3(9Z,12Z,15Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0051445	TG(22:1(13Z)/16/18:3(6Z,9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0046834	TG(22/18:3(9Z,12Z,15Z)/16:1(9Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0047558	TG(24/18:3(9Z,12Z,15Z)/14:1(9Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0046276	TG(22/14/:4(8Z,11Z,14Z,17Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0053267	TG(:2n6/14/22:2(13Z,16Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0050475	TG(:1(11Z)/18:1(11Z)/18:2(9Z,12Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0050339	TG(:1(11Z)/16/:3(5Z,8Z,11Z))	C59H106O6	M+NH4	928.8328	-2.7
HMDB0043957	TG(16//:3n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0047829	TG(14:1(9Z)/22:2(13Z,16Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049263	TG(18:1(11Z)/18:1(11Z)/:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045290	TG(18/18:3(9Z,12Z,15Z)/)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0048700	TG(16:1(9Z)/22:1(13Z)/18:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049224	TG(18:1(11Z)/14:1(9Z)/24:1(15Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044901	TG(18/16:1(9Z)/22:2(13Z,16Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0048595	TG(16:1(9Z)/16:1(9Z)/24:1(15Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0048491	TG(16:1(9Z)/18/22:2(13Z,16Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0043983	TG(16/22/18:3(6Z,9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044758	TG(18/18/:3(5Z,8Z,11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044396	TG(16/22:2(13Z,16Z)/18:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044764	TG(18/18/:3n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0043990	TG(16/22/18:3(9Z,12Z,15Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0042229	TG(14/22/:3n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044127	TG(16/18:1(9Z)/22:2(13Z,16Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0042257	TG(14/24/18:3(6Z,9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044335	TG(16/:3n6/)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0047938	TG(14:1(9Z)/18:1(11Z)/24:1(15Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0042426	TG(14/:3(5Z,8Z,11Z)/22)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0047849	TG(14:1(9Z)/22/:2n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0042264	TG(14/24/18:3(9Z,12Z,15Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0048027	TG(14:1(9Z)/22:1(13Z)/:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0047870	TG(14:1(9Z)/24/18:2(9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0042411	TG(14/:1(11Z)/22:2(13Z,16Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044152	TG(16/:1(11Z)/:2n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0042547	TG(14/18:3(6Z,9Z,12Z)/24)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044476	TG(16/18:3(9Z,12Z,15Z)/22)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044314	TG(16/:2n6/:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0042672	TG(14/22:2(13Z,16Z)/:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0048616	TG(16:1(9Z)/18:1(11Z)/22:1(13Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044789	TG(18//18:3(6Z,9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049143	TG(18:1(11Z)/18/:2n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0005410	TG(18/18:2(9Z,12Z)/:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044206	TG(16/22:1(13Z)/18:2(9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044952	TG(18/18:1(9Z)/:2n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049304	TG(18:1(11Z)/:1(11Z)/18:1(9Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049864	TG(18:1(9Z)/16:1(9Z)/22:1(13Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049162	TG(18:1(11Z)//18:2(9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0005459	TG(18:1(9Z)/18:2(9Z,12Z)/)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049751	TG(18:1(9Z)/16/22:2(13Z,16Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049786	TG(18:1(9Z)//18:2(9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049768	TG(18:1(9Z)/18/:2n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049845	TG(18:1(9Z)/14:1(9Z)/24:1(15Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0005454	TG(18:1(9Z)/18:1(9Z)/:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049882	TG(18:1(9Z)/18:1(11Z)/:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044925	TG(18/18:1(11Z)/:2n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045213	TG(18/22:2(13Z,16Z)/16:1(9Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049244	TG(18:1(11Z)/16:1(9Z)/22:1(13Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049125	TG(18:1(11Z)/16/22:2(13Z,16Z))	C59H108O6	M+NH4	930.8484	-2.1

930.8465

HMDB0044796	TG(18/18:3(9Z,12Z,15Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0048530	TG(16:1(9Z)/22/18:2(9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045134	TG(18/:2n6/18:1(9Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045101	TG(18/18:3(6Z,9Z,12Z)/)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0048510	TG(16:1(9Z)/:2n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044397	TG(16/22:2(13Z,16Z)/18:1(9Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0048701	TG(16:1(9Z)/22:1(13Z)/18:1(9Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0048638	TG(16:1(9Z)/18:1(9Z)/22:1(13Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049284	TG(18:1(11Z)/18:1(9Z)/:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044977	TG(18/:1(11Z)/18:2(9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0005442	TG(16:1(9Z)/:1(11Z)/:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045133	TG(18/:2n6/18:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045574	TG(/18/18:3(9Z,12Z,15Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0042468	TG(14/22:1(13Z)/:2n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044099	TG(16/18:1(11Z)/22:2(13Z,16Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0042757	TG(14/18:3(9Z,12Z,15Z)/24)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0042223	TG(14/22/:3(5Z,8Z,11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0048049	TG(14:1(9Z)/24:1(15Z)/18:1(9Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0042496	TG(14/24:1(15Z)/18:2(9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0042525	TG(14/18:2(9Z,12Z)/24:1(15Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044280	TG(16/18:3(6Z,9Z,12Z)/22)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0042606	TG(14/:3n6/22)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0047983	TG(14:1(9Z)/:1(11Z)/22:1(13Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0042584	TG(14/:2n6/22:1(13Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044260	TG(16/18:2(9Z,12Z)/22:1(13Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0048048	TG(14:1(9Z)/24:1(15Z)/18:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044167	TG(16/:3(5Z,8Z,11Z)/)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0043951	TG(16//:3(5Z,8Z,11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0047961	TG(14:1(9Z)/18:1(9Z)/24:1(15Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045154	TG(18/:3n6/18)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0044992	TG(18/:3(5Z,8Z,11Z)/18)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045873	TG(/18:2(9Z,12Z)/18:1(9Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045567	TG(/18/18:3(6Z,9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0046683	TG(22/:2n6/14:1(9Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0046634	TG(22/18:2(9Z,12Z)/16:1(9Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0046317	TG(22/16/18:3(6Z,9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0046263	TG(22/14/:3(5Z,8Z,11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0046324	TG(22/16/18:3(9Z,12Z,15Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0046269	TG(22/14/:3n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0047015	TG(24/14/18:3(6Z,9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0051918	TG(24:1(15Z)/14/18:2(9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0047366	TG(24/18:2(9Z,12Z)/14:1(9Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0051444	TG(22:1(13Z)/16/18:2(9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0047182	TG(24/14:1(9Z)/18:2(9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0047022	TG(24/14/18:3(9Z,12Z,15Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0046443	TG(22/14:1(9Z)/:2n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0046466	TG(22/16:1(9Z)/18:2(9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0051412	TG(22:1(13Z)/14/:2n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0050344	TG(:1(11Z)/16/:2n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045537	TG(/16/:3(5Z,8Z,11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045698	TG(/16:1(9Z)/:2n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045748	TG(/18:1(9Z)/18:2(9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045872	TG(/18:2(9Z,12Z)/18:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0046000	TG(/22:2(13Z,16Z)/14:1(9Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045923	TG(/:2n6/16:1(9Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0050435	TG(:1(11Z)/14:1(9Z)/22:1(13Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045675	TG(/14:1(9Z)/22:2(13Z,16Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0050309	TG(:1(11Z)/14/22:2(13Z,16Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045722	TG(/18:1(11Z)/18:2(9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0045543	TG(/16/:3n6)	C59H108O6	M+NH4	930.8484	-2.1
HMDB0050361	TG(:1(11Z)/18/18:2(9Z,12Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049303	TG(18:1(11Z)/:1(11Z)/18:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0048721	TG(16:1(9Z)/24:1(15Z)/16:1(9Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0050452	TG(:1(11Z)/16:1(9Z)/:1(11Z))	C59H108O6	M+NH4	930.8484	-2.1
HMDB0049921	TG(18:1(9Z)/:1(11Z)/18:1(9Z))	C59H108O6	M+NH4	930.8484	-2.1

934.7845	HMDB0043334	TG(15/3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0043609	TG(15/22:5(4Z,7Z,Z,13Z,16Z)/3(5Z,8Z,11Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0043503	TG(15/3n6/22:5(4Z,7Z,Z,13Z,16Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0043615	TG(15/22:5(4Z,7Z,Z,13Z,16Z)/3n6)	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0043480	TG(15/2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0043508	TG(15/3n6/22:5(7Z,Z,13Z,16Z,19Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0043788	TG(15/22:6(4Z,7Z,Z,13Z,16Z,19Z)/2n6)	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0043587	TG(15/22:4(7Z,Z,13Z,16Z)/4(5Z,8Z,11Z,14Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0043593	TG(15/22:4(7Z,Z,13Z,16Z)/4(8Z,11Z,14Z,17Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0043531	TG(15/4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0043760	TG(15/22:5(7Z,Z,13Z,16Z,19Z)/3n6)	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0054653	TG(22:4(7Z,Z,13Z,16Z)/15/4(8Z,11Z,14Z,17Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0054025	TG(4(5Z,8Z,11Z,14Z)/15/22:4(7Z,Z,13Z,16Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0053669	TG(3n6/15/22:5(4Z,7Z,Z,13Z,16Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0053674	TG(3n6/15/22:5(7Z,Z,13Z,16Z,19Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0053288	TG(2n6/15/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0050902	TG(3(5Z,8Z,11Z)/15/22:5(7Z,Z,13Z,16Z,19Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0050897	TG(3(5Z,8Z,11Z)/15/22:5(4Z,7Z,Z,13Z,16Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0043329	TG(15/3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0043705	TG(15/4(8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C60H100O6	M+NH4	934.7858	-1.4
	HMDB0043754	TG(15/22:5(7Z,Z,13Z,16Z,19Z)/3(5Z,8Z,11Z))	C60H100O6	M+NH4	934.7858	-1.4
936.7999	HMDB0043580	TG(15/22:4(7Z,Z,13Z,16Z)/3(5Z,8Z,11Z))	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0043733	TG(15/5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0043782	TG(15/22:6(4Z,7Z,Z,13Z,16Z,19Z)/1(11Z))	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0043479	TG(15/2n6/22:5(7Z,Z,13Z,16Z,19Z))	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0043586	TG(15/22:4(7Z,Z,13Z,16Z)/3n6)	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0043306	TG(15/1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0043759	TG(15/22:5(7Z,Z,13Z,16Z,19Z)/2n6)	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0043474	TG(15/2n6/22:5(4Z,7Z,Z,13Z,16Z))	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0043614	TG(15/22:5(4Z,7Z,Z,13Z,16Z)/2n6)	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0054357	TG(22:2(13Z,16Z)/15/5(5Z,8Z,11Z,14Z,17Z))	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0053282	TG(2n6/15/22:5(4Z,7Z,Z,13Z,16Z))	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0053287	TG(2n6/15/22:5(7Z,Z,13Z,16Z,19Z))	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0053668	TG(3n6/15/22:4(7Z,Z,13Z,16Z))	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0050896	TG(3(5Z,8Z,11Z)/15/22:4(7Z,Z,13Z,16Z))	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0050336	TG(1(11Z)/15/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0043565	TG(15/22:2(13Z,16Z)/5(5Z,8Z,11Z,14Z,17Z))	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0043328	TG(15/3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z))	C60H102O6	M+NH4	936.8015	-1.7
	HMDB0043502	TG(15/3n6/22:4(7Z,Z,13Z,16Z))	C60H102O6	M+NH4	936.8015	-1.7
938.8143	HMDB0050335	TG(1(11Z)/15/22:5(7Z,Z,13Z,16Z,19Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0045527	TG(15/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0050330	TG(1(11Z)/15/22:5(4Z,7Z,Z,13Z,16Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0043775	TG(15/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0043305	TG(15/1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0043726	TG(15/5(5Z,8Z,11Z,14Z,17Z)/22:1(13Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0043608	TG(15/22:5(4Z,7Z,Z,13Z,16Z)/1(11Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0043704	TG(15/4(8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0043558	TG(15/22:2(13Z,16Z)/4(5Z,8Z,11Z,14Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0043753	TG(15/22:5(7Z,Z,13Z,16Z,19Z)/1(11Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0043362	TG(15/22:1(13Z)/5(5Z,8Z,11Z,14Z,17Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0043103	TG(15/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0043564	TG(15/22:2(13Z,16Z)/4(8Z,11Z,14Z,17Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0043300	TG(15/1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0043473	TG(15/2n6/22:4(7Z,Z,13Z,16Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0053281	TG(2n6/15/22:4(7Z,Z,13Z,16Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0054024	TG(4(5Z,8Z,11Z,14Z)/15/22:2(13Z,16Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0054356	TG(22:2(13Z,16Z)/15/4(8Z,11Z,14Z,17Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0051438	TG(22:1(13Z)/15/5(5Z,8Z,11Z,14Z,17Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0043530	TG(15/4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0043585	TG(15/22:4(7Z,Z,13Z,16Z)/2n6)	C60H104O6	M+NH4	938.8171	-3.0
	HMDB0053198	TG(18:3(6Z,9Z,12Z)/4(8Z,11Z,14Z,17Z)/4(5Z,8Z,11Z,14Z))	C61H96O6	M+NH4	942.7545	-0.7
	HMDB0055430	TG(18:4(6Z,9Z,12Z,15Z)/3(5Z,8Z,11Z)/4(8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7

HMDB0055421	TG(18:4(6Z,9Z,12Z,15Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055235	TG(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053609	TG(:2n6/:5(5Z,8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0051297	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0051331	TG(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0051341	TG(:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053853	TG(:3n6/18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0051171	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0051314	TG(:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053937	TG(:3n6/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053585	TG(:2n6/18:4(6Z,9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055461	TG(18:4(6Z,9Z,12Z,15Z)/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055277	TG(18:3(9Z,12Z,15Z)/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053120	TG(18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0052649	TG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0050275	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0052782	TG(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0052796	TG(18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0049635	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055415	TG(18:4(6Z,9Z,12Z,15Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055450	TG(18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055283	TG(18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055325	TG(18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055466	TG(18:4(6Z,9Z,12Z,15Z)/:3n6/:4(8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055296	TG(18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0051308	TG(:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0051223	TG(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054850	TG(22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054858	TG(22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054970	TG(22:5(4Z,7Z,Z,13Z,16Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053959	TG(:3n6/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054109	TG(:4(5Z,8Z,11Z,14Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053970	TG(:3n6/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053942	TG(:3n6/18:4(6Z,9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054271	TG(:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055038	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7

HMDB0055695	TG(:5(5Z,8Z,11Z,14Z,17Z)/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0010531	TG(:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054710	TG(22:4(7Z,Z,13Z,16Z)/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055579	TG(:4(8Z,11Z,14Z,17Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055094	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0051348	TG(:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0010528	TG(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054194	TG(:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054915	TG(22:5(4Z,7Z,Z,13Z,16Z)/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054149	TG(:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055612	TG(:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053948	TG(:3n6/18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054787	TG(22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055805	TG(22:5(7Z,Z,13Z,16Z,19Z)/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054215	TG(:4(5Z,8Z,11Z,14Z)/:3n6/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055718	TG(:5(5Z,8Z,11Z,14Z,17Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055031	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053887	TG(:3n6/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0048228	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0044583	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0049040	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0048851	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0044637	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0048915	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0048983	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0049004	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0049025	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0048999	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0049046	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0052768	TG(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0042749	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0042928	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0048382	TG(14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0048360	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H96O6	M+NH4	942.7545	-0.7

HMDB0048365	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0048245	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0042899	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0042923	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0048250	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053075	TG(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053186	TG(18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053107	TG(18:3(6Z,9Z,12Z)/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0052824	TG(18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053160	TG(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053023	TG(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0052763	TG(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0010511	TG(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053230	TG(18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0050237	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053067	TG(18:3(6Z,9Z,12Z)/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0052810	TG(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0052817	TG(18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0049595	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053178	TG(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053147	TG(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053173	TG(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053204	TG(18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055264	TG(18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053211	TG(18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/:3n6)	C61H96O6	M+NH4	942.7545	-0.7
HMDB0052790	TG(18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0052692	TG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0010510	TG(18:3(9Z,12Z,15Z)/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0052735	TG(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0049675	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053080	TG(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0050199	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053114	TG(18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C61H96O6	M+NH4	942.7545	-0.7

HMDB0052754	TG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054291	TG(:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053153	TG(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0010533	TG(:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054977	TG(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055337	TG(18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055302	TG(18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055825	TG(22:5(7Z,Z,13Z,16Z,19Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055721	TG(:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055651	TG(:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055616	TG(:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0053223	TG(18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054188	TG(:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054965	TG(22:5(4Z,7Z,Z,13Z,16Z)/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0054265	TG(:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C61H96O6	M+NH4	942.7545	-0.7
HMDB0055216	TG(18:3(9Z,12Z,15Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055276	TG(18:3(9Z,12Z,15Z)/:3n6/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055414	TG(18:4(6Z,9Z,12Z,15Z)/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055379	TG(18:4(6Z,9Z,12Z,15Z)/18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055460	TG(18:4(6Z,9Z,12Z,15Z)/:2n6/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052816	TG(18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052587	TG(18:2(9Z,12Z)/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049628	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053093	TG(18:3(6Z,9Z,12Z)/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055425	TG(18:4(6Z,9Z,12Z,15Z)/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055234	TG(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053578	TG(:2n6/18:4(6Z,9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053518	TG(:2n6/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053759	TG(:3n6/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0051330	TG(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0050807	TG(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0050771	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055270	TG(18:3(9Z,12Z,15Z)/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055420	TG(18:4(6Z,9Z,12Z,15Z)/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049594	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0005476	TG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C61H98O6	M+NH4	944.7702	-1.2

HMDB0053016	TG(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0010509	TG(18:3(9Z,12Z,15Z)/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049634	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052648	TG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052997	TG(18:3(6Z,9Z,12Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052720	TG(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049614	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053100	TG(18:3(6Z,9Z,12Z)/:3n6/:4(5Z,8Z,11Z,14Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052734	TG(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052775	TG(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052753	TG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052762	TG(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049488	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0050217	TG(18:1(9Z)/:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049589	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053074	TG(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0010496	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049654	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053841	TG(:3n6/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053584	TG(:2n6/18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0051205	TG(:3(5Z,8Z,11Z)/:3n6/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054914	TG(22:5(4Z,7Z,Z,13Z,16Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053803	TG(:3n6/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0010524	TG(:4(5Z,8Z,11Z,14Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055694	TG(:5(5Z,8Z,11Z,14Z,17Z)/16/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054849	TG(22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053958	TG(:3n6/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054717	TG(22:4(7Z,Z,13Z,16Z)/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054786	TG(22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054214	TG(:4(5Z,8Z,11Z,14Z)/:3n6/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054103	TG(:4(5Z,8Z,11Z,14Z)/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055611	TG(:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054778	TG(22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055549	TG(:4(8Z,11Z,14Z,17Z)/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054929	TG(22:5(4Z,7Z,Z,13Z,16Z)/16/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055030	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2

HMDB0054585	TG(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054148	TG(4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055587	TG(4(8Z,11Z,14Z,17Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0051307	TG(:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/:3n6)	C61H98O6	M+NH4	944.7702	-1.2
HMDB0051215	TG(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0051029	TG(:3(5Z,8Z,11Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0051296	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053930	TG(:3n6/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0051170	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053936	TG(:3n6/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053852	TG(:3n6/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0051340	TG(:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0051164	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0051153	TG(:3(5Z,8Z,11Z)/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053481	TG(:2n6/18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0051222	TG(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053846	TG(:3n6/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0051290	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053572	TG(:2n6/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053596	TG(:2n6/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053608	TG(:2n6/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0051323	TG(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0051097	TG(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054108	TG(4(5Z,8Z,11Z,14Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0044636	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049039	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3n6)	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049024	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0045341	TG(18/18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0044577	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049033	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3(5Z,8Z,11Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0048850	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049018	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0048908	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0045445	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0048914	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0048845	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0048697	TG(16:1(9Z)/:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2

HMDB0045393	TG(18/:5(5Z,8Z,11Z,14Z,17Z):5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0044582	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0048998	TG(16:1(9Z):5(5Z,8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0048977	TG(16:1(9Z):4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0044469	TG(16/22:5(4Z,7Z,Z,13Z,16Z):5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0048222	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0048359	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0042748	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0044387	TG(16/:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0048244	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0042922	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0042893	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0042898	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0042719	TG(14/22:4(7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0048227	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0042743	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049427	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0048893	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z):5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0044630	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z):4(5Z,8Z,11Z,14Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053146	TG(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049574	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0050155	TG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052691	TG(18:2(9Z,12Z):4(5Z,8Z,11Z,14Z):4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0050179	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049674	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052727	TG(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052789	TG(18:2(9Z,12Z):5(5Z,8Z,11Z,14Z,17Z):3n6)	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053106	TG(18:3(6Z,9Z,12Z):3n6:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0050230	TG(18:1(9Z):5(5Z,8Z,11Z,14Z,17Z):4(5Z,8Z,11Z,14Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0050274	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052781	TG(18:2(9Z,12Z):4(8Z,11Z,14Z,17Z):4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052643	TG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0050039	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2

HMDB0050097	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0010506	TG(18:3(9Z,12Z,15Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049549	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053197	TG(18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z)/:3n6)	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053066	TG(18:3(6Z,9Z,12Z)/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052809	TG(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052748	TG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0049667	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053172	TG(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0050255	TG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0044555	TG(16/:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0044609	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0048982	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0048829	TG(16:1(9Z)/:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053113	TG(18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z)/:3n6)	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053210	TG(18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/:2n6)	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053022	TG(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052983	TG(18:3(6Z,9Z,12Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0050267	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053061	TG(18:3(6Z,9Z,12Z)/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052802	TG(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0052677	TG(18:2(9Z,12Z)/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0050198	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0050193	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0050236	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055578	TG(:4(8Z,11Z,14Z,17Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054204	TG(:4(5Z,8Z,11Z,14Z)/:2n6/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055477	TG(18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055697	TG(:5(5Z,8Z,11Z,14Z,17Z)/18/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055295	TG(18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055804	TG(22:5(7Z,Z,13Z,16Z,19Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054183	TG(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054177	TG(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054647	TG(22:4(7Z,Z,13Z,16Z)/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054704	TG(22:4(7Z,Z,13Z,16Z)/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2

HMDB0054991	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0010520	TG(:4(5Z,8Z,11Z,14Z)/16:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053875	TG(:3n6/:3n6/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054983	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055582	TG(:4(8Z,11Z,14Z,17Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053886	TG(:3n6/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054118	TG(:4(5Z,8Z,11Z,14Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054976	TG(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054709	TG(22:4(7Z,Z,13Z,16Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0054909	TG(22:5(4Z,7Z,Z,13Z,16Z)/14:22:5(4Z,7Z,Z,13Z,16Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053139	TG(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0051301	TG(:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C61H98O6	M+NH4	944.7702	-1.2
HMDB0053941	TG(:3n6/18:4(6Z,9Z,12Z,15Z)/:3n6)	C61H98O6	M+NH4	944.7702	-1.2
HMDB0055289	TG(18:3(9Z,12Z,15Z)/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052788	TG(18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/:2n6)	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049568	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053009	TG(18:3(6Z,9Z,12Z)/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050247	TG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053086	TG(18:3(6Z,9Z,12Z)/:2n6/:4(5Z,8Z,11Z,14Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053099	TG(18:3(6Z,9Z,12Z)/:3n6/:3n6)	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050038	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049528	TG(18:1(11Z)/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052712	TG(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0010505	TG(18:3(9Z,12Z,15Z)/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053060	TG(18:3(6Z,9Z,12Z)/18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049341	TG(18:1(11Z)/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050799	TG(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0055378	TG(18:4(6Z,9Z,12Z,15Z)/18:22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050806	TG(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050770	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0055383	TG(18:4(6Z,9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0055424	TG(18:4(6Z,9Z,12Z,15Z)/:1(11Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050229	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/:3n6)	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049613	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050173	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050178	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053092	TG(18:3(6Z,9Z,12Z)/:2n6/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052628	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6

HMDB0049573	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049541	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053185	TG(18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0055215	TG(18:3(9Z,12Z,15Z)/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049627	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:3n6)	C61H100O6	M+NH4	946.7858	-1.6
HMDB0055174	TG(18:3(9Z,12Z,15Z)/18:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052670	TG(18:2(9Z,12Z)/:3n6/:4(5Z,8Z,11Z,14Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050033	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0010488	TG(18:2(9Z,12Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052642	TG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050216	TG(18:1(9Z)/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049621	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050210	TG(18:1(9Z)/:4(8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050254	TG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052747	TG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053196	TG(18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z)/:2n6)	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052726	TG(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049481	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050019	TG(18:1(9Z)/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049588	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049487	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050077	TG(18:1(9Z)/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052684	TG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z)/:3n6)	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053112	TG(18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z)/:2n6)	C61H100O6	M+NH4	946.7858	-1.6
HMDB0046173	TG(/:5(5Z,8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054138	TG(:4(5Z,8Z,11Z,14Z)/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0051063	TG(:3(5Z,8Z,11Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050921	TG(:3(5Z,8Z,11Z)/16:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0051204	TG(:3(5Z,8Z,11Z)/:3n6/18:3(9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053758	TG(:3n6/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053753	TG(:3n6/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053834	TG(:3n6/18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0051152	TG(:3(5Z,8Z,11Z)/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053840	TG(:3n6/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0051306	TG(:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/:2n6)	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053565	TG(:2n6/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053781	TG(:3n6/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053427	TG(:2n6/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054052	TG(:4(5Z,8Z,11Z,14Z)/18/:5(5Z,8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054990	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z)/18:3(9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054716	TG(22:4(7Z,Z,13Z,16Z)/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054203	TG(:4(5Z,8Z,11Z,14Z)/:2n6/18:3(9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053874	TG(:3n6/:3n6/18:3(9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054037	TG(:4(5Z,8Z,11Z,14Z)/16:22:5(4Z,7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054117	TG(:4(5Z,8Z,11Z,14Z)/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0055548	TG(:4(8Z,11Z,14Z,17Z)/16:22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0051289	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/:3n6)	C61H100O6	M+NH4	946.7858	-1.6

HMDB0051197	TG(:3(5Z,8Z,11Z)/:3n6/18:3(6Z,9Z,12Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0051187	TG(:3(5Z,8Z,11Z)/:2n6/18:4(6Z,9Z,12Z,15Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0053595	TG(:2n6/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0053505	TG(:2n6/:3n6/18:4(6Z,9Z,12Z,15Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0053769	TG(:3n6/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0053468	TG(:2n6/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0053517	TG(:2n6/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0051045	TG(:3(5Z,8Z,11Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0051322	TG(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0053474	TG(:2n6/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0050619	TG(:1(11Z)/18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0050764	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0050752	TG(:1(11Z)/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0050674	TG(:1(11Z)/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0051096	TG(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0053480	TG(:2n6/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0053687	TG(:3n6/16:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0051214	TG(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0053379	TG(:2n6/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0051028	TG(:3(5Z,8Z,11Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0051089	TG(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0053571	TG(:2n6/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0051163	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/:3n6)	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0051146	TG(:3(5Z,8Z,11Z)/18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0053577	TG(:2n6/18:4(6Z,9Z,12Z,15Z)/:3n6)	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0051023	TG(:3(5Z,8Z,11Z)/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0050788	TG(:1(11Z)/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0049011	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:3(5Z,8Z,11Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0049017	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:3n6)	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0045444	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0048807	TG(16:1(9Z)/:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0048901	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0045314	TG(18/18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0044623	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3(5Z,8Z,11Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0044576	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0044381	TG(16/:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0042892	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0048823	TG(16:1(9Z)/:3n6/22:5(4Z,7Z,Z,13Z,16Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0048886	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0045418	TG(18/22:5(7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0049038	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:2n6)	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0044462	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0044441	TG(16/22:4(7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0045386	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0045366	TG(18/:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0044629	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3n6)	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0048696	TG(16:1(9Z)/:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0049421	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0048691	TG(16:1(9Z)/:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0042718	TG(14/22:4(7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0042713	TG(14/22:4(7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0048205	TG(14:1(9Z)/22:2(13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0049957	TG(18:1(9Z)/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0045335	TG(18/18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0045125	TG(18/18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0048221	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C61H1000O6	M+NH4	946.7858	-1.6
HMDB0044359	TG(16/:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H1000O6	M+NH4	946.7858	-1.6

HMDB0042742	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0048381	TG(14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:2(13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0044191	TG(16/3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0044386	TG(16/4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0044549	TG(16/4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0044468	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049548	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052774	TG(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z)/:3n6)	C61H100O6	M+NH4	946.7858	-1.6
HMDB0055269	TG(18:3(9Z,12Z,15Z)/:2n6/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053015	TG(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z)/:3n6)	C61H100O6	M+NH4	946.7858	-1.6
HMDB0005463	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052991	TG(18:3(6Z,9Z,12Z)/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0055228	TG(18:3(9Z,12Z,15Z)/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052544	TG(18:2(9Z,12Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049607	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052676	TG(18:2(9Z,12Z)/:3n6/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052899	TG(18:3(6Z,9Z,12Z)/18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049653	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049666	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050135	TG(18:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052801	TG(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052996	TG(18:3(6Z,9Z,12Z)/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050096	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052977	TG(18:3(6Z,9Z,12Z)/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052982	TG(18:3(6Z,9Z,12Z)/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0010495	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050154	TG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052586	TG(18:2(9Z,12Z)/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050147	TG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050192	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052662	TG(18:2(9Z,12Z)/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0045340	TG(18/18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0048907	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:3n6)	C61H100O6	M+NH4	946.7858	-1.6
HMDB0048892	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0048844	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0045437	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0048828	TG(16:1(9Z)/:3n6/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049426	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0048976	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0044554	TG(16/4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0044602	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0045204	TG(18/:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053133	TG(18:3(6Z,9Z,12Z)/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6

HMDB0049646	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049647	TG(18:1(11Z)/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050266	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052580	TG(18:2(9Z,12Z)/:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050223	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0052719	TG(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0044608	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0045392	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0049406	TG(18:1(11Z)/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0045283	TG(18/22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054646	TG(22:4(7Z,Z,13Z,16Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0010522	TG(:4(5Z,8Z,11Z,14Z)/18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0046123	TG(/18:4(6Z,9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0055435	TG(18:4(6Z,9Z,12Z,15Z)/22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054703	TG(22:4(7Z,Z,13Z,16Z)/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0055581	TG(:4(8Z,11Z,14Z,17Z)/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0055586	TG(:4(8Z,11Z,14Z,17Z)/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054982	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z)/18:3(9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054777	TG(22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0055552	TG(:4(8Z,11Z,14Z,17Z)/18/:5(5Z,8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0051827	TG(22:1(13Z)/18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054724	TG(22:4(7Z,Z,13Z,16Z)/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054042	TG(:4(5Z,8Z,11Z,14Z)/16/22:5(7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053802	TG(:3n6/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054128	TG(:4(5Z,8Z,11Z,14Z)/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054733	TG(22:4(7Z,Z,13Z,16Z)/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054928	TG(22:5(4Z,7Z,Z,13Z,16Z)/16/:4(8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054505	TG(22:2(13Z,16Z)/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054419	TG(22:2(13Z,16Z)/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054641	TG(22:4(7Z,Z,13Z,16Z)/14/22:5(4Z,7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054663	TG(22:4(7Z,Z,13Z,16Z)/16/:5(5Z,8Z,11Z,14Z,17Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054102	TG(:4(5Z,8Z,11Z,14Z)/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054575	TG(22:2(13Z,16Z)/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054584	TG(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053863	TG(:3n6/:2n6/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054935	TG(22:5(4Z,7Z,Z,13Z,16Z)/18/18:4(6Z,9Z,12Z,15Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0051283	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0051157	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053929	TG(:3n6/18:3(9Z,12Z,15Z)/:3n6)	C61H100O6	M+NH4	946.7858	-1.6
HMDB0054122	TG(:4(5Z,8Z,11Z,14Z)/18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C61H100O6	M+NH4	946.7858	-1.6
HMDB0053845	TG(:3n6/18:3(6Z,9Z,12Z)/:3n6)	C61H100O6	M+NH4	946.7858	-1.6
HMDB0050798	TG(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052655	TG(18:2(9Z,12Z)/:2n6/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053002	TG(18:3(6Z,9Z,12Z)/:1(11Z)/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053014	TG(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z)/:2n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049600	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052538	TG(18:2(9Z,12Z)/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049520	TG(18:1(11Z)/22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3

HMDB0050032	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049540	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050246	TG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049480	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/:3n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050057	TG(18:1(9Z)/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050089	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/:3n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050228	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/:2n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050780	TG(:1(11Z)/:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0055240	TG(18:3(9Z,12Z,15Z)/22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0055382	TG(18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050751	TG(:1(11Z)/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0046097	TG(/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045991	TG(/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050655	TG(:1(11Z)/:3n6/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050541	TG(:1(11Z)/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050618	TG(:1(11Z)/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049334	TG(18:1(11Z)/:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053171	TG(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050172	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052711	TG(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053085	TG(18:3(6Z,9Z,12Z)/:2n6/:3n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053098	TG(18:3(6Z,9Z,12Z)/:3n6/:2n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052579	TG(18:2(9Z,12Z)/:3(5Z,8Z,11Z)/:3n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049340	TG(18:1(11Z)/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049661	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053073	TG(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0010494	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052543	TG(18:2(9Z,12Z)/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052911	TG(18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052976	TG(18:3(6Z,9Z,12Z)/18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052761	TG(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050203	TG(18:1(9Z)/:4(8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052705	TG(18:2(9Z,12Z)/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049446	TG(18:1(11Z)/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050134	TG(18:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049606	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/:3n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053008	TG(18:3(6Z,9Z,12Z)/:1(11Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049950	TG(18:1(9Z)/:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052572	TG(18:2(9Z,12Z)/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049474	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052669	TG(18:2(9Z,12Z)/:3n6/:3n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050076	TG(18:1(9Z)/:3n6/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049645	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050070	TG(18:1(9Z)/:3n6/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049899	TG(18:1(9Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050469	TG(:1(11Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053768	TG(:3n6/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051162	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/:2n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053833	TG(:3n6/18:2(9Z,12Z)/:3n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053576	TG(:2n6/18:4(6Z,9Z,12Z,15Z)/:2n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051288	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/:2n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051186	TG(:3(5Z,8Z,11Z)/:2n6/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053378	TG(:2n6/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051196	TG(:3(5Z,8Z,11Z)/:3n6/18:2(9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053301	TG(:2n6/16:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051139	TG(:3(5Z,8Z,11Z)/18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051022	TG(:3(5Z,8Z,11Z)/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053373	TG(:2n6/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051062	TG(:3(5Z,8Z,11Z)/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050915	TG(:3(5Z,8Z,11Z)/16:22:5(4Z,7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053473	TG(:2n6/18:3(6Z,9Z,12Z)/:3n6)	C61H102O6	M+NH4	948.8015	-1.3

HMDB0051079	TG:(3(5Z,8Z,11Z)/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053697	TG(:3n6/18/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053403	TG(:2n6/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051038	TG(:3(5Z,8Z,11Z)/18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053681	TG(:3n6/16/22:5(4Z,7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053504	TG(:2n6/:3n6/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051044	TG(:3(5Z,8Z,11Z)/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051145	TG(:3(5Z,8Z,11Z)/18:2(9Z,12Z)/:3n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053390	TG(:2n6/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053774	TG(:3n6/18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053762	TG(:3n6/18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053492	TG(:2n6/:2n6/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050612	TG(:1(11Z)/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0046147	TG(/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045915	TG(/18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0046165	TG(/:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050757	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050673	TG(:1(11Z)/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050787	TG(:1(11Z)/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050666	TG(:1(11Z)/:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050763	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/:3n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0046122	TG(/18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0046172	TG(/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050745	TG(:1(11Z)/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0046116	TG(/18:4(6Z,9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053752	TG(:3n6/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051088	TG(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050937	TG(:3(5Z,8Z,11Z)/18/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051179	TG(:3(5Z,8Z,11Z)/:2n6/18:3(6Z,9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053780	TG(:3n6/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051056	TG(:3(5Z,8Z,11Z)/18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053426	TG(:2n6/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053564	TG(:2n6/18:3(9Z,12Z,15Z)/:3n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053467	TG(:2n6/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053686	TG(:3n6/16/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050920	TG(:3(5Z,8Z,11Z)/16/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050600	TG(:1(11Z)/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045308	TG(18/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045385	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/:3n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049301	TG(18:1(11Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048997	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0044455	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048199	TG(14:1(9Z)/22:2(13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048243	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:2(13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0044353	TG(16/:3n6/22:5(4Z,7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0042921	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:2(13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0044358	TG(16/:3n6/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0044185	TG(16/:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0044548	TG(16/:4(8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045334	TG(18/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049032	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:1(11Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048879	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045282	TG(18/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045436	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048885	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/:3n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045313	TG(18/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049400	TG(18:1(11Z)/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045365	TG(18/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045410	TG(18/22:5(7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048675	TG(16:1(9Z)/:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045359	TG(18/:4(8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0044190	TG(16/:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048374	TG(14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:1(13Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045203	TG(18/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0044331	TG(16/:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3

HMDB0044380	TG(16:4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048358	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:2(13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0042712	TG(14/22:4(7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048204	TG(14:1(9Z)/22:2(13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0042689	TG(14/22:2(13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048044	TG(14:1(9Z)/22:1(13Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048822	TG(16:1(9Z)/:3n6/22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053035	TG(18:3(6Z,9Z,12Z)/22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049626	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:2n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0055173	TG(18:3(9Z,12Z,15Z)/18/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050127	TG(18:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0055227	TG(18:3(9Z,12Z,15Z)/:1(11Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049567	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052898	TG(18:3(6Z,9Z,12Z)/18/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049956	TG(18:1(9Z)/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0010478	TG(18:2(9Z,12Z)/18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049527	TG(18:1(11Z)/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052893	TG(18:3(6Z,9Z,12Z)/18/22:5(4Z,7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050018	TG(18:1(9Z)/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052990	TG(18:3(6Z,9Z,12Z)/18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050146	TG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050083	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053132	TG(18:3(6Z,9Z,12Z)/22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0055179	TG(18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052773	TG(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z)/:2n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052553	TG(18:2(9Z,12Z)/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050013	TG(18:1(9Z)/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052661	TG(18:2(9Z,12Z)/:2n6/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049466	TG(18:1(11Z)/:3n6/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0010487	TG(18:2(9Z,12Z)/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0010465	TG(18:1(9Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049460	TG(18:1(11Z)/:3n6/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0052683	TG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z)/:2n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050209	TG(18:1(9Z)/:4(8Z,11Z,14Z,17Z)/:3n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045417	TG(18/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0044434	TG(16/22:4(7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045098	TG(18/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0044461	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/:3n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048801	TG(16:1(9Z)/:2n6/22:5(4Z,7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049016	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:2n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048690	TG(16:1(9Z)/:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048906	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:2n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045015	TG(18/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045256	TG(18/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049280	TG(18:1(11Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048806	TG(16:1(9Z)/:2n6/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045379	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0005413	TG(18/:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0044440	TG(16/22:4(7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045177	TG(18/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045275	TG(18/22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045119	TG(18/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0048871	TG(16:1(9Z)/22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0044601	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/:3n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049405	TG(18:1(11Z)/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0044628	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:2n6)	C61H102O6	M+NH4	948.8015	-1.3
HMDB0045124	TG(18/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049420	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0044595	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/:3(5Z,8Z,11Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053461	TG(:2n6/18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050261	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0049660	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0055288	TG(18:3(9Z,12Z,15Z)/22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3

HMDB0055387	TG(18:4(6Z,9Z,12Z,15Z)/22:18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0055551	TG(:4(8Z,11Z,14Z,17Z)/18:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054640	TG(22:4(7Z,Z,13Z,16Z)/14:22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054051	TG(:4(5Z,8Z,11Z,14Z)/18:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054662	TG(22:4(7Z,Z,13Z,16Z)/16:4(8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054670	TG(22:4(7Z,Z,13Z,16Z)/18:18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054732	TG(22:4(7Z,Z,13Z,16Z)/18:1(9Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054137	TG(:4(5Z,8Z,11Z,14Z)/:1(11Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051826	TG(22:1(13Z)/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051542	TG(22:1(13Z)/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053862	TG(:3n6/:2n6/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054418	TG(22:2(13Z,16Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0046875	TG(22:18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054504	TG(22:2(13Z,16Z)/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051691	TG(22:1(13Z)/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054723	TG(22:4(7Z,Z,13Z,16Z)/18:1(11Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051810	TG(22:1(13Z)/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054934	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054036	TG(:4(5Z,8Z,11Z,14Z)/16:22:4(7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054349	TG(22:2(13Z,16Z)/14:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054495	TG(22:2(13Z,16Z)/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053791	TG(:3n6/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054413	TG(22:2(13Z,16Z)/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0051819	TG(22:1(13Z)/18:4(6Z,9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054574	TG(22:2(13Z,16Z)/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054061	TG(:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054427	TG(22:2(13Z,16Z)/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0054045	TG(:4(5Z,8Z,11Z,14Z)/18:4(5Z,8Z,11Z,14Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0053125	TG(18:3(6Z,9Z,12Z)/22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C61H102O6	M+NH4	948.8015	-1.3
HMDB0050605	TG(:1(11Z)/18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052448	TG(18:2(9Z,12Z)/18:22:5(4Z,7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049937	TG(18:1(9Z)/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050012	TG(18:1(9Z)/18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049587	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052904	TG(18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049620	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:1(11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050069	TG(18:1(9Z)/:3n6/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0010468	TG(18:1(9Z)/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049439	TG(18:1(11Z)/:2n6/:4(5Z,8Z,11Z,14Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052892	TG(18:3(6Z,9Z,12Z)/18:22:4(7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049459	TG(18:1(11Z)/:3n6/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050222	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/:1(11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052641	TG(18:2(9Z,12Z)/18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045990	TG(/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045965	TG(/:3n6/18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0055184	TG(18:3(9Z,12Z,15Z)/22:18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050468	TG(:1(11Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050593	TG(:1(11Z)/18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0046115	TG(/18:4(6Z,9Z,12Z,15Z)/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050762	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/:2n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0046164	TG(/:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0046109	TG(/18:4(6Z,9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050505	TG(:1(11Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0010486	TG(18:2(9Z,12Z)/18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052668	TG(18:2(9Z,12Z)/:3n6/:2n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052704	TG(18:2(9Z,12Z)/22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049333	TG(18:1(11Z)/:3(5Z,8Z,11Z)/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049893	TG(18:1(9Z)/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053059	TG(18:3(6Z,9Z,12Z)/18:2(9Z,12Z)/22:2(13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050088	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/:2n6)	C61H104O6	M+NH4	950.8171	-2.0

HMDB0052578	TG(18:2(9Z,12Z)/:3(5Z,8Z,11Z)/:2n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049453	TG(18:1(11Z)/:3n6/:3(5Z,8Z,11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050191	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052467	TG(18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053001	TG(18:3(6Z,9Z,12Z)/:1(11Z)/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050126	TG(18:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049327	TG(18:1(11Z)/:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049445	TG(18:1(11Z)/:2n6/:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053084	TG(18:3(6Z,9Z,12Z)/:2n6/:2n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052923	TG(18:3(6Z,9Z,12Z)/22:18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049913	TG(18:1(9Z)/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0055178	TG(18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049943	TG(18:1(9Z)/:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052453	TG(18:2(9Z,12Z)/18:22:5(7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049507	TG(18:1(11Z)/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049949	TG(18:1(9Z)/:3(5Z,8Z,11Z)/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049898	TG(18:1(9Z)/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052746	TG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049605	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/:2n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052600	TG(18:2(9Z,12Z)/22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049320	TG(18:1(11Z)/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050611	TG(:1(11Z)/18:3(6Z,9Z,12Z)/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051818	TG(22:1(13Z)/18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050930	TG(:3(5Z,8Z,11Z)/18:4(5Z,8Z,11Z,14Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051178	TG(:3(5Z,8Z,11Z)/:2n6/18:2(9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053300	TG(:2n6/16:22:5(7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053690	TG(:3n6/18:4(5Z,8Z,11Z,14Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053402	TG(:2n6/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053460	TG(:2n6/18:2(9Z,12Z)/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050936	TG(:3(5Z,8Z,11Z)/18:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053389	TG(:2n6/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051071	TG(:3(5Z,8Z,11Z)/:1(11Z)/18:3(6Z,9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051037	TG(:3(5Z,8Z,11Z)/18:1(11Z)/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053563	TG(:2n6/18:3(9Z,12Z,15Z)/:2n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053491	TG(:2n6/:2n6/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053295	TG(:2n6/16:22:5(4Z,7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051557	TG(22:1(13Z)/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053696	TG(:3n6/18:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053383	TG(:2n6/18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050914	TG(:3(5Z,8Z,11Z)/16:22:4(7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053312	TG(:2n6/18:5(5Z,8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053414	TG(:2n6/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053372	TG(:2n6/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051144	TG(:3(5Z,8Z,11Z)/18:2(9Z,12Z)/:2n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051055	TG(:3(5Z,8Z,11Z)/18:1(9Z)/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053472	TG(:2n6/18:3(6Z,9Z,12Z)/:2n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051078	TG(:3(5Z,8Z,11Z)/:1(11Z)/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050953	TG(:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053680	TG(:3n6/16:22:4(7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050654	TG(:1(11Z)/:3n6/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0046090	TG(/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0046146	TG(/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050738	TG(:1(11Z)/18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045983	TG(/:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045809	TG(/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045914	TG(/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050665	TG(:1(11Z)/:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0046209	TG(/22:6(4Z,7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045889	TG(/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050355	TG(:1(11Z)/16:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050744	TG(:1(11Z)/18:3(9Z,12Z,15Z)/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0046096	TG(/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053396	TG(:2n6/18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045908	TG(/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050463	TG(:1(11Z)/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0

HMDB0050486	TG:(1(11Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050647	TG:(1(11Z)/:3n6/18:3(6Z,9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050540	TG:(1(11Z)/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0046139	TG(/:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050636	TG:(1(11Z)/:2n6/18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050599	TG:(1(11Z)/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050779	TG:(1(11Z)/:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045709	TG(/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050533	TG:(1(11Z)/:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050056	TG(18:1(9Z)/:2n6/:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045014	TG(18/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0042683	TG(14/22:2(13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048043	TG(14:1(9Z)/22:1(13Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048329	TG(14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/24:1(15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0042741	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/22:2(13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0044330	TG(16/:2n6/22:5(7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0042688	TG(14/22:2(13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0042891	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/22:2(13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048351	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:1(13Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048065	TG(14:1(9Z)/24:1(15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0042479	TG(14/22:1(13Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0044325	TG(16/:2n6/22:5(4Z,7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0044352	TG(16/:3n6/22:4(7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0042914	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:1(13Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048864	TG(16:1(9Z)/22:2(13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045118	TG(18/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049010	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:1(11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0044427	TG(16/22:4(7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045430	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049279	TG(18:1(11Z)/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0044936	TG(18/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045150	TG(18/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045352	TG(18/:4(8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0047860	TG(14:1(9Z)/22/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048038	TG(14:1(9Z)/22:1(13Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048236	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:1(13Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048198	TG(14:1(9Z)/22:2(13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045196	TG(18/:4(5Z,8Z,11Z,14Z)/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0044460	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/:2n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0044184	TG(16/:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048220	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/22:2(13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0044163	TG(16/:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045008	TG(18/:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049779	TG(18:1(9Z)/18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049479	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/:2n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045190	TG(18/:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048800	TG(16:1(9Z)/:2n6/22:4(7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049274	TG(18:1(11Z)/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048900	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:1(11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0044622	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:1(11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045431	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048843	TG(16:1(9Z)/:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048990	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:1(13Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0044575	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0005471	TG(18:2(9Z,12Z)/:1(11Z)/:4(5Z,8Z,11Z,14Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049535	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052697	TG(18:2(9Z,12Z)/22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052654	TG(18:2(9Z,12Z)/:2n6/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052910	TG(18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052571	TG(18:2(9Z,12Z)/:1(11Z)/:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050050	TG(18:1(9Z)/:2n6/:4(5Z,8Z,11Z,14Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050208	TG(18:1(9Z)/:4(8Z,11Z,14Z,17Z)/:2n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052537	TG(18:2(9Z,12Z)/18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049519	TG(18:1(11Z)/22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049640	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C61H104O6	M+NH4	950.8171	-2.0

HMDB0050063	TG(18:1(9Z)/:3n6/:3(5Z,8Z,11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053034	TG(18:3(6Z,9Z,12Z)/22:1(13Z)/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045274	TG(18/22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049154	TG(18:1(11Z)/18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049399	TG(18:1(11Z)/18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045092	TG(18/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049300	TG(18:1(11Z)/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048717	TG(16:1(9Z)/22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0044413	TG(16/22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048870	TG(16:1(9Z)/22:2(13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0044600	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/:2n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048521	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045307	TG(18/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049295	TG(18:1(11Z)/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045176	TG(18/:3n6/:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048975	TG(16:1(9Z)/:4(8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048669	TG(16:1(9Z)/:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045097	TG(18/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0044963	TG(18/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045384	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/:2n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045409	TG(18/22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045170	TG(18/:3n6/:4(5Z,8Z,11Z,14Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0044433	TG(16/22:4(7Z,Z,13Z,16Z)/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045358	TG(18/:4(8Z,11Z,14Z,17Z)/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045248	TG(18/22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048884	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/:2n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0048674	TG(16:1(9Z)/:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0045255	TG(18/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050115	TG(18:1(9Z)/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050141	TG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049639	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0049534	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0055239	TG(18:3(9Z,12Z,15Z)/22:1(13Z)/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0046850	TG(22/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053761	TG(:3n6/18:1(11Z)/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053773	TG(:3n6/18:1(9Z)/:3n6)	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051423	TG(22:1(13Z)/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0054101	TG(:4(5Z,8Z,11Z,14Z)/16:1(9Z)/22:2(13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051809	TG(22:1(13Z)/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0054435	TG(22:2(13Z,16Z)/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053707	TG(:3n6//18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0046867	TG(22/18:4(6Z,9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0054412	TG(22:2(13Z,16Z)/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0046874	TG(22/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0054343	TG(22:2(13Z,16Z)/14/22:5(4Z,7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0054494	TG(22:2(13Z,16Z)/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0054348	TG(22:2(13Z,16Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0054445	TG(22:2(13Z,16Z)/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0054426	TG(22:2(13Z,16Z)/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051674	TG(22:1(13Z)/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0054060	TG(:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0054367	TG(22:2(13Z,16Z)/16:5(5Z,8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0054669	TG(22:4(7Z,Z,13Z,16Z)/18/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053790	TG(:3n6/:1(11Z)/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0046958	TG(22/22:6(4Z,7Z,Z,13Z,16Z,19Z)/14:1(9Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051541	TG(22:1(13Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051802	TG(22:1(13Z)/18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051683	TG(22:1(13Z)/18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0046454	TG(22/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0046675	TG(22/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051690	TG(22:1(13Z)/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051536	TG(22:1(13Z)/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0052041	TG(24:1(15Z)/14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050241	TG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0051031	TG(:3(5Z,8Z,11Z)/18:1(11Z)/:3(5Z,8Z,11Z))	C61H104O6	M+NH4	950.8171	-2.0

HMDB0051049	TG:(3(5Z,8Z,11Z)/18:1(9Z)/:3(5Z,8Z,11Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0053027	TG(18:3(6Z,9Z,12Z)/22:1(13Z)/18:3(6Z,9Z,12Z))	C61H104O6	M+NH4	950.8171	-2.0
HMDB0050498	TG(:1(11Z)/18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049936	TG(18:1(9Z)/:1(11Z)/:4(8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0052696	TG(18:2(9Z,12Z)/22:2(13Z,16Z)/18:2(9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0052922	TG(18:3(6Z,9Z,12Z)/22/18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0005469	TG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049499	TG(18:1(11Z)/22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049506	TG(18:1(11Z)/22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0052592	TG(18:2(9Z,12Z)/22:1(13Z)/18:3(6Z,9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0010467	TG(18:1(9Z)/18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050068	TG(18:1(9Z)/:3n6/:2n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0052903	TG(18:3(6Z,9Z,12Z)/:3n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049566	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049360	TG(18:1(11Z)/22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049797	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050610	TG(:1(11Z)/18:3(6Z,9Z,12Z)/:2n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050646	TG(:1(11Z)/:3n6/18:2(9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045553	TG(/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045703	TG(/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045733	TG(/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0046083	TG(/18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0046183	TG(/22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050485	TG(:1(11Z)/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045801	TG(/:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049580	TG(18:1(11Z)/18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050114	TG(18:1(9Z)/22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049892	TG(18:1(9Z)/18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050043	TG(18:1(9Z)/:2n6/:3(5Z,8Z,11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050049	TG(18:1(9Z)/:2n6/:3n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050107	TG(18:1(9Z)/22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0052564	TG(18:2(9Z,12Z)/:1(11Z)/:3n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0052466	TG(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050082	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/:1(11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0052599	TG(18:2(9Z,12Z)/22:1(13Z)/18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0052480	TG(18:2(9Z,12Z)/22/18:4(6Z,9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049313	TG(18:1(11Z)/:1(11Z)/:4(5Z,8Z,11Z,14Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049948	TG(18:1(9Z)/:3(5Z,8Z,11Z)/:2n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049332	TG(18:1(11Z)/:3(5Z,8Z,11Z)/:2n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0052975	TG(18:3(6Z,9Z,12Z)/18:1(11Z)/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049599	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/:1(11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049432	TG(18:1(11Z)/:2n6/:3(5Z,8Z,11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049473	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/:1(11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049458	TG(18:1(11Z)/:3n6/:2n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0052653	TG(18:2(9Z,12Z)/:2n6/:2n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049514	TG(18:1(11Z)/22:4(7Z,Z,13Z,16Z)/18:1(9Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049319	TG(18:1(11Z)/:1(11Z)/:4(8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050171	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050202	TG(18:1(9Z)/:4(8Z,11Z,14Z,17Z)/:1(11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049438	TG(18:1(11Z)/:2n6/:3n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049173	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050184	TG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0052626	TG(18:2(9Z,12Z)/18:2(9Z,12Z)/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0005458	TG(18:1(9Z)/:1(11Z)/:4(5Z,8Z,11Z,14Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0051556	TG(22:1(13Z)/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0053311	TG(:2n6/18:4(8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0053382	TG(:2n6/18:1(11Z)/:3n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0051054	TG(:3(5Z,8Z,11Z)/18:1(9Z)/:2n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0053459	TG(:2n6/18:2(9Z,12Z)/:2n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0053395	TG(:2n6/18:1(9Z)/:3n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0053323	TG(:2n6//18:4(6Z,9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050929	TG(:3(5Z,8Z,11Z)/18/:3n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0053305	TG(:2n6/18/:4(5Z,8Z,11Z,14Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050586	TG(:1(11Z)/18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045982	TG(/:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8

HMDB0050504	TG:(1(11Z)/18:1(9Z):4(8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0053413	TG(:2n6/:1(11Z)/18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0051021	TG(:3(5Z,8Z,11Z)/16:1(9Z)/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0046279	TG(22/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0047630	TG(24/:5(5Z,8Z,11Z,14Z,17Z)/14:1(9Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0054342	TG(22:2(13Z,16Z)/14/22:4(7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0046448	TG(22/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0051801	TG(22:1(13Z)/18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0051036	TG(:3(5Z,8Z,11Z)/18:1(11Z):2n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0053751	TG(:3n6/16:1(9Z)/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050945	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050952	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0053294	TG(:2n6/16/22:4(7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0051070	TG(:3(5Z,8Z,11Z):1(11Z)/18:2(9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050522	TG(:1(11Z):1(11Z)/18:4(6Z,9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045808	TG(/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045957	TG(/:3n6/18:3(6Z,9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0046089	TG(/18:3(9Z,12Z,15Z):3n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0046158	TG(/:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0046114	TG(/18:4(6Z,9Z,12Z,15Z):2n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045964	TG(/:3n6/18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050479	TG(:1(11Z)/18:1(11Z):4(5Z,8Z,11Z,14Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045888	TG(/18:2(9Z,12Z):4(8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0046159	TG(/:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045939	TG(/:2n6/18:4(6Z,9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050349	TG(:1(11Z)/16/22:5(4Z,7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045901	TG(/18:3(6Z,9Z,12Z):3(5Z,8Z,11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050628	TG(:1(11Z):2n6/18:3(6Z,9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045708	TG(/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045759	TG(/18:1(9Z):5(5Z,8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045882	TG(/18:2(9Z,12Z):4(5Z,8Z,11Z,14Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050354	TG(:1(11Z)/16/22:5(7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050635	TG(:1(11Z):2n6/18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0046138	TG(/:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050743	TG(:1(11Z)/18:3(9Z,12Z,15Z):2n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045907	TG(/18:3(6Z,9Z,12Z):3n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0046053	TG(/22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050462	TG(:1(11Z)/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050372	TG(:1(11Z)/18/:5(5Z,8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050592	TG(:1(11Z)/18:2(9Z,12Z):3n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050532	TG(:1(11Z):3(5Z,8Z,11Z)/18:2(9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049773	TG(18:1(9Z)/18/22:5(4Z,7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048836	TG(16:1(9Z):4(5Z,8Z,11Z,14Z)/22:1(13Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0042682	TG(14/22:2(13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0042711	TG(14/22:4(7Z,Z,13Z,16Z)/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048213	TG(14:1(9Z)/22:4(7Z,Z,13Z,16Z)/22:1(13Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044157	TG(16/:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048064	TG(14:1(9Z)/24:1(15Z):4(8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048037	TG(14:1(9Z)/22:1(13Z)/22:4(7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0047854	TG(14:1(9Z)/22/22:5(4Z,7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0047859	TG(14:1(9Z)/22/22:5(7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044547	TG(16/:4(8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0043967	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0042478	TG(14/22:1(13Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0042239	TG(14/22/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0047881	TG(14:1(9Z)/24/:5(5Z,8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048863	TG(16:1(9Z)/22:2(13Z,16Z):3n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044406	TG(16/22:2(13Z,16Z):4(5Z,8Z,11Z,14Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045247	TG(18/22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044324	TG(16/:2n6/22:4(7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0042906	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048058	TG(14:1(9Z)/24:1(15Z):4(5Z,8Z,11Z,14Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044379	TG(16/:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0042473	TG(14/22:1(13Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044162	TG(16/:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8

HMDB0048168	TG(14:1(9Z):/4(5Z,8Z,11Z,14Z)/24:1(15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048306	TG(14:1(9Z):/4(8Z,11Z,14Z,17Z)/24:1(15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0042507	TG(14/24:1(15Z):/5(5Z,8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0042734	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/22:1(13Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0042855	TG(14:/5(5Z,8Z,11Z,14Z,17Z)/24:1(15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0042884	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/22:1(13Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049975	TG(18:1(9Z)/22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048515	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048857	TG(16:1(9Z)/22:2(13Z,16Z):/3(5Z,8Z,11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048541	TG(16:1(9Z)/22:/5(5Z,8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044962	TG(18/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049419	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045195	TG(18:/4(5Z,8Z,11Z,14Z):/2n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045143	TG(18:/2n6:/4(5Z,8Z,11Z,14Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044957	TG(18/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045269	TG(18/22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045169	TG(18:/3n6:/3n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048710	TG(16:1(9Z)/22:1(13Z)/:/4(5Z,8Z,11Z,14Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044432	TG(16/22:4(7Z,Z,13Z,16Z):/2n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045001	TG(18:/3(5Z,8Z,11Z):/3(5Z,8Z,11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0052447	TG(18:2(9Z,12Z)/18/22:4(7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0052989	TG(18:3(6Z,9Z,12Z)/18:1(9Z)/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0053000	TG(18:3(6Z,9Z,12Z):/1(11Z):/2n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0050031	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048520	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049148	TG(18:1(11Z)/18/22:5(4Z,7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045333	TG(18/18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049273	TG(18:1(11Z)/18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045007	TG(18:/3(5Z,8Z,11Z):/3n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049153	TG(18:1(11Z)/18/22:5(7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044217	TG(16/22:1(13Z):/5(5Z,8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044594	TG(16/22:5(7Z,Z,13Z,16Z,19Z):/1(11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045378	TG(18:/5(5Z,8Z,11Z,14Z,17Z):/1(11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045404	TG(18/22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045403	TG(18/22:5(7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048878	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z):/1(11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048821	TG(16:1(9Z):/3n6/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045091	TG(18/18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044935	TG(18/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044615	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048737	TG(16:1(9Z)/24:1(15Z)/18:4(6Z,9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048716	TG(16:1(9Z)/22:1(13Z):/4(8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0049294	TG(18:1(11Z)/18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048968	TG(16:1(9Z):/4(8Z,11Z,14Z,17Z)/22:1(13Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045163	TG(18:/3n6:/3(5Z,8Z,11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044454	TG(16/22:5(4Z,7Z,Z,13Z,16Z):/1(11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048668	TG(16:1(9Z):/1(11Z)/22:4(7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044568	TG(16:/5(5Z,8Z,11Z,14Z,17Z)/22:1(13Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045149	TG(18:/2n6:/4(8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044774	TG(18/18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045357	TG(18:/4(8Z,11Z,14Z,17Z):/2n6)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045229	TG(18/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044930	TG(18/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048689	TG(16:1(9Z):/3(5Z,8Z,11Z)/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044412	TG(16/22:2(13Z,16Z):/4(8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0044988	TG(18:/1(11Z):/5(5Z,8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0048947	TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/24:1(15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045268	TG(18/22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0051417	TG(22:1(13Z)/14/22:5(4Z,7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0045424	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18)	C61H106O6	M+NH4	952.8328	-2.8
HMDB0055183	TG(18:3(9Z,12Z,15Z)/22/18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0054444	TG(22:2(13Z,16Z)/18:1(9Z)/18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0051455	TG(22:1(13Z)/16:/5(5Z,8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0046453	TG(22/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
HMDB0054366	TG(22:2(13Z,16Z)/16:/4(8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8

	HMDB0052915	TG(18:3(6Z,9Z,12Z)/22/18:3(6Z,9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0053689	TG(:3n6/18/:3n6)	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0046674	TG(22/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0046933	TG(22/22:5(7Z,Z,13Z,16Z,19Z)/14:1(9Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0054375	TG(22:2(13Z,16Z)/18/18:4(6Z,9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0051666	TG(22:1(13Z)/18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0053706	TG(:3n6//18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0051929	TG(24:1(15Z)/14/:5(5Z,8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0052055	TG(24:1(15Z)/16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0047193	TG(24/14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0046667	TG(22/18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0052040	TG(24:1(15Z)/14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0046849	TG(22/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0054035	TG(:4(5Z,8Z,11Z,14Z)/16/22:2(13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0046909	TG(22/:5(5Z,8Z,11Z,14Z,17Z)/16:1(9Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0052034	TG(24:1(15Z)/14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0046650	TG(22/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0051572	TG(22:1(13Z)/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0046842	TG(22/18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0051673	TG(22:1(13Z)/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0046808	TG(22/22:5(4Z,7Z,Z,13Z,16Z)/14:1(9Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0046477	TG(22/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0051422	TG(22:1(13Z)/14/22:5(7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0046866	TG(22/18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0051535	TG(22:1(13Z)/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0051589	TG(22:1(13Z)/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0051550	TG(22:1(13Z)/16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0051682	TG(22:1(13Z)/18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0054434	TG(22:2(13Z,16Z)/18:1(11Z)/18:3(9Z,12Z,15Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0050121	TG(18:1(9Z)/22:4(7Z,Z,13Z,16Z)/18:1(9Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0049778	TG(18:1(9Z)/18/22:5(7Z,Z,13Z,16Z,19Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0049513	TG(18:1(11Z)/22:4(7Z,Z,13Z,16Z)/18:1(11Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0050756	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C61H106O6	M+NH4	952.8328	-2.8
	HMDB0050923	TG(:3(5Z,8Z,11Z)/18/:3(5Z,8Z,11Z))	C61H106O6	M+NH4	952.8328	-2.8
958.8183	HMDB0008782	PC(24/24)	C56H112NO8P	M+H	958.8198	-1.6
	HMDB0042471	TG(14/22:1(13Z)/22:2(13Z,16Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0045291	TG(18/18:3(9Z,12Z,15Z)/22)	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0048639	TG(16:1(9Z)/18:1(9Z)/24:1(15Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0048532	TG(16:1(9Z)/22/:2n6)	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0049286	TG(18:1(11Z)/18:1(9Z)/22:1(13Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0044791	TG(18//:3n6)	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0044018	TG(16/24/18:3(9Z,12Z,15Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0045214	TG(18/22:2(13Z,16Z)/18:1(11Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0049146	TG(18:1(11Z)/18/22:2(13Z,16Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0044208	TG(16/22:1(13Z)/:2n6)	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0045215	TG(18/22:2(13Z,16Z)/18:1(9Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0044979	TG(18/:1(11Z)/:2n6)	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0044823	TG(18/22/18:3(9Z,12Z,15Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0048722	TG(16:1(9Z)/24:1(15Z)/18:1(11Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0044011	TG(16/24/18:3(6Z,9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0043979	TG(16/22/:3(5Z,8Z,11Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0048617	TG(16:1(9Z)/18:1(11Z)/24:1(15Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0048029	TG(14:1(9Z)/22:1(13Z)/22:1(13Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0044281	TG(16/18:3(6Z,9Z,12Z)/24)	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0042674	TG(14/22:2(13Z,16Z)/22:1(13Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0042585	TG(14/:2n6/24:1(15Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0042607	TG(14/:3n6/24)	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0047984	TG(14:1(9Z)/:1(11Z)/24:1(15Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0042498	TG(14/24:1(15Z)/:2n6)	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0048723	TG(16:1(9Z)/24:1(15Z)/18:1(9Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0048513	TG(16:1(9Z)//22:2(13Z,16Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0048552	TG(16:1(9Z)/24/18:2(9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0044785	TG(18//:3(5Z,8Z,11Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0044993	TG(18/:3(5Z,8Z,11Z)/)	C61H112O6	M+NH4	958.8797	-2.4

HMDB0049265	TG(18:1(11Z)/18:1(11Z)/22:1(13Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0044234	TG(16/24:1(15Z)/18:2(9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0043985	TG(16/22/:3n6)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0045083	TG(18/18:2(9Z,12Z)/22:1(13Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0049806	TG(18:1(9Z)/22/18:2(9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0049183	TG(18:1(11Z)/22/18:2(9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0049865	TG(18:1(9Z)/16:1(9Z)/24:1(15Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0049164	TG(18:1(11Z)/:/2n6)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0049884	TG(18:1(9Z)/18:1(11Z)/22:1(13Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0049305	TG(18:1(11Z)/:1(11Z)/:1(11Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0005457	TG(18:1(9Z)/:1(11Z)/:1(11Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0050436	TG(:1(11Z)/14:1(9Z)/24:1(15Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0045569	TG(/18/:3n6)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0045724	TG(/18:1(11Z)/:2n6)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0045874	TG(/18:2(9Z,12Z)/:1(11Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0045600	TG(/18:3(9Z,12Z,15Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0045563	TG(/18/:3(5Z,8Z,11Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0050363	TG(:1(11Z)/18/:2n6)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0049771	TG(18:1(9Z)/18/22:2(13Z,16Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0049788	TG(18:1(9Z)/:/2n6)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0044398	TG(16/22:2(13Z,16Z)/:1(11Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0048660	TG(16:1(9Z)/:1(11Z)/22:1(13Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0045155	TG(18/:3n6/)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0048702	TG(16:1(9Z)/22:1(13Z)/:1(11Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0045031	TG(18/22:1(13Z)/18:2(9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0044955	TG(18/18:1(9Z)/22:2(13Z,16Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0049245	TG(18:1(11Z)/16:1(9Z)/24:1(15Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0044928	TG(18/18:1(11Z)/22:2(13Z,16Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0044816	TG(18/22/18:3(6Z,9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0045102	TG(18/18:3(6Z,9Z,12Z)/22)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0045135	TG(18/:2n6/:1(11Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0005468	TG(18:2(9Z,12Z)/:/1(11Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0010466	TG(18:1(9Z)/18:1(9Z)/22:1(13Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0049346	TG(18:1(11Z)/22:1(13Z)/18:1(9Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0050454	TG(:1(11Z)/16:1(9Z)/22:1(13Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0044155	TG(16/:1(11Z)/22:2(13Z,16Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0042253	TG(14/24/:3(5Z,8Z,11Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0044261	TG(16/18:2(9Z,12Z)/24:1(15Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0048050	TG(14:1(9Z)/24:1(15Z)/:1(11Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0044316	TG(16/:2n6/22:1(13Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0044168	TG(16/:3(5Z,8Z,11Z)/22)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0042427	TG(14/:3(5Z,8Z,11Z)/24)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0044336	TG(16/:3n6/22)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0042259	TG(14/24/:3n6)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0047852	TG(14:1(9Z)/22/22:2(13Z,16Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0044477	TG(16/18:3(9Z,12Z,15Z)/24)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0047872	TG(14:1(9Z)/24/:2n6)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0045925	TG(/:2n6/18:1(9Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0046075	TG(/18:3(9Z,12Z,15Z)/)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0045893	TG(/18:3(6Z,9Z,12Z)/)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0050380	TG(:1(11Z)/18:2(9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0045750	TG(/18:1(9Z)/:2n6)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0046491	TG(22/18:1(11Z)/18:2(9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0051461	TG(22:1(13Z)/18/18:2(9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0047017	TG(24/14/:3n6)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0046468	TG(22/16:1(9Z)/:2n6)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0047184	TG(24/14:1(9Z)/:2n6)	C61H112O6	M+NH4	958.8797	-2.4
HMDB0046684	TG(22/:2n6/16:1(9Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0046342	TG(22/18/18:3(6Z,9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0046349	TG(22/18/18:3(9Z,12Z,15Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0047070	TG(24/16/18:3(9Z,12Z,15Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0047206	TG(24/16:1(9Z)/18:2(9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0046516	TG(22/18:1(9Z)/18:2(9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0047011	TG(24/14/:3(5Z,8Z,11Z))	C61H112O6	M+NH4	958.8797	-2.4
HMDB0046319	TG(22/16/:3n6)	C61H112O6	M+NH4	958.8797	-2.4

	HMDB0047367	TG(24/18:2(9Z,12Z)/16:1(9Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0047414	TG(24/:2n6/14:1(9Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0046635	TG(22/18:2(9Z,12Z)/18:1(11Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0045924	TG(/:2n6/18:1(11Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0045774	TG(/:1(11Z)/18:2(9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0050347	TG(:1(11Z)/16/22:2(13Z,16Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0045593	TG(/18:3(6Z,9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0046001	TG(/22:2(13Z,16Z)/16:1(9Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0045701	TG(/16:1(9Z)/22:2(13Z,16Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0051446	TG(22:1(13Z)/16/:2n6)	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0046313	TG(22/16/:3(5Z,8Z,11Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0051415	TG(22:1(13Z)/14/22:2(13Z,16Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0046758	TG(22/22:2(13Z,16Z)/14:1(9Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0047063	TG(24/16/18:3(6Z,9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0051950	TG(24:1(15Z)/16/18:2(9Z,12Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0046446	TG(22/14:1(9Z)/22:2(13Z,16Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0046636	TG(22/18:2(9Z,12Z)/18:1(9Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0051920	TG(24:1(15Z)/14/:2n6)	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0049961	TG(18:1(9Z)/22:1(13Z)/18:1(9Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0049345	TG(18:1(11Z)/22:1(13Z)/18:1(11Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0051936	TG(24:1(15Z)/15/:2n6)	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0051527	TG(22:1(13Z)/14:1(9Z)/22:1(13Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0050490	TG(:1(11Z)/18:1(9Z)/:1(11Z))	C61H112O6	M+NH4	958.8797	-2.4
	HMDB0050471	TG(:1(11Z)/18:1(11Z)/:1(11Z))	C61H112O6	M+NH4	958.8797	-2.4
960.7997	HMDB0043590	TG(15/22:4(7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C62H102O6	M+NH4	960.8015	-1.8
	HMDB0043763	TG(15/22:5(4Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C62H102O6	M+NH4	960.8015	-1.8
	HMDB0043618	TG(15/22:5(4Z,7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C62H102O6	M+NH4	960.8015	-1.8
	HMDB0043595	TG(15/22:4(7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C62H102O6	M+NH4	960.8015	-1.8
	HMDB0054650	TG(22:4(7Z,Z,13Z,16Z)/15/22:5(4Z,7Z,Z,13Z,16Z))	C62H102O6	M+NH4	960.8015	-1.8
	HMDB0054655	TG(22:4(7Z,Z,13Z,16Z)/15/22:5(7Z,Z,13Z,16Z,19Z))	C62H102O6	M+NH4	960.8015	-1.8
	HMDB0044148	TG(16/:1(11Z)/22:1(13Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0044093	TG(16/18:1(11Z)/24:1(15Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0047823	TG(14:1(9Z)/24:1(15Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0048547	TG(16:1(9Z)/24/18:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0044229	TG(16/24:1(15Z)/18:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0044010	TG(16/24/18:2(9Z,12Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0048526	TG(16:1(9Z)/22/:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0043984	TG(16/22/:2n6)	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0044895	TG(18/16:1(9Z)/24:1(15Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0045026	TG(18/22:1(13Z)/18:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0044391	TG(16/22:2(13Z,16Z)/)	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0043959	TG(16//22:2(13Z,16Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0047845	TG(14:1(9Z)/22/22:1(13Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0044253	TG(16/18:2(9Z,12Z)/24)	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0042405	TG(14/:1(11Z)/24:1(15Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0042231	TG(14/22/22:2(13Z,16Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0042577	TG(14/:2n6/24)	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0044121	TG(16/18:1(9Z)/24:1(15Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0042492	TG(14/24:1(15Z)/:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0044308	TG(16/:2n6/22)	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0047866	TG(14:1(9Z)/24/:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0042258	TG(14/24/:2n6)	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0042666	TG(14/22:2(13Z,16Z)/22)	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0042464	TG(14/22:1(13Z)/22:1(13Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0044948	TG(18/18:1(9Z)/22:1(13Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0045051	TG(18/24:1(15Z)/16:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0049119	TG(18:1(11Z)/16/24:1(15Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0049158	TG(18:1(11Z)/:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0005467	TG(18:2(9Z,12Z)/)	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0049178	TG(18:1(11Z)/22/18:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0005450	TG(18:1(9Z)/:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0049764	TG(18:1(9Z)/18/22:1(13Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0049745	TG(18:1(9Z)/16/24:1(15Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0050303	TG(:1(11Z)/14/24:1(15Z))	C61H114O6	M+NH4	960.8954	-2.6
	HMDB0045819	TG(/22:1(13Z)/16:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6

960.8929

HMDB0045867	TG(/18:2(9Z,12Z)/)	C61H114O6	M+NH4	960.8954	-2.6
HMDB0045769	TG(/:1(11Z)/18:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0005407	TG(18/:1(11Z):1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0044202	TG(16/22:1(13Z)/:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0045075	TG(18/18:2(9Z,12Z)/22)	C61H114O6	M+NH4	960.8954	-2.6
HMDB0044815	TG(18/22/18:2(9Z,12Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0045128	TG(18/:2n6)	C61H114O6	M+NH4	960.8954	-2.6
HMDB0048485	TG(16:1(9Z)/18/24:1(15Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0049139	TG(18:1(11Z)/18/22:1(13Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0044790	TG(18/:2n6)	C61H114O6	M+NH4	960.8954	-2.6
HMDB0044921	TG(18/18:1(11Z)/22:1(13Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0048506	TG(16:1(9Z)/22:1(13Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0048546	TG(16:1(9Z)/24/18:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0045025	TG(18/22:1(13Z)/18:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0044766	TG(18/18/22:2(13Z,16Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0044228	TG(16/24:1(15Z)/18:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0050340	TG(:1(11Z)/16/22:1(13Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0045208	TG(18/22:2(13Z,16Z)/18)	C61H114O6	M+NH4	960.8954	-2.6
HMDB0046511	TG(22/18:1(9Z)/18:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0047247	TG(24/18:1(9Z)/16:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0045592	TG(/18:2(9Z,12Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0045768	TG(/:1(11Z)/18:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0046510	TG(22/18:1(9Z)/18:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0046341	TG(22/18/18:2(9Z,12Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0047178	TG(24/14:1(9Z)/:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0046486	TG(22/18:1(11Z)/18:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0046534	TG(22/:1(11Z)/16:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0046462	TG(22/16:1(9Z)/:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0046485	TG(22/18:1(11Z)/18:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0046439	TG(22/14:1(9Z)/22:1(13Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0047062	TG(24/16/18:2(9Z,12Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0046271	TG(22/14/22:2(13Z,16Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0047270	TG(24/:1(11Z)/14:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0046318	TG(22/16/:2n6)	C61H114O6	M+NH4	960.8954	-2.6
HMDB0047223	TG(24/18:1(11Z)/16:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0045718	TG(/18:1(11Z):1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0045545	TG(/16/22:2(13Z,16Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0045844	TG(/24:1(15Z)/14:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0045669	TG(/14:1(9Z)/24:1(15Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0045568	TG(/18/:2n6)	C61H114O6	M+NH4	960.8954	-2.6
HMDB0045744	TG(/18:1(9Z)/:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0045694	TG(/16:1(9Z)/22:1(13Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0047016	TG(24/14/:2n6)	C61H114O6	M+NH4	960.8954	-2.6
HMDB0047200	TG(24/16:1(9Z)/18:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0046583	TG(22/22:1(13Z)/14:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0047201	TG(24/16:1(9Z)/18:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0051408	TG(22:1(13Z)/14/22:1(13Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0050357	TG(:1(11Z)/18:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0049801	TG(18:1(9Z)/22/18:1(9Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0049177	TG(18:1(11Z)/22/18:1(11Z))	C61H114O6	M+NH4	960.8954	-2.6
HMDB0055063	TG(22:5(4Z,7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055662	TG(:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0054259	TG(:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0054228	TG(:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0054274	TG(:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0053995	TG(:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055097	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3

966.7542

HMDB0055104	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z)/4(8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0054279	TG(:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055118	TG(22:5(4Z,7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055632	TG(:4(8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0054294	TG(:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0054861	TG(22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0054314	TG(:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0054877	TG(22:4(7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055619	TG(:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055111	TG(22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0054324	TG(:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055750	TG(:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0053973	TG(:3n6/:5(5Z,8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055041	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0010540	TG(:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055654	TG(:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0053951	TG(:3n6/18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0010538	TG(:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0054304	TG(:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0054197	TG(:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055658	TG(:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0054284	TG(:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0051385	TG(:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0051317	TG(:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0053233	TG(18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0053240	TG(18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0053220	TG(18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0052827	TG(18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0052799	TG(18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0053246	TG(18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0053215	TG(18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0053123	TG(18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3

HMDB0049049	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0053207	TG(18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0053163	TG(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0051351	TG(:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055474	TG(18:4(6Z,9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055433	TG(18:4(6Z,9Z,12Z,15Z)/:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0010516	TG(18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))[iso6]	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055334	TG(18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055490	TG(18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055328	TG(18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055305	TG(18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055520	TG(18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055510	TG(18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055469	TG(18:4(6Z,9Z,12Z,15Z)/:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055340	TG(18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055485	TG(18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055346	TG(18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0054298	TG(:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0010555	TG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055666	TG(:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055733	TG(:5(5Z,8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0055757	TG(:5(5Z,8Z,11Z,14Z,17Z)/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H96O6	M+NH4	966.7545	-0.3
HMDB0053587	TG(:2n6/18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055614	TG(:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053889	TG(:3n6/:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055597	TG(:4(8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054151	TG(:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053950	TG(:3n6/18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055618	TG(:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054227	TG(:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054217	TG(:4(5Z,8Z,11Z,14Z)/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055627	TG(:4(8Z,11Z,14Z,17Z)/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054268	TG(:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054814	TG(22:4(7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3

HMDB0051377	TG:(3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0051299	TG:(3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053855	TG:(3n6/18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0051316	TG:(3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0051367	TG:(3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0051384	TG:(3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0051311	TG:(3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0051333	TG:(3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0051344	TG:(3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0051225	TG:(3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053611	TG:(2n6/:5(5Z,8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053939	TG:(3n6/18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053635	TG:(2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054860	TG(22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055096	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053961	TG:(3n6/:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053972	TG:(3n6/:5(5Z,8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053983	TG:(3n6/22:5(7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055040	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054191	TG(:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054876	TG(22:4(7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054852	TG(22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0010530	TG(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0010537	TG(:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054273	TG(:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055033	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054258	TG(:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055110	TG(22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055062	TG(22:5(4Z,7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055753	TG(:5(5Z,8Z,11Z,14Z,17Z)/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053945	TG:(3n6/18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054979	TG(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054293	TG(:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3

968.7689

HMDB0055653	TG(4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054789	TG(22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054313	TG(4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053966	TG(:3n6/:5(5Z,8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055007	TG(22:5(4Z,7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055055	TG(22:5(4Z,7Z,Z,13Z,16Z)/:3n6/18:4(6Z,9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055723	TG(:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0010535	TG(:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0051173	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0049048	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0049637	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053201	TG(18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053122	TG(18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0052820	TG(18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0050239	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0052694	TG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053239	TG(18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3n6)	C63H98O6	M+NH4	968.7702	-1.3
HMDB0049677	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0052826	TG(18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053149	TG(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0049043	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0049027	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0048917	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0044639	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0052812	TG(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053226	TG(18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0052737	TG(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055463	TG(18:4(6Z,9Z,12Z,15Z)/:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055484	TG(18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055304	TG(18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0010515	TG(18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055432	TG(18:4(6Z,9Z,12Z,15Z)/:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055339	TG(18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3

HMDB0055237	TG(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055298	TG(18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055279	TG(18:3(9Z,12Z,15Z)/:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055327	TG(18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0051277	TG(:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055468	TG(18:4(6Z,9Z,12Z,15Z)/:3n6/22:5(7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0052798	TG(18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053206	TG(18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0052793	TG(18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053156	TG(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053214	TG(18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053162	TG(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053232	TG(18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053117	TG(18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053025	TG(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053109	TG(18:3(6Z,9Z,12Z)/:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0052784	TG(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0050277	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0051350	TG(:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054278	TG(:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0005478	TG(:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054248	TG(:4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055631	TG(:4(8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055661	TG(:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055829	TG(22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054196	TG(:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053994	TG(:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0053923	TG(:3n6/22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054868	TG(22:4(7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055897	TG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0054287	TG(:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C63H98O6	M+NH4	968.7702	-1.3
HMDB0055427	TG(18:4(6Z,9Z,12Z,15Z)/:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6

HMDB0051326	TG(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051376	TG(:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051224	TG(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051332	TG(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051276	TG(:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051293	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053849	TG(:3n6/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053574	TG(:2n6/18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053604	TG(:2n6/:5(5Z,8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053586	TG(:2n6/18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053843	TG(:3n6/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053634	TG(:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053581	TG(:2n6/18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051310	TG(:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053622	TG(:2n6/22:5(7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051218	TG(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053854	TG(:3n6/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0050809	TG(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055236	TG(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0050773	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053598	TG(:2n6/:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051172	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051207	TG(:3(5Z,8Z,11Z)/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0050845	TG(:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053610	TG(:2n6/:5(5Z,8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051298	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053483	TG(:2n6/18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051359	TG(:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051099	TG(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053938	TG(:3n6/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051343	TG(:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:3n6)	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053520	TG(:2n6/:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051269	TG(:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053933	TG(:3n6/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051259	TG(:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054150	TG(:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054867	TG(22:4(7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053888	TG(:3n6/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6

HMDB0055032	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z)/4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054587	TG(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z)/5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055047	TG(22:5(4Z,7Z,Z,13Z,16Z)/2n6/18:4(6Z,9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053911	TG(:3n6/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0010526	TG(:4(5Z,8Z,11Z,14Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054180	TG(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0010534	TG(:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055722	TG(:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053877	TG(:3n6/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054931	TG(22:5(4Z,7Z,Z,13Z,16Z)/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054120	TG(:4(5Z,8Z,11Z,14Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054247	TG(:4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054978	TG(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054813	TG(22:4(7Z,Z,13Z,16Z)/4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053557	TG(:2n6/22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051366	TG(:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051155	TG(:3(5Z,8Z,11Z)/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051167	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054190	TG(:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053954	TG(:3n6/:4(8Z,11Z,14Z,17Z)/4(5Z,8Z,11Z,14Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053922	TG(:3n6/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054805	TG(22:4(7Z,Z,13Z,16Z)/3n6/18:4(6Z,9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055613	TG(:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055584	TG(:4(8Z,11Z,14Z,17Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054985	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z)/5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053982	TG(:3n6/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053882	TG(:3n6/:4(5Z,8Z,11Z,14Z)/4(5Z,8Z,11Z,14Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055054	TG(22:5(4Z,7Z,Z,13Z,16Z)/3n6/18:3(9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0010543	TG(22:5(7Z,Z,13Z,16Z,19Z)/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054605	TG(22:2(13Z,16Z)/5(5Z,8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055297	TG(18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z)/4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0044638	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0044471	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0048911	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0049021	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0045447	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6

970.7843

HMDB0049026	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053103	TG(18:3(6Z,9Z,12Z)/:3n6/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0052693	TG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0052805	TG(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0050157	TG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053200	TG(18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0050219	TG(18:1(9Z)/:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0049631	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0052722	TG(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0052589	TG(18:2(9Z,12Z)/:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0048895	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0049042	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0048916	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0044633	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0044611	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0045395	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0052730	TG(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053116	TG(18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0050257	TG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053024	TG(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0049656	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0052792	TG(18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0052783	TG(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053155	TG(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/:3n6)	C63H100O6	M+NH4	970.7858	-1.6
HMDB0049676	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0050233	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0050099	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053148	TG(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0049670	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0049636	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0050270	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055462	TG(18:4(6Z,9Z,12Z,15Z)/:2n6/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055479	TG(18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055278	TG(18:3(9Z,12Z,15Z)/:3n6/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6

HMDB0050276	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053108	TG(18:3(6Z,9Z,12Z)/:3n6/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0050238	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0052819	TG(18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3n6)	C63H100O6	M+NH4	970.7858	-1.6
HMDB0052811	TG(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053095	TG(18:3(6Z,9Z,12Z)/:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053019	TG(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053225	TG(18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/:3n6)	C63H100O6	M+NH4	970.7858	-1.6
HMDB0049551	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0052778	TG(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0049616	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053238	TG(18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:2n6)	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053142	TG(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0052679	TG(18:2(9Z,12Z)/:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0052736	TG(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0049490	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0052688	TG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055272	TG(18:3(9Z,12Z,15Z)/:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054851	TG(22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0051337	TG(:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055699	TG(:5(5Z,8Z,11Z,14Z,17Z)/18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055828	TG(22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055729	TG(:5(5Z,8Z,11Z,14Z,17Z)/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055626	TG(:4(8Z,11Z,14Z,17Z)/:3n6/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055596	TG(:4(8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053944	TG(:3n6/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054780	TG(22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054751	TG(22:4(7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054788	TG(22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054267	TG(:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055589	TG(:4(8Z,11Z,14Z,17Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054206	TG(:4(5Z,8Z,11Z,14Z)/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0055622	TG(:4(8Z,11Z,14Z,17Z)/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053960	TG(:3n6/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0010529	TG(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054993	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054216	TG(:4(5Z,8Z,11Z,14Z)/:3n6/:4(8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053805	TG(:3n6/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H100O6	M+NH4	970.7858	-1.6

HMDB0055006	TG(22:5(4Z,7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054719	TG(22:4(7Z,Z,13Z,16Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054144	TG(:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053965	TG(:3n6/:5(5Z,8Z,11Z,14Z,17Z)/:3n6)	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054210	TG(:4(5Z,8Z,11Z,14Z)/:3n6/:4(5Z,8Z,11Z,14Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0054973	TG(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H100O6	M+NH4	970.7858	-1.6
HMDB0053513	TG(:2n6/:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053573	TG(:2n6/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051092	TG(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050731	TG(:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053482	TG(:2n6/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053580	TG(:2n6/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051268	TG(:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053621	TG(:2n6/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051154	TG(:3(5Z,8Z,11Z)/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053591	TG(:2n6/:4(8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053603	TG(:2n6/:5(5Z,8Z,11Z,14Z,17Z)/:3n6)	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053519	TG(:2n6/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051189	TG(:3(5Z,8Z,11Z)/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051065	TG(:3(5Z,8Z,11Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050826	TG(:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053544	TG(:2n6/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053771	TG(:3n6/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051047	TG(:3(5Z,8Z,11Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050844	TG(:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051258	TG(:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053568	TG(:2n6/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053783	TG(:3n6/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050790	TG(:1(11Z)/:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0055271	TG(18:3(9Z,12Z,15Z)/:2n6/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050802	TG(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050676	TG(:1(11Z)/:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050754	TG(:1(11Z)/18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050767	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0055437	TG(18:4(6Z,9Z,12Z,15Z)/22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0055478	TG(18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0046125	TG(/18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0046175	TG(/:5(5Z,8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053477	TG(:2n6/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051166	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051149	TG(:3(5Z,8Z,11Z)/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051251	TG(:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C63H102O6	M+NH4	972.8015	-1.8

HMDB0046225	TG(/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050772	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0055385	TG(18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0055291	TG(18:3(9Z,12Z,15Z)/22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0055426	TG(18:4(6Z,9Z,12Z,15Z)/:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051342	TG(:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:2n6)	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051829	TG(22:1(13Z)/18:4(6Z,9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054750	TG(22:4(7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054665	TG(22:4(7Z,Z,13Z,16Z)/16:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0055621	TG(:4(8Z,11Z,14Z,17Z)/:2n6/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0055554	TG(:4(8Z,11Z,14Z,17Z)/18:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053865	TG(:3n6/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054930	TG(22:5(4Z,7Z,Z,13Z,16Z)/16:22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0010525	TG(:4(5Z,8Z,11Z,14Z)/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0055588	TG(:4(8Z,11Z,14Z,17Z)/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054114	TG(:4(5Z,8Z,11Z,14Z)/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051861	TG(22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054054	TG(:4(5Z,8Z,11Z,14Z)/18:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054586	TG(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054992	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0055698	TG(:5(5Z,8Z,11Z,14Z,17Z)/18:22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054507	TG(22:2(13Z,16Z)/18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054237	TG(:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054595	TG(22:2(13Z,16Z)/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054718	TG(22:4(7Z,Z,13Z,16Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054277	TG(:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054735	TG(22:4(7Z,Z,13Z,16Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054726	TG(22:4(7Z,Z,13Z,16Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051325	TG(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z)/:3n6)	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051206	TG(:3(5Z,8Z,11Z)/:3n6/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053837	TG(:3n6/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051200	TG(:3(5Z,8Z,11Z)/:3n6/:4(5Z,8Z,11Z,14Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053932	TG(:3n6/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053556	TG(:2n6/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051358	TG(:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051098	TG(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050837	TG(:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C63H102O6	M+NH4	972.8015	-1.8

972.7997

HMDB0051292	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054119	TG(:4(5Z,8Z,11Z,14Z)/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0055592	TG(:4(8Z,11Z,14Z,17Z)/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053597	TG(:2n6/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053842	TG(:3n6/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051217	TG(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z)/:3n6)	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053507	TG(:2n6/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053429	TG(:2n6/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053848	TG(:3n6/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053470	TG(:2n6/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050098	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0044632	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0045206	TG(18/:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0044443	TG(16/22:4(7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0045394	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0044465	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0044610	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0045420	TG(18/22:5(7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0045446	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049484	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0052777	TG(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050093	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049959	TG(18:1(9Z)/:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050213	TG(18:1(9Z)/:4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049469	TG(18:1(11Z)/:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053018	TG(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053102	TG(18:3(6Z,9Z,12Z)/:3n6/22:4(7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049615	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0045440	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0045368	TG(18/:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0048894	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0052678	TG(18:2(9Z,12Z)/:3n6/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0044605	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049020	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0045285	TG(18/22:5(4Z,7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0044470	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0048910	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8

HMDB0048889	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0045389	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053213	TG(18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050621	TG(:1(11Z)/18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049630	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050269	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3n6)	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049669	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3n6)	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050250	TG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049649	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053154	TG(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/:2n6)	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053011	TG(18:3(6Z,9Z,12Z)/:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050150	TG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049489	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053094	TG(18:3(6Z,9Z,12Z)/:2n6/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050808	TG(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053141	TG(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z)/:3n6)	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049530	TG(18:1(11Z)/22:4(7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049655	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050232	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0055230	TG(18:3(9Z,12Z,15Z)/:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050137	TG(18:1(9Z)/22:4(7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049663	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3(5Z,8Z,11Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0052715	TG(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0052729	TG(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/:3n6)	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050079	TG(18:1(9Z)/:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0052673	TG(18:2(9Z,12Z)/:3n6/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0052583	TG(18:2(9Z,12Z)/:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053224	TG(18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/:2n6)	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049544	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053089	TG(18:3(6Z,9Z,12Z)/:2n6/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049343	TG(18:1(11Z)/:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050256	TG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050156	TG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050263	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3(5Z,8Z,11Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0052804	TG(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/:3n6)	C63H102O6	M+NH4	972.8015	-1.8
HMDB0052664	TG(18:2(9Z,12Z)/:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0052818	TG(18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:2n6)	C63H102O6	M+NH4	972.8015	-1.8
HMDB0050218	TG(18:1(9Z)/:4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049550	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8

HMDB0052588	TG(18:2(9Z,12Z)/:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053135	TG(18:3(6Z,9Z,12Z)/22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0052687	TG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0049610	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0052721	TG(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051319	TG(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0051211	TG(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0010542	TG(22:5(7Z,Z,13Z,16Z,19Z)/16/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0055701	TG(:5(5Z,8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053876	TG(:3n6/:3n6/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054179	TG(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054713	TG(22:4(7Z,Z,13Z,16Z)/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054199	TG(:4(5Z,8Z,11Z,14Z)/:2n6/:4(5Z,8Z,11Z,14Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054796	TG(22:4(7Z,Z,13Z,16Z)/:2n6/18:4(6Z,9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054125	TG(:4(5Z,8Z,11Z,14Z)/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054140	TG(:4(5Z,8Z,11Z,14Z)/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054205	TG(:4(5Z,8Z,11Z,14Z)/:2n6/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054577	TG(22:2(13Z,16Z)/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054804	TG(22:4(7Z,Z,13Z,16Z)/:3n6/18:3(9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0055046	TG(22:5(4Z,7Z,Z,13Z,16Z)/:2n6/18:3(9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053798	TG(:3n6/:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054984	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053804	TG(:3n6/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054604	TG(22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054937	TG(22:5(4Z,7Z,Z,13Z,16Z)/18/:5(5Z,8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0055583	TG(:4(8Z,11Z,14Z,17Z)/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053870	TG(:3n6/:3n6/:4(5Z,8Z,11Z,14Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054999	TG(22:5(4Z,7Z,Z,13Z,16Z)/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054535	TG(22:2(13Z,16Z)/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053910	TG(:3n6/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054779	TG(22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0054925	TG(22:5(4Z,7Z,Z,13Z,16Z)/16/22:5(4Z,7Z,Z,13Z,16Z))	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053881	TG(:3n6/:4(5Z,8Z,11Z,14Z)/:3n6)	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053953	TG(:3n6/:4(8Z,11Z,14Z,17Z)/:3n6)	C63H102O6	M+NH4	972.8015	-1.8
HMDB0053782	TG(:3n6/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053405	TG(:2n6/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053500	TG(:2n6/:3n6/:4(5Z,8Z,11Z,14Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053590	TG(:2n6/:4(8Z,11Z,14Z,17Z)/:3n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051148	TG(:3(5Z,8Z,11Z)/18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051091	TG(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z)/:3n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051241	TG(:3(5Z,8Z,11Z)/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050712	TG(:1(11Z)/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051188	TG(:3(5Z,8Z,11Z)/:2n6/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4

HMDB0053422	TG(:2n6/:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050836	TG(:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053469	TG(:2n6/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051309	TG(:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050730	TG(:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051081	TG(:3(5Z,8Z,11Z)/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050939	TG(:3(5Z,8Z,11Z)/18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053476	TG(:2n6/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051182	TG(:3(5Z,8Z,11Z)/:2n6/:4(5Z,8Z,11Z,14Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053543	TG(:2n6/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051041	TG(:3(5Z,8Z,11Z)/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053770	TG(:3n6/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050825	TG(:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050723	TG(:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050753	TG(:1(11Z)/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0046124	TG(/18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0055384	TG(18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0046069	TG(/22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0046224	TG(/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0055242	TG(18:3(9Z,12Z,15Z)/22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0046149	TG(/:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050801	TG(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:3n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050543	TG(:1(11Z)/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0046174	TG(/:5(5Z,8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050795	TG(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050748	TG(:1(11Z)/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0055389	TG(18:4(6Z,9Z,12Z,15Z)/22:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045993	TG(/:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0046199	TG(/22:5(7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0046119	TG(/18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050620	TG(:1(11Z)/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0046168	TG(/:5(5Z,8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0005466	TG(:1(11Z)/:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045917	TG(/18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050783	TG(:1(11Z)/:4(8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050789	TG(:1(11Z)/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0046217	TG(/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050766	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0046877	TG(22/18:4(6Z,9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054465	TG(22:2(13Z,16Z)/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051812	TG(22:1(13Z)/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054672	TG(22:4(7Z,Z,13Z,16Z)/18/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054659	TG(22:4(7Z,Z,13Z,16Z)/16/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054525	TG(22:2(13Z,16Z)/:3n6/18:4(6Z,9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054506	TG(22:2(13Z,16Z)/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054734	TG(22:4(7Z,Z,13Z,16Z)/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054497	TG(22:2(13Z,16Z)/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054160	TG(:4(5Z,8Z,11Z,14Z)/22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051828	TG(22:1(13Z)/18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4

HMDB0053943	TG(:3n6/18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054139	TG(:4(5Z,8Z,11Z,14Z)/:1(11Z)/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053793	TG(:3n6/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054053	TG(:4(5Z,8Z,11Z,14Z)/18/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054534	TG(22:2(13Z,16Z)/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054576	TG(22:2(13Z,16Z)/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0055553	TG(:4(8Z,11Z,14Z,17Z)/18/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054063	TG(:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053864	TG(:3n6/:2n6/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0052311	TG(24:1(15Z)/18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053899	TG(:3n6/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054124	TG(:4(5Z,8Z,11Z,14Z)/18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051822	TG(22:1(13Z)/18:4(6Z,9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054664	TG(22:4(7Z,Z,13Z,16Z)/16/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051064	TG(:3(5Z,8Z,11Z)/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053699	TG(:3n6/18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053392	TG(:2n6/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051216	TG(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z)/:2n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051059	TG(:3(5Z,8Z,11Z)/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053428	TG(:2n6/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051199	TG(:3(5Z,8Z,11Z)/:3n6/:3n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053464	TG(:2n6/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051250	TG(:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053602	TG(:2n6/:5(5Z,8Z,11Z,14Z,17Z)/:2n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053494	TG(:2n6/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051046	TG(:3(5Z,8Z,11Z)/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054429	TG(22:2(13Z,16Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054936	TG(22:5(4Z,7Z,Z,13Z,16Z)/18/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053512	TG(:2n6/:4(5Z,8Z,11Z,14Z)/:3n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051324	TG(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z)/:2n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053836	TG(:3n6/18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053765	TG(:3n6/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053777	TG(:3n6/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050818	TG(:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053506	TG(:2n6/:3n6/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053567	TG(:2n6/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0052803	TG(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/:2n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045284	TG(18/22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045362	TG(18/:4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045258	TG(18/22:4(7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049041	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:2(13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0044442	TG(16/22:4(7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045200	TG(18/:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045413	TG(18/22:5(7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045017	TG(18/:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045388	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0044604	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045367	TG(18/:4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045179	TG(18/:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049958	TG(18:1(9Z)/:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053134	TG(18:3(6Z,9Z,12Z)/22:2(13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0052672	TG(18:2(9Z,12Z)/:3n6/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050059	TG(18:1(9Z)/:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049529	TG(18:1(11Z)/22:4(7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049953	TG(18:1(9Z)/:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4

HMDB0053010	TG(18:3(6Z,9Z,12Z):1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049537	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z):3(5Z,8Z,11Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050212	TG(18:1(9Z):4(8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0044464	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045205	TG(18:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0048888	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045419	TG(18/22:5(7Z,Z,13Z,16Z,19Z):4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045278	TG(18/22:5(4Z,7Z,Z,13Z,16Z):4(5Z,8Z,11Z,14Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045433	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z):3(5Z,8Z,11Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0048873	TG(16:1(9Z)/22:2(13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0044437	TG(16/22:4(7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0045439	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z):3n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0055290	TG(18:3(9Z,12Z,15Z)/22:2(13Z,16Z):4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050073	TG(18:1(9Z):3n6/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049648	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z):3n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050136	TG(18:1(9Z)/22:4(7Z,Z,13Z,16Z):4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049668	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z):2n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050130	TG(18:1(9Z)/22:4(7Z,Z,13Z,16Z):4(5Z,8Z,11Z,14Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050078	TG(18:1(9Z):3n6/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053199	TG(18:3(6Z,9Z,12Z):4(8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050243	TG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z):3(5Z,8Z,11Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050149	TG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z):3n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050268	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z):2n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0055181	TG(18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053128	TG(18:3(6Z,9Z,12Z)/22:2(13Z,16Z):4(5Z,8Z,11Z,14Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050602	TG(:1(11Z)/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0046099	TG(/18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0055436	TG(18:4(6Z,9Z,12Z,15Z)/22:1(13Z):4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050657	TG(:1(11Z):3n6/5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050615	TG(:1(11Z)/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050675	TG(:1(11Z):4(5Z,8Z,11Z,14Z):4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0052663	TG(18:2(9Z,12Z):2n6/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049337	TG(18:1(11Z):3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049642	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z):3(5Z,8Z,11Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0052574	TG(18:2(9Z,12Z):1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050249	TG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z):3n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0052658	TG(18:2(9Z,12Z):2n6/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053005	TG(18:3(6Z,9Z,12Z):1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0055229	TG(18:3(9Z,12Z,15Z):1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053140	TG(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z):2n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053115	TG(18:3(6Z,9Z,12Z):4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049468	TG(18:1(11Z):3n6/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049523	TG(18:1(11Z)/22:4(7Z,Z,13Z,16Z):4(5Z,8Z,11Z,14Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049342	TG(18:1(11Z):3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0052728	TG(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z):2n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049609	TG(18:1(11Z):4(8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0052913	TG(18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0052582	TG(18:2(9Z,12Z):3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4

HMDB0049483	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049448	TG(18:1(11Z)/:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0052791	TG(18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053037	TG(18:3(6Z,9Z,12Z)/22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0052707	TG(18:2(9Z,12Z)/22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050092	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053088	TG(18:3(6Z,9Z,12Z)/:2n6/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049463	TG(18:1(11Z)/:3n6/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0052714	TG(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z)/:3n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0049543	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/:3n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050143	TG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051844	TG(22:1(13Z)/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051085	TG(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051193	TG(:3(5Z,8Z,11Z)/:3n6/:3(5Z,8Z,11Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054712	TG(22:4(7Z,Z,13Z,16Z)/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0055441	TG(18:4(6Z,9Z,12Z,15Z)/24:1(15Z)/18:4(6Z,9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054725	TG(22:4(7Z,Z,13Z,16Z)/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054742	TG(22:4(7Z,Z,13Z,16Z)/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051742	TG(22:1(13Z)/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054189	TG(:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0046925	TG(22/:5(5Z,8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054594	TG(22:2(13Z,16Z)/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054943	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051693	TG(22:1(13Z)/18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0055557	TG(:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051860	TG(22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054048	TG(:4(5Z,8Z,11Z,14Z)/18/22:5(4Z,7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053858	TG(:3n6/:2n6/:4(5Z,8Z,11Z,14Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0055591	TG(:4(8Z,11Z,14Z,17Z)/:1(11Z)/:4(8Z,11Z,14Z,17Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054795	TG(22:4(7Z,Z,13Z,16Z)/:2n6/18:3(9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0051853	TG(22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054266	TG(:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054236	TG(:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054113	TG(:4(5Z,8Z,11Z,14Z)/18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054998	TG(22:5(4Z,7Z,Z,13Z,16Z)/:1(11Z)/18:3(9Z,12Z,15Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0054133	TG(:4(5Z,8Z,11Z,14Z)/:1(11Z)/:4(5Z,8Z,11Z,14Z))	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053797	TG(:3n6/:3(5Z,8Z,11Z)/:3n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0053869	TG(:3n6/:3n6/:3n6)	C63H104O6	M+NH4	974.8171	-2.4
HMDB0050711	TG(:1(11Z)/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050782	TG(:1(11Z)/:4(8Z,11Z,14Z,17Z)/:3n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050662	TG(:1(11Z)/:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0055186	TG(18:3(9Z,12Z,15Z)/22/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0055388	TG(18:4(6Z,9Z,12Z,15Z)/22/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046093	TG(/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046216	TG(/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045992	TG(/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8

HMDB0046068	TG(/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045911	TG(/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050596	TG(:1(11Z)/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046198	TG(/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053579	TG(:2n6/18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053698	TG(:3n6/18:22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051090	TG(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z)/:2n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051165	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053386	TG(:2n6/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053416	TG(:2n6/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051080	TG(:3(5Z,8Z,11Z)/:1(11Z)/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053399	TG(:2n6/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051291	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053314	TG(:2n6/18:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053391	TG(:2n6/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050488	TG(:1(11Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045811	TG(/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050638	TG(:1(11Z)/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050536	TG(:1(11Z)/:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046142	TG(/:4(8Z,11Z,14Z,17Z)/:4(5Z,8Z,11Z,14Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050656	TG(:1(11Z)/:3n6/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050776	TG(:1(11Z)/:4(8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050542	TG(:1(11Z)/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046191	TG(/22:5(7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050507	TG(:1(11Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0055241	TG(18:3(9Z,12Z,15Z)/22:1(13Z)/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050747	TG(:1(11Z)/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050668	TG(:1(11Z)/:4(5Z,8Z,11Z,14Z)/:3n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046167	TG(/:5(5Z,8Z,11Z,14Z,17Z)/:3n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0055247	TG(18:3(9Z,12Z,15Z)/24:1(15Z)/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045916	TG(/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046148	TG(/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050800	TG(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:2n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050614	TG(:1(11Z)/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0005420	TG(/:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046161	TG(/:5(5Z,8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050650	TG(:1(11Z)/:3n6/:4(5Z,8Z,11Z,14Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050601	TG(:1(11Z)/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046098	TG(/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046043	TG(/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053421	TG(:2n6/:3(5Z,8Z,11Z)/:3n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054047	TG(:4(5Z,8Z,11Z,14Z)/18:22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054159	TG(:4(5Z,8Z,11Z,14Z)/22:1(13Z)/18:3(9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053898	TG(:3n6/22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054679	TG(22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051725	TG(22:1(13Z)/:3n6/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051852	TG(22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054437	TG(22:2(13Z,16Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050938	TG(:3(5Z,8Z,11Z)/18:22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050704	TG(:1(11Z)/22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053693	TG(:3n6/18:22:5(4Z,7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050722	TG(:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053792	TG(:3n6/:1(11Z)/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051811	TG(22:1(13Z)/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051805	TG(22:1(13Z)/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053857	TG(:3n6/:2n6/:3n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046852	TG(22/18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052303	TG(24:1(15Z)/18:4(6Z,9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054515	TG(22:2(13Z,16Z)/:2n6/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051734	TG(22:1(13Z)/:4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051623	TG(22:1(13Z)/:3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054423	TG(22:2(13Z,16Z)/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054741	TG(22:4(7Z,Z,13Z,16Z)/:1(11Z)/18:3(9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054524	TG(22:2(13Z,16Z)/:3n6/18:3(9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8

HMDB0051198	TG:(3(5Z,8Z,11Z)/:3n6/:2n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053531	TG:(2n6/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053404	TG:(2n6/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053499	TG:(2n6/:3n6/:3n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053847	TG:(3n6/18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050817	TG:(1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053931	TG:(3n6/18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053487	TG:(2n6/:2n6/:4(5Z,8Z,11Z,14Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050933	TG:(3(5Z,8Z,11Z)/18/22:5(4Z,7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053493	TG:(2n6/:2n6/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053463	TG:(2n6/18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053776	TG:(3n6/18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051074	TG:(3(5Z,8Z,11Z)/:1(11Z)/:4(5Z,8Z,11Z,14Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051240	TG:(3(5Z,8Z,11Z)/22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051181	TG:(3(5Z,8Z,11Z)/:2n6/:3n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051175	TG:(3(5Z,8Z,11Z)/:2n6/:3(5Z,8Z,11Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053589	TG:(2n6/:4(8Z,11Z,14Z,17Z)/:2n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053511	TG:(2n6/:4(5Z,8Z,11Z,14Z)/:2n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051040	TG:(3(5Z,8Z,11Z)/18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051233	TG:(3(5Z,8Z,11Z)/22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051058	TG:(3(5Z,8Z,11Z)/18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051302	TG:(3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053764	TG:(3n6/18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051115	TG:(3(5Z,8Z,11Z)/22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050955	TG:(3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046118	TG(/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0048719	TG(16:1(9Z)/22:1(13Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045412	TG(18/22:5(7Z,Z,13Z,16Z,19Z)/:3n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045152	TG(18/:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0044631	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:2(13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0048867	TG(16:1(9Z)/22:2(13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045173	TG(18/:3n6/22:5(4Z,7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0048872	TG(16:1(9Z)/22:2(13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0048909	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:2(13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0044436	TG(16/22:4(7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045016	TG(18/:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0048067	TG(14:1(9Z)/24:1(15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049019	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:2(13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0044415	TG(16/22:2(13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045257	TG(18/22:4(7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045199	TG(18/:4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045277	TG(18/22:5(4Z,7Z,Z,13Z,16Z)/:3n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045271	TG(18/22:5(4Z,7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045011	TG(18/:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045178	TG(18/:3n6/22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049034	TG(16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:1(13Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045251	TG(18/22:4(7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045361	TG(18/:4(8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045438	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:2n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0048375	TG(14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/24:1(15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045406	TG(18/22:5(7Z,Z,13Z,16Z,19Z)/:3(5Z,8Z,11Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0045891	TG(/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053127	TG(18:3(6Z,9Z,12Z)/22:2(13Z,16Z)/:3n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049952	TG(18:1(9Z)/:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050148	TG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:2n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052568	TG(18:2(9Z,12Z)/:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049462	TG(18:1(11Z)/:3n6/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049516	TG(18:1(11Z)/22:4(7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052907	TG(18:3(6Z,9Z,12Z)//22:5(4Z,7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052469	TG(18:2(9Z,12Z)//22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050248	TG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:2n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049336	TG(18:1(11Z)/:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049447	TG(18:1(11Z)/:2n6/22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053030	TG(18:3(6Z,9Z,12Z)/22:1(13Z)/:4(5Z,8Z,11Z,14Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046061	TG(/22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C63H106O6	M+NH4	976.8328	-1.8

HMDB0045967	TG(/:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049647	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/:2n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049542	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/:2n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0055180	TG(18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050053	TG(18:1(9Z)/:2n6/22:5(4Z,7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053101	TG(18:3(6Z,9Z,12Z)/:3n6/22:2(13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049662	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:1(11Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053036	TG(18:3(6Z,9Z,12Z)/22:1(13Z)/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050072	TG(18:1(9Z)/:3n6/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053004	TG(18:3(6Z,9Z,12Z)/:1(11Z)/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052925	TG(18:3(6Z,9Z,12Z)/22:/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050058	TG(18:1(9Z)/:2n6/22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053017	TG(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z)/22:2(13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052686	TG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050262	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:1(11Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049509	TG(18:1(11Z)/22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052706	TG(18:2(9Z,12Z)/22:2(13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049322	TG(18:1(11Z)/:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052602	TG(18:2(9Z,12Z)/22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052912	TG(18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049629	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052657	TG(18:2(9Z,12Z)/:2n6/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052713	TG(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z)/:2n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050129	TG(18:1(9Z)/22:4(7Z,Z,13Z,16Z)/:3n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049522	TG(18:1(11Z)/22:4(7Z,Z,13Z,16Z)/:3n6)	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050117	TG(18:1(9Z)/22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049442	TG(18:1(11Z)/:2n6/22:5(4Z,7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052573	TG(18:2(9Z,12Z)/:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0049939	TG(18:1(9Z)/:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052776	TG(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050231	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052700	TG(18:2(9Z,12Z)/22:2(13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0050123	TG(18:1(9Z)/22:4(7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053049	TG(18:3(6Z,9Z,12Z)/24:1(15Z)/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046870	TG(22/18:4(6Z,9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0055393	TG(18:4(6Z,9Z,12Z,15Z)/24/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0055556	TG(/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054447	TG(22:2(13Z,16Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052043	TG(24:1(15Z)/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051676	TG(22:1(13Z)/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053815	TG(/:3n6/22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046917	TG(22:/:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054942	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054178	TG(/:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z)/22:2(13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054658	TG(22:4(7Z,Z,13Z,16Z)/16/22:4(7Z,Z,13Z,16Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051692	TG(22:1(13Z)/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046900	TG(22:/:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051836	TG(22:1(13Z)/:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046750	TG(22:/:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054496	TG(22:2(13Z,16Z)/18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046677	TG(22/18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054671	TG(22:4(7Z,Z,13Z,16Z)/18:/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052310	TG(24:1(15Z)/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046876	TG(22/18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053786	TG(/:3n6/:1(11Z)/:4(5Z,8Z,11Z,14Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054369	TG(22:2(13Z,16Z)/16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0046924	TG(22:/:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054464	TG(22:2(13Z,16Z)/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052183	TG(24:1(15Z)/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051559	TG(22:1(13Z)/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0047599	TG(24/18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054072	TG(/:4(5Z,8Z,11Z,14Z)/22/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054062	TG(/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051821	TG(22:1(13Z)/18:4(6Z,9Z,12Z,15Z)/:3n6)	C63H106O6	M+NH4	976.8328	-1.8

HMDB0051843	TG(22:1(13Z)/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054428	TG(22:2(13Z,16Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051741	TG(22:1(13Z)/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0052295	TG(24:1(15Z)/18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053709	TG(:3n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0051686	TG(22:1(13Z)/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0054056	TG(:4(5Z,8Z,11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C63H106O6	M+NH4	976.8328	-1.8
HMDB0053486	TG(:2n6/:2n6/:3n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050374	TG(:1(11Z)/18:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045910	TG(/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050643	TG(:1(11Z)/:3n6/:3(5Z,8Z,11Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046210	TG(/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050693	TG(:1(11Z)/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046166	TG(/:5(5Z,8Z,11Z,14Z,17Z)/:2n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0055191	TG(18:3(9Z,12Z,15Z)/24:18:4(6Z,9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050535	TG(:1(11Z)/:3(5Z,8Z,11Z)/:3n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045960	TG(/:3n6/:4(5Z,8Z,11Z,14Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045810	TG(/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050595	TG(:1(11Z)/18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050765	TG(:1(11Z)/18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053313	TG(:2n6/18:22:5(7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050971	TG(:3(5Z,8Z,11Z)/22:18:4(6Z,9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050482	TG(:1(11Z)/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050637	TG(:1(11Z)/:2n6/:4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046141	TG(/:4(8Z,11Z,14Z,17Z)/:3n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050524	TG(:1(11Z)/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045735	TG(/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046092	TG(/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045804	TG(/:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050501	TG(:1(11Z)/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045966	TG(/:3n6/:4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046211	TG(/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050631	TG(:1(11Z)/:2n6/:4(5Z,8Z,11Z,14Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045985	TG(/:4(5Z,8Z,11Z,14Z)/:3n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050781	TG(:1(11Z)/:4(8Z,11Z,14Z,17Z)/:2n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046190	TG(/22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045761	TG(/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0055185	TG(18:3(9Z,12Z,15Z)/22/:4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045941	TG(/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053126	TG(18:3(6Z,9Z,12Z)/22:2(13Z,16Z)/:2n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049502	TG(18:1(11Z)/22:2(13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049799	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049608	TG(18:1(11Z)/:4(8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046035	TG(/22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045979	TG(/:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046060	TG(/22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046042	TG(/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046135	TG(/:4(8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050506	TG(:1(11Z)/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050649	TG(:1(11Z)/:3n6/:3n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050667	TG(:1(11Z)/:4(5Z,8Z,11Z,14Z)/:2n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045890	TG(/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045885	TG(/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050487	TG(:1(11Z)/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050529	TG(:1(11Z)/:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049175	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0054377	TG(22:2(13Z,16Z)/18/:5(5Z,8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0047575	TG(24:18:3(9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046749	TG(22/:4(5Z,8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051724	TG(22:1(13Z)/:3n6/18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052302	TG(24:1(15Z)/18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052042	TG(24:1(15Z)/14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052294	TG(24:1(15Z)/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046670	TG(22/18:3(6Z,9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C63H108O6	M+NH4	978.8484	-2.7

HMDB0051675	TG(22:1(13Z)/18:2(9Z,12Z)/4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053708	TG(:3n6//:4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052057	TG(24:1(15Z)/16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046899	TG(22/:4(8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053814	TG(:3n6/22:1(13Z)/18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046725	TG(22/:3n6/18:4(6Z,9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0054071	TG(:4(5Z,8Z,11Z,14Z)/22/18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046863	TG(22/18:4(6Z,9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0054368	TG(22:2(13Z,16Z)/16/22:5(7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046652	TG(22/18:2(9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0054678	TG(22:4(7Z,Z,13Z,16Z)//18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052175	TG(24:1(15Z)/18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046869	TG(22/18:4(6Z,9Z,12Z,15Z)/:3n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051591	TG(22:1(13Z)/18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0054112	TG(:4(5Z,8Z,11Z,14Z)/18:1(11Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053385	TG(:2n6/18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053398	TG(:2n6/18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053498	TG(:2n6/:3n6/:2n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053415	TG(:2n6/:1(11Z)/:4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051147	TG(:3(5Z,8Z,11Z)/18:2(9Z,12Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053835	TG(:3n6/18:2(9Z,12Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053692	TG(:3n6/18:22:4(7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053325	TG(:2n6//:5(5Z,8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053420	TG(:2n6/:3(5Z,8Z,11Z)/:2n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051073	TG(:3(5Z,8Z,11Z)/:1(11Z)/:3n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051114	TG(:3(5Z,8Z,11Z)/22:1(13Z)/18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050932	TG(:3(5Z,8Z,11Z)/18/22:4(7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053530	TG(:2n6/22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050703	TG(:1(11Z)/22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053308	TG(:2n6/18/22:5(4Z,7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053409	TG(:2n6/:1(11Z)/:4(5Z,8Z,11Z,14Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053440	TG(:2n6/22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053566	TG(:2n6/18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051180	TG(:3(5Z,8Z,11Z)/:2n6/:2n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050948	TG(:3(5Z,8Z,11Z)//:4(5Z,8Z,11Z,14Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053475	TG(:2n6/18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051232	TG(:3(5Z,8Z,11Z)/22:2(13Z,16Z)/18:2(9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050954	TG(:3(5Z,8Z,11Z)//:4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051107	TG(:3(5Z,8Z,11Z)/22:1(13Z)/18:3(6Z,9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051284	TG(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z)/22:1(13Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051158	TG(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z)/22:1(13Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049933	TG(18:1(9Z)/:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0044409	TG(16/22:2(13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0048887	TG(16:1(9Z)/22:4(7Z,Z,13Z,16Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0044603	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045231	TG(18/22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0042915	TG(14/22:6(4Z,7Z,Z,13Z,16Z,19Z)/24:1(15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0042509	TG(14/24:1(15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0048237	TG(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/24:1(15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0048352	TG(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/24:1(15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0048061	TG(14:1(9Z)/24:1(15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0047883	TG(14:1(9Z)/24/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0048066	TG(14:1(9Z)/24:1(15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049012	TG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:1(13Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045151	TG(18/:2n6/22:5(7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0048866	TG(16:1(9Z)/22:2(13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045146	TG(18/:2n6/22:5(4Z,7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0048739	TG(16:1(9Z)/24:1(15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0044990	TG(18/:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0044414	TG(16/22:2(13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0048902	TG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:1(13Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0048718	TG(16:1(9Z)/22:1(13Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045432	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:1(11Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0044219	TG(16/22:1(13Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045276	TG(18/22:5(4Z,7Z,Z,13Z,16Z)/:2n6)	C63H108O6	M+NH4	978.8484	-2.7

HMDB0049977	TG(18:1(9Z)/22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052924	TG(18:3(6Z,9Z,12Z)/22:/4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049641	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/:1(11Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049482	TG(18:1(11Z)/:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053029	TG(18:3(6Z,9Z,12Z)/22:1(13Z)/:3n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049441	TG(18:1(11Z)/:2n6/22:4(7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052918	TG(18:3(6Z,9Z,12Z)/22:/4(5Z,8Z,11Z,14Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049316	TG(18:1(11Z)/:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050128	TG(18:1(9Z)/22:4(7Z,Z,13Z,16Z)/:2n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049321	TG(18:1(11Z)/:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053087	TG(18:3(6Z,9Z,12Z)/:2n6/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052595	TG(18:2(9Z,12Z)/22:1(13Z)/:4(5Z,8Z,11Z,14Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049362	TG(18:1(11Z)/22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053048	TG(18:3(6Z,9Z,12Z)/24:1(15Z)/18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049938	TG(18:1(9Z)/:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049508	TG(18:1(11Z)/22:2(13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050242	TG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/:1(11Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049536	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/:1(11Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052601	TG(18:2(9Z,12Z)/22:1(13Z)/:4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052615	TG(18:2(9Z,12Z)/24:1(15Z)/18:4(6Z,9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050091	TG(18:1(9Z)/:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049622	TG(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:1(13Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050110	TG(18:1(9Z)/22:2(13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050211	TG(18:1(9Z)/:4(8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0049521	TG(18:1(11Z)/22:4(7Z,Z,13Z,16Z)/:2n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052468	TG(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0044463	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045387	TG(18:/5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045244	TG(18/22:4(7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0048991	TG(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/24:1(15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0048543	TG(16:1(9Z)/22/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045411	TG(18/22:5(7Z,Z,13Z,16Z,19Z)/:2n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0044624	TG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:1(13Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045010	TG(18:/3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045250	TG(18/22:4(7Z,Z,13Z,16Z)/:3n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0048713	TG(16:1(9Z)/22:1(13Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052463	TG(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052581	TG(18:2(9Z,12Z)/:3(5Z,8Z,11Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052699	TG(18:2(9Z,12Z)/22:2(13Z,16Z)/:3n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052937	TG(18:3(6Z,9Z,12Z)/24/18:4(6Z,9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052671	TG(18:2(9Z,12Z)/:3n6/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052906	TG(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052482	TG(18:2(9Z,12Z)/22:/5(5Z,8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050052	TG(18:1(9Z)/:2n6/22:4(7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050224	TG(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:1(13Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050142	TG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/:1(11Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050116	TG(18:1(9Z)/22:2(13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052567	TG(18:2(9Z,12Z)/:1(11Z)/22:4(7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0045172	TG(18:/3n6/22:4(7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051931	TG(24:1(15Z)/14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0047407	TG(24/18:3(6Z,9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0047678	TG(24/22:6(4Z,7Z,Z,13Z,16Z,19Z)/14:1(9Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0054446	TG(22:2(13Z,16Z)/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051685	TG(22:1(13Z)/18:3(6Z,9Z,12Z)/:3n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052182	TG(24:1(15Z)/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051820	TG(22:1(13Z)/18:4(6Z,9Z,12Z,15Z)/:2n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0047591	TG(24/18:4(6Z,9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051553	TG(22:1(13Z)/16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053719	TG(:3n6/22/18:4(6Z,9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0054422	TG(22:2(13Z,16Z)/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051622	TG(22:1(13Z)/:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046742	TG(22:/4(5Z,8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0055246	TG(18:3(9Z,12Z,15Z)/24:1(15Z)/18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046575	TG(22:/3(5Z,8Z,11Z)/18:4(6Z,9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0054363	TG(22:2(13Z,16Z)/16/22:5(4Z,7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7

HMDB0052037	TG(24:1(15Z)/14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051558	TG(22:1(13Z)/16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051457	TG(22:1(13Z)/16:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0047195	TG(24/14:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052167	TG(24:1(15Z)/18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046892	TG(22:4(8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051835	TG(22:1(13Z)/:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053702	TG(:3n6//:4(5Z,8Z,11Z,14Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0047598	TG(24/18:4(6Z,9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0054455	TG(22:2(13Z,16Z)/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0054123	TG(:4(5Z,8Z,11Z,14Z)/18:1(9Z)/22:2(13Z,16Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046479	TG(22/16:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0052287	TG(24:1(15Z)/18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046959	TG(22/22:6(4Z,7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046845	TG(22/18:3(9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051733	TG(22:1(13Z)/:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051615	TG(22:1(13Z)/:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051574	TG(22:1(13Z)/18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046851	TG(22/18:3(9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046676	TG(22/18:3(6Z,9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051717	TG(22:1(13Z)/:3n6/18:3(6Z,9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051708	TG(22:1(13Z)/:2n6/18:4(6Z,9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0046916	TG(22/:5(5Z,8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051669	TG(22:1(13Z)/18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0054436	TG(22:2(13Z,16Z)/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0054514	TG(22:2(13Z,16Z)/:2n6/18:3(9Z,12Z,15Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051804	TG(22:1(13Z)/18:3(9Z,12Z,15Z)/:3n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0050794	TG(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/:1(11Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0051067	TG(:3(5Z,8Z,11Z)/:1(11Z)/:3(5Z,8Z,11Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053785	TG(:3n6/:1(11Z)/:3n6)	C63H108O6	M+NH4	978.8484	-2.7
HMDB0053041	TG(18:3(6Z,9Z,12Z)/24:1(15Z)/18:3(6Z,9Z,12Z))	C63H108O6	M+NH4	978.8484	-2.7
HMDB0156071	2-amino-4-{[2-(5-[4-(2-amino-2-carboxyethyl)-2,6-diiodophenoxy]-2-hydroxy-3-iodophenyl)sulfanyl]-1-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl]-C-hydroxycarbonimidoyl}butanoic acid	C25H27I3N4O10S	M+Na	978.8474	-2.7
HMDB0046091	TG(/18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045978	TG(/:4(5Z,8Z,11Z,14Z)/:1(11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045573	TG(/18/22:5(4Z,7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046110	TG(/18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050408	TG(:1(11Z)/22/18:4(6Z,9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050739	TG(:1(11Z)/18:3(9Z,12Z,15Z)/22:1(13Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050516	TG(:1(11Z)/:1(11Z)/:3n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050559	TG(:1(11Z)/22:1(13Z)/18:3(9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050684	TG(:1(11Z)/22:2(13Z,16Z)/18:2(9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050367	TG(:1(11Z)/18/22:4(7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050552	TG(:1(11Z)/22:1(13Z)/18:3(6Z,9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045578	TG(/18/22:5(7Z,Z,13Z,16Z,19Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0005419	TG(/:1(11Z)/:4(5Z,8Z,11Z,14Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045933	TG(/:2n6/:3n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045802	TG(/:3(5Z,8Z,11Z)/:2n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045927	TG(/:2n6/:3(5Z,8Z,11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046029	TG(/22:4(7Z,Z,13Z,16Z)/18:1(9Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050629	TG(:1(11Z)/:2n6/:2n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050510	TG(:1(11Z)/:1(11Z)/:3(5Z,8Z,11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045835	TG(22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045958	TG(/:3n6/:2n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050390	TG(:1(11Z)/:4(8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046009	TG(22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046028	TG(/22:4(7Z,Z,13Z,16Z)/18:1(11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050025	TG(18:1(9Z)/18:3(6Z,9Z,12Z)/24:1(15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049328	TG(18:1(11Z)/:3(5Z,8Z,11Z)/22:1(13Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0052593	TG(18:2(9Z,12Z)/22:1(13Z)/:2n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0052494	TG(18:2(9Z,12Z)/24/18:3(9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049792	TG(18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050165	TG(18:1(9Z)/18:3(9Z,12Z,15Z)/24:1(15Z))	C63H112O6	M+NH4	982.8797	-2.9

HMDB0050108	TG(18:1(9Z)/22:2(13Z,16Z)/:2n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049560	TG(18:1(11Z)/18:3(9Z,12Z,15Z)/24:1(15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049500	TG(18:1(11Z)/22:2(13Z,16Z)/:2n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049454	TG(18:1(11Z)/:3n6/22:1(13Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050064	TG(18:1(9Z)/:3n6/22:1(13Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049213	TG(18:1(11Z)/24/18:4(6Z,9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049348	TG(18:1(11Z)/22:1(13Z)/:3(5Z,8Z,11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0052566	TG(18:2(9Z,12Z)/:1(11Z)/22:2(13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049810	TG(18:1(9Z)/22/:4(5Z,8Z,11Z,14Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049380	TG(18:1(11Z)/24:1(15Z)/18:3(9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049440	TG(18:1(11Z)/:2n6/22:2(13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0052474	TG(18:2(9Z,12Z)/22/:3n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0052916	TG(18:3(6Z,9Z,12Z)/22/:2n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049193	TG(18:1(11Z)/22/:4(8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049835	TG(18:1(9Z)/24/18:4(6Z,9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050051	TG(18:1(9Z)/:2n6/22:2(13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049944	TG(18:1(9Z)/:3(5Z,8Z,11Z)/22:1(13Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049969	TG(18:1(9Z)/22:1(13Z)/:3n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045784	TG(/:1(11Z)/:4(8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047382	TG(24/18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046472	TG(22/16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0052079	TG(24:1(15Z)/18:1(9Z)/18:3(6Z,9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047239	TG(24/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0052063	TG(24:1(15Z)/18:1(11Z)/18:3(6Z,9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046736	TG(22/:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046566	TG(22/:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046328	TG(22/16/22:5(7Z,Z,13Z,16Z,19Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051583	TG(22:1(13Z)/18:1(9Z)/:3n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046501	TG(22/18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051465	TG(22:1(13Z)/18/:4(5Z,8Z,11Z,14Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051667	TG(22:1(13Z)/18:2(9Z,12Z)/:2n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047375	TG(24/18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051471	TG(22:1(13Z)/18/:4(8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046699	TG(22/:2n6/18:3(9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047263	TG(24/18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046784	TG(22/22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047510	TG(24/22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051975	TG(24:1(15Z)/18/18:4(6Z,9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0054384	TG(22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046692	TG(22/:2n6/18:3(6Z,9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051954	TG(24:1(15Z)/16/:4(5Z,8Z,11Z,14Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046862	TG(22/18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046352	TG(22/18/:5(5Z,8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047216	TG(24/16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0053397	TG(:2n6/18:1(9Z)/22:2(13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051032	TG(:3(5Z,8Z,11Z)/18:1(11Z)/22:1(13Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046134	TG(/:4(8Z,11Z,14Z,17Z)/:1(11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050594	TG(:1(11Z)/18:2(9Z,12Z)/22:2(13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045603	TG(/:5(5Z,8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045754	TG(/18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045909	TG(/18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046016	TG(/22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050606	TG(:1(11Z)/18:3(6Z,9Z,12Z)/22:1(13Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045728	TG(/18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051050	TG(:3(5Z,8Z,11Z)/18:1(9Z)/22:1(13Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0053335	TG(:2n6/22/18:3(9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051960	TG(24:1(15Z)/16/:4(8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046520	TG(22/18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0053407	TG(:2n6/:1(11Z)/:2n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050931	TG(:3(5Z,8Z,11Z)/18/22:2(13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050962	TG(:3(5Z,8Z,11Z)/22/18:2(9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050946	TG(:3(5Z,8Z,11Z)/:2n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0053384	TG(:2n6/18:1(11Z)/22:2(13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0053691	TG(:3n6/18/22:2(13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0053317	TG(:2n6/:3n6)	C63H112O6	M+NH4	982.8797	-2.9

HMDB0051015	TG(:3(5Z,8Z,11Z)/16:1(9Z)/24:1(15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050384	TG(:1(11Z)/:4(5Z,8Z,11Z,14Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0042502	TG(14/24:1(15Z)/22:4(7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0042705	TG(14/22:4(7Z,Z,13Z,16Z)/24:1(15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0042877	TG(14/22:5(7Z,Z,13Z,16Z,19Z)/24)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047876	TG(14:1(9Z)/24/22:4(7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0042268	TG(14/24/22:5(7Z,Z,13Z,16Z,19Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0042263	TG(14/24/22:5(4Z,7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0044373	TG(16/:4(5Z,8Z,11Z,14Z)/24:1(15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0042727	TG(14/22:5(4Z,7Z,Z,13Z,16Z)/24)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0052487	TG(18:2(9Z,12Z)/24/18:3(6Z,9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045191	TG(18/:4(5Z,8Z,11Z,14Z)/22:1(13Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0044800	TG(18//22:5(7Z,Z,13Z,16Z,19Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049413	TG(18:1(11Z)/18:3(6Z,9Z,12Z)/24:1(15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045223	TG(18/22:2(13Z,16Z)/:3n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0048731	TG(16:1(9Z)/24:1(15Z)/:3n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045353	TG(18/:4(8Z,11Z,14Z,17Z)/22:1(13Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0044541	TG(16/:4(8Z,11Z,14Z,17Z)/24:1(15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0044238	TG(16/24:1(15Z)/:4(5Z,8Z,11Z,14Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0048683	TG(16:1(9Z)/:3(5Z,8Z,11Z)/24:1(15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0044983	TG(18/:1(11Z)/22:4(7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045067	TG(18/24:1(15Z)/18:4(6Z,9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045171	TG(18/:3n6/22:2(13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049354	TG(18:1(11Z)/22:1(13Z)/:3n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049373	TG(18:1(11Z)/24:1(15Z)/18:3(6Z,9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049187	TG(18:1(11Z)/22/:4(5Z,8Z,11Z,14Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0052606	TG(18:2(9Z,12Z)/24:1(15Z)/18:2(9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049168	TG(18:1(11Z)//22:4(7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049816	TG(18:1(9Z)/22/:4(8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049987	TG(18:1(9Z)/24:1(15Z)/18:3(6Z,9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049994	TG(18:1(9Z)/24:1(15Z)/18:3(9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0049963	TG(18:1(9Z)/22:1(13Z)/:3(5Z,8Z,11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045243	TG(18/22:4(7Z,Z,13Z,16Z)/:1(11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045009	TG(18/:3(5Z,8Z,11Z)/22:2(13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045327	TG(18/18:4(6Z,9Z,12Z,15Z)/24:1(15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0048815	TG(16:1(9Z)/:3n6/24:1(15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045372	TG(18/:5(5Z,8Z,11Z,14Z,17Z)/22)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0044448	TG(16/22:5(4Z,7Z,Z,13Z,16Z)/22)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0044212	TG(16/22:1(13Z)/22:4(7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0048725	TG(16:1(9Z)/24:1(15Z)/:3(5Z,8Z,11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0044428	TG(16/22:4(7Z,Z,13Z,16Z)/22:1(13Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0044561	TG(16/:5(5Z,8Z,11Z,14Z,17Z)/24)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0044795	TG(18//22:5(4Z,7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045263	TG(18/22:5(4Z,7Z,Z,13Z,16Z)/)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045035	TG(18/22:1(13Z)/:4(5Z,8Z,11Z,14Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045398	TG(18/22:5(7Z,Z,13Z,16Z,19Z)/)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0043994	TG(16/22/22:5(7Z,Z,13Z,16Z,19Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0044244	TG(16/24:1(15Z)/:4(8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0048562	TG(16:1(9Z)/24/:4(8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0048556	TG(16:1(9Z)/24/:4(5Z,8Z,11Z,14Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0043989	TG(16/22/22:5(4Z,7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045217	TG(18/22:2(13Z,16Z)/:3(5Z,8Z,11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0044588	TG(16/22:5(7Z,Z,13Z,16Z,19Z)/22)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0048865	TG(16:1(9Z)/22:2(13Z,16Z)/22:2(13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0048536	TG(16:1(9Z)/22/22:4(7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0045041	TG(18/22:1(13Z)/:4(8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0044826	TG(18/22/:5(5Z,8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0044021	TG(16/24/:5(5Z,8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046735	TG(22/:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046153	TG(/:5(5Z,8Z,11Z,14Z,17Z)/)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0054421	TG(22:2(13Z,16Z)/16:1(9Z)/22:2(13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046495	TG(22/18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051699	TG(22:1(13Z)/:2n6/18:2(9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0052049	TG(24:1(15Z)/16:1(9Z)/:3n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047021	TG(24/14/22:5(4Z,7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9

HMDB0046638	TG(22/18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047566	TG(24/18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046644	TG(22/18:2(9Z,12Z)/:3n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046886	TG(22/:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0052905	TG(18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0052070	TG(24:1(15Z)/18:1(11Z)/18:3(9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047585	TG(24/18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047026	TG(24/14:22:5(7Z,Z,13Z,16Z,19Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047073	TG(24/16/:5(5Z,8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047188	TG(24/14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046885	TG(22/:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051605	TG(22:1(13Z)/:1(11Z)/18:3(9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047463	TG(24/:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047398	TG(24/18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046526	TG(22/18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051924	TG(24:1(15Z)/14:22:4(7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047584	TG(24/18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051487	TG(22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051598	TG(22:1(13Z)/:1(11Z)/18:3(6Z,9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047607	TG(24/:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046550	TG(22/:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051450	TG(22:1(13Z)/16:22:4(7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0051566	TG(22:1(13Z)/18:1(11Z)/:3n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046668	TG(22/18:3(6Z,9Z,12Z)/:2n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0052086	TG(24:1(15Z)/18:1(9Z)/18:3(9Z,12Z,15Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046323	TG(22/16:22:5(4Z,7Z,Z,13Z,16Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0052158	TG(24:1(15Z)/18:2(9Z,12Z)/18:2(9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046843	TG(22/18:3(9Z,12Z,15Z)/:2n6)	C63H112O6	M+NH4	982.8797	-2.9
HMDB0046716	TG(22/:3n6/18:2(9Z,12Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0047210	TG(24/16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050528	TG(:1(11Z)/:3(5Z,8Z,11Z)/:1(11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0050642	TG(:1(11Z)/:3n6/:1(11Z))	C63H112O6	M+NH4	982.8797	-2.9
HMDB0048052	TG(14:1(9Z)/24:1(15Z)/22:1(13Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045292	TG(18/18:3(9Z,12Z,15Z)/24)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045103	TG(18/18:3(6Z,9Z,12Z)/24)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045058	TG(18/24:1(15Z)/18:2(9Z,12Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0044013	TG(16/24/:3n6)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045084	TG(18/18:2(9Z,12Z)/24:1(15Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0044211	TG(16/22:1(13Z)/22:2(13Z,16Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0048661	TG(16:1(9Z)/:1(11Z)/24:1(15Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0044982	TG(18/:1(11Z)/22:2(13Z,16Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049287	TG(18:1(11Z)/18:1(9Z)/24:1(15Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0044400	TG(16/22:2(13Z,16Z)/22:1(13Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045156	TG(18/:3n6/22)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0044236	TG(16/24:1(15Z)/:2n6)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045137	TG(18/:2n6/22:1(13Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0048554	TG(16:1(9Z)/24/:2n6)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0044337	TG(16/:3n6/24)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0044994	TG(18/:3(5Z,8Z,11Z)/22)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0044843	TG(18/24/18:3(6Z,9Z,12Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0044812	TG(18/22/:3(5Z,8Z,11Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0048535	TG(16:1(9Z)/22/22:2(13Z,16Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0044007	TG(16/24/:3(5Z,8Z,11Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0044850	TG(18/24/18:3(9Z,12Z,15Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049266	TG(18:1(11Z)/18:1(11Z)/24:1(15Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0048724	TG(16:1(9Z)/24:1(15Z)/:1(11Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0044818	TG(18/22/:3n6)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045033	TG(18/22:1(13Z)/:2n6)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0048704	TG(16:1(9Z)/22:1(13Z)/22:1(13Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045216	TG(18/22:2(13Z,16Z)/:1(11Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049808	TG(18:1(9Z)/22/:2n6)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045826	TG(22:1(13Z)/18:2(9Z,12Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045626	TG(22/18:3(9Z,12Z,15Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0050455	TG(:1(11Z)/16:1(9Z)/24:1(15Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045589	TG(/:3(5Z,8Z,11Z))	C63H116O6	M+NH4	986.9110	-1.5

HMDB0045926	TG(/:2n6/:1(11Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0046002	TG(/22:2(13Z,16Z)/18:1(11Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0046076	TG(/18:3(9Z,12Z,15Z)/22)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045619	TG(/22/18:3(6Z,9Z,12Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0050366	TG(:1(11Z)/18/22:2(13Z,16Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0050492	TG(:1(11Z)/18:1(9Z)/22:1(13Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0050473	TG(:1(11Z)/18:1(11Z)/22:1(13Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045727	TG(/18:1(11Z)/22:2(13Z,16Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045776	TG(/:1(11Z)/:2n6)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049204	TG(18:1(11Z)/24/18:2(9Z,12Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049885	TG(18:1(9Z)/18:1(11Z)/24:1(15Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049185	TG(18:1(11Z)/22/:2n6)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049307	TG(18:1(11Z)/:1(11Z)/22:1(13Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049924	TG(18:1(9Z)/:1(11Z)/22:1(13Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049167	TG(18:1(11Z)//22:2(13Z,16Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049791	TG(18:1(9Z)//22:2(13Z,16Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049826	TG(18:1(9Z)/24/18:2(9Z,12Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049905	TG(18:1(9Z)/18:1(9Z)/24:1(15Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049367	TG(18:1(11Z)/24:1(15Z)/18:1(9Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049962	TG(18:1(9Z)/22:1(13Z)/:1(11Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049347	TG(18:1(11Z)/22:1(13Z)/:1(11Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045595	TG(/:3n6)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0048030	TG(14:1(9Z)/22:1(13Z)/24:1(15Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0044317	TG(16/:2n6/24:1(15Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0047875	TG(14:1(9Z)/24/22:2(13Z,16Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0044169	TG(16/:3(5Z,8Z,11Z)/24)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0042501	TG(14/24:1(15Z)/22:2(13Z,16Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0042675	TG(14/22:2(13Z,16Z)/24:1(15Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045945	TG(/:3n6/)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045789	TG(/:3(5Z,8Z,11Z)/)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0005464	TG(:1(11Z)/:1(11Z)/:1(11Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0050382	TG(:1(11Z)//:2n6)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0046518	TG(22/18:1(9Z)/:2n6)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0046374	TG(22//18:3(9Z,12Z,15Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0051463	TG(22:1(13Z)/18/:2n6)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0047486	TG(24/22:2(13Z,16Z)/14:1(9Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0051966	TG(24:1(15Z)/18/18:2(9Z,12Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0047094	TG(24/18/18:3(9Z,12Z,15Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0046344	TG(22/18/:3n6)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0051952	TG(24:1(15Z)/16/:2n6)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0046686	TG(22/:2n6/18:1(9Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0047059	TG(24/16/:3(5Z,8Z,11Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0046685	TG(22/:2n6/18:1(11Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0047087	TG(24/18/18:3(6Z,9Z,12Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0051449	TG(22:1(13Z)/16/22:2(13Z,16Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0046541	TG(22/:1(11Z)/18:2(9Z,12Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045753	TG(/18:1(9Z)/22:2(13Z,16Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045894	TG(/18:3(6Z,9Z,12Z)/22)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0050399	TG(:1(11Z)/22/18:2(9Z,12Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0046003	TG(/22:2(13Z,16Z)/18:1(9Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0045876	TG(/18:2(9Z,12Z)/22:1(13Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0051923	TG(24:1(15Z)/14/22:2(13Z,16Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0047254	TG(24/18:1(9Z)/18:2(9Z,12Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0046637	TG(22/18:2(9Z,12Z)/:1(11Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0046759	TG(22/22:2(13Z,16Z)/16:1(9Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0047230	TG(24/18:1(11Z)/18:2(9Z,12Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0047369	TG(24/18:2(9Z,12Z)/18:1(9Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0047368	TG(24/18:2(9Z,12Z)/18:1(11Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0047208	TG(24/16:1(9Z)/:2n6)	C63H116O6	M+NH4	986.9110	-1.5
HMDB0051478	TG(22:1(13Z)//18:2(9Z,12Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049981	TG(18:1(9Z)/24:1(15Z)/18:1(9Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0049366	TG(18:1(11Z)/24:1(15Z)/18:1(11Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0047415	TG(24/:2n6/16:1(9Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0046471	TG(22/16:1(9Z)/22:2(13Z,16Z))	C63H116O6	M+NH4	986.9110	-1.5
HMDB0047065	TG(24/16/:3n6)	C63H116O6	M+NH4	986.9110	-1.5

	HMDB0046493	TG(22/18:1(11Z)/:2n6)	C63H116O6	M+NH4	986.9110	-1.5
	HMDB0051528	TG(22:1(13Z)/14:1(9Z)/24:1(15Z))	C63H116O6	M+NH4	986.9110	-1.5
	HMDB0046367	TG(22//18:3(6Z,9Z,12Z))	C63H116O6	M+NH4	986.9110	-1.5
	HMDB0046338	TG(22/18/:3(5Z,8Z,11Z))	C63H116O6	M+NH4	986.9110	-1.5
	HMDB0047187	TG(24/14:1(9Z)/22:2(13Z,16Z))	C63H116O6	M+NH4	986.9110	-1.5
	HMDB0051544	TG(22:1(13Z)/16:1(9Z)/22:1(13Z))	C63H116O6	M+NH4	986.9110	-1.5
988.9243	HMDB0045076	TG(18/18:2(9Z,12Z)/24)	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0044949	TG(18/18:1(9Z)/24:1(15Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0044204	TG(16/22:1(13Z)/22:1(13Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0045129	TG(18/:2n6/22)	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0044392	TG(16/22:2(13Z,16Z)/22)	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0044842	TG(18/24/18:2(9Z,12Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0044922	TG(18/18:1(11Z)/24:1(15Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0044975	TG(18/:1(11Z)/22:1(13Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0048507	TG(16:1(9Z)//24:1(15Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0048548	TG(16:1(9Z)/24:1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0044149	TG(16/:1(11Z)/24:1(15Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0042494	TG(14/24:1(15Z)/22:1(13Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0044309	TG(16/:2n6/24)	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0047846	TG(14:1(9Z)/22/24:1(15Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0047868	TG(14:1(9Z)/24/22:1(13Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0042261	TG(14/24/22:2(13Z,16Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0042465	TG(14/22:1(13Z)/24:1(15Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0042667	TG(14/22:2(13Z,16Z)/24)	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0045209	TG(18/22:2(13Z,16Z)/)	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0043987	TG(16/22/22:2(13Z,16Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0045027	TG(18/22:1(13Z)/:1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0049179	TG(18:1(11Z)/22/:1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0049765	TG(18:1(9Z)/18/24:1(15Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0045720	TG(/18:1(11Z)/22:1(13Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0045695	TG(/16:1(9Z)/24:1(15Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0050341	TG(:1(11Z)/16/24:1(15Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0045868	TG(/18:2(9Z,12Z)/22)	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0045746	TG(/18:1(9Z)/22:1(13Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0045820	TG(/22:1(13Z)/18:1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0050359	TG(:1(11Z)/18/22:1(13Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0049802	TG(18:1(9Z)/22/:1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0049784	TG(18:1(9Z)//22:1(13Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0049160	TG(18:1(11Z)//22:1(13Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0048528	TG(16:1(9Z)/22/22:1(13Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0044012	TG(16/24/:2n6)	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0045052	TG(18/24:1(15Z)/18:1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0044817	TG(18/22/:2n6)	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0044793	TG(18//22:2(13Z,16Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0049140	TG(18:1(11Z)/18/24:1(15Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0044230	TG(16/24:1(15Z)/:1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0045053	TG(18/24:1(15Z)/18:1(9Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0049199	TG(18:1(11Z)/24/18:1(9Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0045571	TG(/18/22:2(13Z,16Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0045594	TG(//:2n6)	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0047225	TG(24/18:1(11Z)/18:1(9Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0046440	TG(22/14:1(9Z)/24:1(15Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0047180	TG(24/14:1(9Z)/22:1(13Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0047086	TG(24/18/18:2(9Z,12Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0046608	TG(22/24:1(15Z)/14:1(9Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0047318	TG(24/22:1(13Z)/14:1(9Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0047224	TG(24/18:1(11Z)/18:1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0051409	TG(22:1(13Z)/14/24:1(15Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0047249	TG(24/18:1(9Z)/18:1(9Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0046321	TG(22/16/22:2(13Z,16Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0047271	TG(24/:1(11Z)/16:1(9Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0046584	TG(22/22:1(13Z)/16:1(9Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0045919	TG(/:2n6/)	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0045618	TG(/22/18:2(9Z,12Z))	C63H118O6	M+NH4	988.9267	-2.4
	HMDB0045845	TG(/24:1(15Z)/16:1(9Z))	C63H118O6	M+NH4	988.9267	-2.4

HMDB0045821	TG(22:1(13Z)/18:1(9Z))	C63H118O6	M+NH4	988.9267	-2.4
HMDB0005418	TG(/:1(11Z):1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
HMDB0046512	TG(22/18:1(9Z):1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
HMDB0046343	TG(22/18/:2n6)	C63H118O6	M+NH4	988.9267	-2.4
HMDB0047248	TG(24/18:1(9Z)/18:1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
HMDB0047202	TG(24/16:1(9Z):1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
HMDB0046536	TG(22/:1(11Z)/18:1(9Z))	C63H118O6	M+NH4	988.9267	-2.4
HMDB0046487	TG(22/18:1(11Z):1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
HMDB0046464	TG(22/16:1(9Z)/22:1(13Z))	C63H118O6	M+NH4	988.9267	-2.4
HMDB0049198	TG(18:1(11Z)/24/18:1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
HMDB0049821	TG(18:1(9Z)/24/18:1(9Z))	C63H118O6	M+NH4	988.9267	-2.4
HMDB0046366	TG(22/18:2(9Z,12Z))	C63H118O6	M+NH4	988.9267	-2.4
HMDB0047019	TG(24/14/22:2(13Z,16Z))	C63H118O6	M+NH4	988.9267	-2.4
HMDB0047064	TG(24/16/:2n6)	C63H118O6	M+NH4	988.9267	-2.4
HMDB0046535	TG(22/:1(11Z)/18:1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
HMDB0051442	TG(22:1(13Z)/16/22:1(13Z))	C63H118O6	M+NH4	988.9267	-2.4
HMDB0050376	TG(:1(11Z)/:1(11Z))	C63H118O6	M+NH4	988.9267	-2.4
HMDB0055057	TG(22:5(4Z,7Z,Z,13Z,16Z):3n6/:5(5Z,8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054862	TG(22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054878	TG(22:4(7Z,Z,13Z,16Z):5(5Z,8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0053963	TG(:3n6/:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054250	TG(:4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z):5(5Z,8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0053974	TG(:3n6/:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054315	TG(:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055734	TG(:5(5Z,8Z,11Z,14Z,17Z)/:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0053969	TG(:3n6/:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055098	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054816	TG(22:4(7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055642	TG(:4(8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0053925	TG(:3n6/22:5(4Z,7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054300	TG(:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054295	TG(:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054290	TG(:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0053990	TG(:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055629	TG(:4(8Z,11Z,14Z,17Z)/:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054791	TG(22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054870	TG(22:4(7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054219	TG(:4(5Z,8Z,11Z,14Z)/:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055009	TG(22:5(4Z,7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054153	TG(:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054894	TG(22:4(7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C65H100O6	M+NH4	994.7858	-1.6

994.7842

HMDB0055663	TG(4(8Z,11Z,14Z,17Z):4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0055064	TG(22:5(4Z,7Z,Z,13Z,16Z):4(5Z,8Z,11Z,14Z):4(8Z,11Z,14Z,17Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0053985	TG(:3n6/22:5(7Z,Z,13Z,16Z,19Z):5(5Z,8Z,11Z,14Z,17Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0054224	TG(4(5Z,8Z,11Z,14Z):4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0054854	TG(22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0054229	TG(4(5Z,8Z,11Z,14Z):4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0055633	TG(4(8Z,11Z,14Z,17Z):4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0054260	TG(4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z):4(8Z,11Z,14Z,17Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0054886	TG(22:4(7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0010547	TG(22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0053996	TG(:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z):4(8Z,11Z,14Z,17Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0055599	TG(4(8Z,11Z,14Z,17Z):3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0053891	TG(:3n6/4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0055079	TG(22:5(4Z,7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0055086	TG(22:5(4Z,7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0055035	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0055341	TG(18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0052814	TG(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0053229	TG(18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0050279	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0053159	TG(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0052739	TG(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0053242	TG(18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0052823	TG(18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0053234	TG(18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0053151	TG(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0052828	TG(18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0049679	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0053164	TG(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0055486	TG(18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0055306	TG(18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6
HMDB0055300	TG(18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H1000O6	M+NH4	994.7858	-1.6

HMDB0055112	TG(22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055042	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054841	TG(22:4(7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055755	TG(:5(5Z,8Z,11Z,14Z,17Z)/:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055758	TG(:5(5Z,8Z,11Z,14Z,17Z)/:3n6/22:5(7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054857	TG(22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z)/22:5(4Z,Z,13Z,16Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055126	TG(22:5(4Z,7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0053637	TG(:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0051386	TG(:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0053613	TG(:2n6/:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0051369	TG(:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0051335	TG(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0051352	TG(:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0051227	TG(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0051347	TG(:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0051279	TG(:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0051380	TG(:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054254	TG(:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0010548	TG(22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0054309	TG(:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055646	TG(:4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055671	TG(:4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055852	TG(22:5(7Z,Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055911	TG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055913	TG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055093	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z)/22:5(4Z,Z,13Z,16Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0055037	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z)/22:5(4Z,Z,13Z,16Z))	C65H100O6	M+NH4	994.7858	-1.6
HMDB0051209	TG(:3(5Z,8Z,11Z)/:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054790	TG(22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054885	TG(22:4(7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055628	TG(:4(8Z,11Z,14Z,17Z)/:3n6/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054848	TG(22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053913	TG(:3n6/22:4(7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8

HMDB0054208	TG(:4(5Z,8Z,11Z,14Z):2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054289	TG(:4(5Z,8Z,11Z,14Z):4(8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054218	TG(:4(5Z,8Z,11Z,14Z):3n6/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053978	TG(:3n6/22:5(7Z,Z,13Z,16Z,19Z):4(5Z,8Z,11Z,14Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053807	TG(:3n6/:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053885	TG(:3n6/:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054869	TG(22:4(7Z,Z,13Z,16Z):4(8Z,11Z,14Z,17Z):4(8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0051329	TG(:3(5Z,8Z,11Z):4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053636	TG(:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z):4(8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053630	TG(:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z):4(5Z,8Z,11Z,14Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053559	TG(:2n6/22:5(4Z,7Z,Z,13Z,16Z):5(5Z,8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053957	TG(:3n6/:4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054753	TG(22:4(7Z,Z,13Z,16Z):3(5Z,8Z,11Z):5(5Z,8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055008	TG(22:5(4Z,7Z,Z,13Z,16Z):3(5Z,8Z,11Z):4(8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055731	TG(:5(5Z,8Z,11Z,14Z,17Z):1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055598	TG(:4(8Z,11Z,14Z,17Z):3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054213	TG(:4(5Z,8Z,11Z,14Z):3n6/22:5(4Z,7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054223	TG(:4(5Z,8Z,11Z,14Z):4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054832	TG(22:4(7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055078	TG(22:5(4Z,7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054807	TG(22:4(7Z,Z,13Z,16Z):3n6/:5(5Z,8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055754	TG(:5(5Z,8Z,11Z,14Z,17Z):2n6/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053984	TG(:3n6/22:5(7Z,Z,13Z,16Z,19Z):4(8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055832	TG(22:5(7Z,Z,13Z,16Z,19Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053918	TG(:3n6/22:5(4Z,7Z,Z,13Z,16Z):4(5Z,8Z,11Z,14Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053962	TG(:3n6/:4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053879	TG(:3n6/:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054249	TG(:4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z):4(8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054853	TG(22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055049	TG(22:5(4Z,7Z,Z,13Z,16Z):2n6/:5(5Z,8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053890	TG(:3n6/:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053924	TG(:3n6/22:5(4Z,7Z,Z,13Z,16Z):4(8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054589	TG(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053968	TG(:3n6/:5(5Z,8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055034	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054625	TG(22:2(13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054785	TG(22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054995	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8

996.7997

HMDB0054152	TG(:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055056	TG(22:5(4Z,7Z,Z,13Z,16Z)/:3n6/:4(8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0010545	TG(22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0052808	TG(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0052733	TG(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0049678	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053150	TG(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0050278	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0050273	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0050159	TG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053145	TG(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0049553	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0052813	TG(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0052724	TG(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0050259	TG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0045449	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0052738	TG(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0049658	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053228	TG(18:3(6Z,9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0052822	TG(18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0051272	TG(:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0050847	TG(:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0051368	TG(:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053522	TG(:2n6/:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0051221	TG(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0051334	TG(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0051346	TG(:3(5Z,8Z,11Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053624	TG(:2n6/22:5(7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0051379	TG(:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3n6)	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053612	TG(:2n6/:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0051101	TG(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053600	TG(:2n6/:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053158	TG(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8

HMDB0049673	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055299	TG(18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0050811	TG(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055481	TG(18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0051261	TG(:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0051362	TG(:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053607	TG(:2n6/:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0051226	TG(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0051278	TG(:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0051373	TG(:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3(5Z,8Z,11Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0010556	TG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0010546	TG(22:5(7Z,Z,13Z,16Z,19Z)/18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055624	TG(:4(8Z,11Z,14Z,17Z)/:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055641	TG(:4(8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055765	TG(:5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054840	TG(22:4(7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054147	TG(:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054607	TG(22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054782	TG(22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0055029	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054815	TG(22:4(7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054987	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054243	TG(:4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0054856	TG(22:4(7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053989	TG(:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3n6)	C65H102O6	M+NH4	996.8015	-1.8
HMDB0053629	TG(:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3n6)	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054207	TG(:4(5Z,8Z,11Z,14Z)/:2n6/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053867	TG(:3n6/:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054142	TG(:4(5Z,8Z,11Z,14Z)/:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054737	TG(22:4(7Z,Z,13Z,16Z)/18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054212	TG(:4(5Z,8Z,11Z,14Z)/:3n6/22:4(7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054202	TG(:4(5Z,8Z,11Z,14Z)/:2n6/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0055048	TG(22:5(4Z,7Z,Z,13Z,16Z)/:2n6/:4(8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054606	TG(22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z)/:4(8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054986	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054239	TG(:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1

HMDB0054831	TG(22:4(7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0051100	TG(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0051254	TG(:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0051208	TG(:3(5Z,8Z,11Z)/:3n6/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0050846	TG(:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053552	TG(:2n6/22:5(4Z,7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053594	TG(:2n6/:4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053516	TG(:2n6/:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0051260	TG(:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053521	TG(:2n6/:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0051328	TG(:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053623	TG(:2n6/22:5(7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0050840	TG(:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0051191	TG(:3(5Z,8Z,11Z)/:2n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054588	TG(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0055594	TG(:4(8Z,11Z,14Z,17Z)/:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054146	TG(:4(5Z,8Z,11Z,14Z)/:3(5Z,8Z,11Z)/22:4(7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054939	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054728	TG(22:4(7Z,Z,13Z,16Z)/18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054798	TG(22:4(7Z,Z,13Z,16Z)/:2n6/:5(5Z,8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0055071	TG(22:5(4Z,7Z,Z,13Z,16Z)/22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0055637	TG(:4(8Z,11Z,14Z,17Z)/22:2(13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053806	TG(:3n6/:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054624	TG(22:2(13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0055623	TG(:4(8Z,11Z,14Z,17Z)/:2n6/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0051831	TG(22:1(13Z)/18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053873	TG(:3n6/:3n6/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053878	TG(:3n6/:3n6/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054565	TG(22:2(13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0055730	TG(:5(5Z,8Z,11Z,14Z,17Z)/:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0051863	TG(22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0055814	TG(22:5(7Z,Z,13Z,16Z,19Z)/18:22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053906	TG(:3n6/22:4(7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054776	TG(22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0055703	TG(:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054615	TG(22:2(13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053956	TG(:3n6/:4(8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053884	TG(:3n6/:4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054994	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1

998.8150

HMDB0054752	TG(22:4(7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z)/:4(8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0054583	TG(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053431	TG(:2n6/:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0052732	TG(18:2(9Z,12Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053241	TG(18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:2(13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0052723	TG(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0049532	TG(18:1(11Z)/22:4(7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0050139	TG(18:1(9Z)/22:4(7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0049672	TG(18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0049657	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053144	TG(18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053137	TG(18:3(6Z,9Z,12Z)/22:2(13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0049552	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0049547	TG(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0052718	TG(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0049652	TG(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0045422	TG(18/22:5(7Z,Z,13Z,16Z,19Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0045448	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0045287	TG(18/22:5(4Z,7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0045443	TG(18/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0050253	TG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0050158	TG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0050272	TG(18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0050258	TG(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0051271	TG(:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z)/:3n6)	C65H104O6	M+NH4	998.8171	-2.1
HMDB0051095	TG(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0050828	TG(:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0051203	TG(:3(5Z,8Z,11Z)/:3n6/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053617	TG(:2n6/22:5(7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0051220	TG(:3(5Z,8Z,11Z)/:4(5Z,8Z,11Z,14Z)/22:4(7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053599	TG(:2n6/:4(8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053606	TG(:2n6/:5(5Z,8Z,11Z,14Z,17Z)/22:4(7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0051361	TG(:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z)/:3n6)	C65H104O6	M+NH4	998.8171	-2.1
HMDB0051378	TG(:3(5Z,8Z,11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:2n6)	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053558	TG(:2n6/22:5(4Z,7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053509	TG(:2n6/:3n6/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
HMDB0053546	TG(:2n6/22:4(7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1

	HMDB0050153	TG(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0052807	TG(18:2(9Z,12Z)/22:5(7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0046227	TG(/22:6(4Z,7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0055293	TG(18:3(9Z,12Z,15Z)/22:2(13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0050805	TG(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0050810	TG(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0055480	TG(18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0046177	TG(/:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0050678	TG(:1(11Z)/:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0050792	TG(:1(11Z)/:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0055439	TG(18:4(6Z,9Z,12Z,15Z)/22:1(13Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0050733	TG(:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0051895	TG(22:1(13Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0051265	TG(:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z)/:3(5Z,8Z,11Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0051355	TG(:3(5Z,8Z,11Z)/22:5(7Z,Z,13Z,16Z,19Z)/:3(5Z,8Z,11Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0010544	TG(22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0054579	TG(22:2(13Z,16Z)/18:3(9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0054989	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0055737	TG(:5(5Z,8Z,11Z,14Z,17Z)/22:1(13Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0054806	TG(22:4(7Z,Z,13Z,16Z)/:3n6/:4(8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0053912	TG(:3n6/22:4(7Z,Z,13Z,16Z)/:4(8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0054509	TG(22:2(13Z,16Z)/18:3(6Z,9Z,12Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0054537	TG(22:2(13Z,16Z)/:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0054597	TG(22:2(13Z,16Z)/:4(8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0054299	TG(:4(5Z,8Z,11Z,14Z)/:5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0055001	TG(22:5(4Z,7Z,Z,13Z,16Z)/:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0053801	TG(:3n6/:3(5Z,8Z,11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0055831	TG(22:5(7Z,Z,13Z,16Z,19Z)/18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0054981	TG(22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0053977	TG(:3n6/22:5(7Z,Z,13Z,16Z,19Z)/:3n6)	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0054847	TG(22:4(7Z,Z,13Z,16Z)/18:3(9Z,12Z,15Z)/22:4(7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0054784	TG(22:4(7Z,Z,13Z,16Z)/18:3(6Z,9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C65H104O6	M+NH4	998.8171	-2.1
	HMDB0053917	TG(:3n6/22:5(4Z,7Z,Z,13Z,16Z)/:3n6)	C65H104O6	M+NH4	998.8171	-2.1
m/z detected	HMDB ID	Metabolites	Formula	Adduct ions	m/z calculated	Error, ppm
	HMDB0165479	2,3-dihydroxy-2-methylpropanenitrile	C4H7NO2	M-H	100.0404	1.0

100.0405	HMDB0036458	1-Aminocyclopropanecarboxylic acid	C4H7NO2	M-H	100.0404	1.0
	HMDB0029615	(S)-2-Azetidinecarboxylic acid	C4H7NO2	M-H	100.0404	1.0
	HMDB0029387	L-3-Aminodihydro-2(3H)-furanone	C4H7NO2	M-H	100.0404	1.0
	HMDB0061870	N-Methylene-ethenamine	C3H5N	M+FA-H	100.0404	1.0
101.0245	HMDB0000060	Acetoacetic acid	C4H6O3	M-H	101.0244	0.8
	HMDB0172027	Tocris538	C4H6O3	M-H	101.0244	0.8
	HMDB0172028	3-Methyloxirane-2-carboxylic acid	C4H6O3	M-H	101.0244	0.8
	HMDB0168831	methyl oxirane-2-carboxylate	C4H6O3	M-H	101.0244	0.8
	HMDB0171690	ethyl glyoxylate	C4H6O3	M-H	101.0244	0.8
	HMDB0178247	5469-16-9	C4H6O3	M-H	101.0244	0.8
	HMDB0031646	Acetic anhydride	C4H6O3	M-H	101.0244	0.8
	HMDB0003381	4-Hydroxycrotonic acid	C4H6O3	M-H	101.0244	0.8
	HMDB0002217	(S)-Methylmalonic acid semialdehyde	C4H6O3	M-H	101.0244	0.8
	HMDB0001259	Succinic acid semialdehyde	C4H6O3	M-H	101.0244	0.8
	HMDB0001172	2-Methyl-3-oxopropanoic acid	C4H6O3	M-H	101.0244	0.8
	HMDB0000005	2-Ketobutyric acid	C4H6O3	M-H	101.0244	0.8
	HMDB0184570	dihydro-4-hydroxy-3(2h)-furanone	C4H6O3	M-H	101.0244	0.8
	HMDB0180697	2-Propyn-1-ol	C3H4O	M+FA-H	101.0244	0.8
	HMDB0041822	Acrolein	C3H4O	M+FA-H	101.0244	0.8
101.0609	HMDB0034237	Propyl acetate	C5H10O2	M-H	101.0608	0.9
	HMDB0041992	Pivalic acid	C5H10O2	M-H	101.0608	0.9
	HMDB0059678	1-Hydroxy-2-pentanone	C5H10O2	M-H	101.0608	0.9
	HMDB0061989	2-hydroxy-3-pentanone	C5H10O2	M-H	101.0608	0.9
	HMDB0167011	2-methyl-3-butene-1,2-diol	C5H10O2	M-H	101.0608	0.9
	HMDB0167012	1,2-epoxy-3-hydroxy-3-methylbutane	C5H10O2	M-H	101.0608	0.9
	HMDB0175213	2-ethylidene-propane-1,3-diol	C5H10O2	M-H	101.0608	0.9
	HMDB0175214	MBDO	C5H10O2	M-H	101.0608	0.9
	HMDB0032230	2,4-Dimethyl-1,3-dioxolane	C5H10O2	M-H	101.0608	0.9
	HMDB0033890	Methyl butyrate	C5H10O2	M-H	101.0608	0.9
	HMDB0000892	Valeric acid	C5H10O2	M-H	101.0608	0.9
	HMDB0000718	Isovaleric acid	C5H10O2	M-H	101.0608	0.9
	HMDB0002176	Ethylmethylacetic acid	C5H10O2	M-H	101.0608	0.9
	HMDB0031516	3-Hydroxy-2-pentanone	C5H10O2	M-H	101.0608	0.9
	HMDB0031175	Tetrahydro-2-furanmethanol	C5H10O2	M-H	101.0608	0.9
	HMDB0039799	Tetrahydro-2-methyl-3-furanol	C5H10O2	M-H	101.0608	0.9
	HMDB0031247	2-Methylpropyl formate	C5H10O2	M-H	101.0608	0.9
	HMDB0033742	(S)-2-Methylbutanoic acid	C5H10O2	M-H	101.0608	0.9
	HMDB0031241	Isopropyl acetate	C5H10O2	M-H	101.0608	0.9
	HMDB0031249	Methyl isobutyrate	C5H10O2	M-H	101.0608	0.9
	HMDB0030058	Ethyl propionate	C5H10O2	M-H	101.0608	0.9
	HMDB0040575	Butyl formate	C5H10O2	M-H	101.0608	0.9
	HMDB0175215	(2,3-Dimethyloxiranyl)methanol	C5H10O2	M-H	101.0608	0.9
	HMDB0161203	isovalerate	C5H9O2	M-H	101.0608	1.0
102.0562	HMDB0000092	Dimethylglycine	C4H9NO2	M-H	102.0561	1.4
	HMDB0094692	N-Methylalanine	C4H9NO2	M-H	102.0561	1.4
	HMDB0240305	N-acetyethanolamine	C4H9NO2	M-H	102.0561	1.4
	HMDB0167365	3-hydroxybutanimidic acid	C4H9NO2	M-H	102.0561	1.4
	HMDB0167367	2-hydroxybutanamide	C4H9NO2	M-H	102.0561	1.4
	HMDB0167366	4-hydroxybutanamide	C4H9NO2	M-H	102.0561	1.4
	HMDB0001906	2-Aminoisobutyric acid	C4H9NO2	M-H	102.0561	1.4
	HMDB0000650	D-alpha-Aminobutyric acid	C4H9NO2	M-H	102.0561	1.4
	HMDB0061050	D-alpha-Aminobutyric acid	C4H9NO2	M-H	102.0561	1.4
	HMDB0000452	L-alpha-Aminobutyric acid	C4H9NO2	M-H	102.0561	1.4
	HMDB0002166	(S)-beta-Aminoisobutyric acid	C4H9NO2	M-H	102.0561	1.4
	HMDB0000112	gamma-Aminobutyric acid	C4H9NO2	M-H	102.0561	1.4
	HMDB0002299	(R)-beta-Aminoisobutyric acid	C4H9NO2	M-H	102.0561	1.4
	HMDB0003911	3-Aminoisobutanoic acid	C4H9NO2	M-H	102.0561	1.4
	HMDB0038394	O-Acetyethanolamine	C4H9NO2	M-H	102.0561	1.4
	HMDB0031329	Butyl nitrite	C4H9NO2	M-H	102.0561	1.4
	HMDB0031654	3-Aminobutanoic acid	C4H9NO2	M-H	102.0561	1.4
	HMDB0094693	3-Aminobutanoic acid	C4H9NO2	M-H	102.0561	1.4
	HMDB0041945	N-Ethylglycine	C4H9NO2	M-H	102.0561	1.4
	HMDB0168957	Allylamine	C3H7N	M+FA-H	102.0561	1.5
	HMDB0029572	Diethyl disulfide	C4H10S2	M-H20-H	103.0040	-1.0
	HMDB0031157	2,3-Butanedithiol	C4H10S2	M-H20-H	103.0040	-1.0

103.0039	HMDB0033552	1,3-Butanedithiol	C4H10S2	M-H2O-H	103.0040	-1.0
	HMDB0031872	Methyl propyl disulfide	C4H10S2	M-H2O-H	103.0040	-1.0
	HMDB0031708	1,2-Bis(methylthio)ethane	C4H10S2	M-H2O-H	103.0040	-1.0
	HMDB0041492	1,2-Butanedithiol	C4H10S2	M-H2O-H	103.0040	-1.0
	HMDB0006938	Tartronate semialdehyde	C3H4O4	M-H	103.0037	2.1
	HMDB0001352	Hydroxypyruvic acid	C3H4O4	M-H	103.0037	2.1
103.0402	HMDB0000691	Malonic acid	C3H4O4	M-H	103.0037	2.1
	HMDB0000008	(S)-2-hydroxybutyric acid	C4H8O3	M-H	103.0401	1.3
	HMDB0165470	2-Butanone, 1,3-dihydroxy-	C4H8O3	M-H	103.0401	1.3
	HMDB0165469	3,4-dihydroxy-2-butanone	C4H8O3	M-H	103.0401	1.3
	HMDB0059748	2-Methyl-3-hydroxypropanoate	C4H8O3	M-H	103.0401	1.3
	HMDB0000710	4-Hydroxybutyric acid	C4H8O3	M-H	103.0401	1.3
	HMDB0000442	(S)-3-Hydroxybutyric acid	C4H8O3	M-H	103.0401	1.3
	HMDB0000357	3-Hydroxybutyric acid	C4H8O3	M-H	103.0401	1.3
	HMDB0062640	3-Hydroxyisobutyric acid	C4H8O3	M-H	103.0401	1.3
	HMDB0126088	3-Hydroxyisobutyric acid	C4H8O3	M-H	103.0401	1.3
	HMDB0000336	(R)-3-Hydroxyisobutyric acid	C4H8O3	M-H	103.0401	1.3
	HMDB0000023	(S)-3-Hydroxyisobutyric acid	C4H8O3	M-H	103.0401	1.3
	HMDB0000011	(R)-3-Hydroxybutyric acid	C4H8O3	M-H	103.0401	1.3
	HMDB0031212	Ethoxyacetic acid	C4H8O3	M-H	103.0401	1.3
	HMDB0000729	alpha-Hydroxyisobutyric acid	C4H8O3	M-H	103.0401	1.3
	HMDB0001659	Acetone	C3H6O	M+FA-H	103.0401	1.3
	HMDB0003366	Propanal	C3H6O	M+FA-H	103.0401	1.3
	HMDB0062143	oxetane	C3H6O	M+FA-H	103.0401	1.3
	HMDB0031558	Methyloxirane	C3H6O	M+FA-H	103.0401	1.3
	HMDB0031652	Allyl alcohol	C3H6O	M+FA-H	103.0401	1.3
104.0355	HMDB0000187	L-Serine	C3H7NO3	M-H	104.0353	1.8
	HMDB0062263	L-Serine	C3H7NO3	M-H	104.0353	1.8
	HMDB0003406	D-Serine	C3H7NO3	M-H	104.0353	1.8
	HMDB0003656	Acetaldehyde oxime	C2H5NO	M+FA-H	104.0353	1.8
	HMDB0001122	N-Methylformamide	C2H5NO	M+FA-H	104.0353	1.8
	HMDB0031645	Acetamide	C2H5NO	M+FA-H	104.0353	1.8
107.0503	HMDB0001858	p-Cresol	C7H8O	M-H	107.0502	0.6
	HMDB0002048	m-Cresol	C7H8O	M-H	107.0502	0.6
	HMDB0002055	o-Cresol	C7H8O	M-H	107.0502	0.6
	HMDB0003119	Benzyl alcohol	C7H8O	M-H	107.0502	0.6
	HMDB0033895	Anisole	C7H8O	M-H	107.0502	0.6
109.0296	HMDB0000957	Pyrocatechol	C6H6O2	M-H	109.0295	0.9
	HMDB0032037	1,3-Benzenediol	C6H6O2	M-H	109.0295	0.9
	HMDB0033002	5-Methyl-2-furancarboxaldehyde	C6H6O2	M-H	109.0295	0.9
	HMDB0031180	(E,E)-2,4-Hexadienedial	C6H6O2	M-H	109.0295	0.9
	HMDB0033127	2-Acetylfuran	C6H6O2	M-H	109.0295	0.9
	HMDB0002434	Hydroquinone	C6H6O2	M-H	109.0295	0.9
109.0660	HMDB0187589	2-Cyclohexene-1,4-dione	C6H6O2	M-H	109.0295	0.9
	HMDB0061891	(E,Z)-2,4-Heptadienal	C7H10O	M-H	109.0659	1.0
	HMDB0040278	2-Isopropylfuran	C7H10O	M-H	109.0659	1.0
	HMDB0031541	3-Methyl-2-cyclohexen-1-one	C7H10O	M-H	109.0659	1.0
	HMDB0029721	2,3,5-Trimethylfuran	C7H10O	M-H	109.0659	1.0
	HMDB0029728	2-Ethyl-5-methylfuran	C7H10O	M-H	109.0659	1.0
110.0249	HMDB0040277	2-Propylfuran	C7H10O	M-H	109.0659	1.0
	HMDB0004230	Pyrrole-2-carboxylic acid	C5H5NO2	M-H	110.0248	1.3
111.0089	HMDB0038175	2-Acetyloxazole	C5H5NO2	M-H	110.0248	1.3
	HMDB0000444	3-Furoic acid	C5H4O3	M-H	111.0088	1.2
	HMDB0032994	3-Hydroxy-2H-pyran-2-one	C5H4O3	M-H	111.0088	1.2
	HMDB0039437	2,3-Dihydroxy-2,4-cyclopentadien-1-one	C5H4O3	M-H	111.0088	1.2
	HMDB0000617	2-Furoic acid	C5H4O3	M-H	111.0088	1.2
111.0201	HMDB0000300	Uracil	C4H4N2O2	M-H	111.0200	0.9
	HMDB0060760	4-Carboxypyrazole	C4H4N2O2	M-H	111.0200	0.9
	HMDB0001164	trans-1,2-Dihydrobenzene-1,2-diol	C6H8O2	M-H	111.0452	1.3
	HMDB0032233	2,5-Dimethyl-3(2H)-furanone	C6H8O2	M-H	111.0452	1.3
	HMDB0029581	(2E,4E)-2,4-Hexadienoic acid	C6H8O2	M-H	111.0452	1.3
	HMDB0031543	3-Methyl-1,2-cyclopentanedione	C6H8O2	M-H	111.0452	1.3
	HMDB0031759	(E)-4-Oxo-2-hexen-1-al	C6H8O2	M-H	111.0452	1.3
	HMDB0040260	5,5-Dimethyl-2(5H)-furanone	C6H8O2	M-H	111.0452	1.3
	HMDB0034247	2-(Methoxymethyl)furan	C6H8O2	M-H	111.0452	1.3

111.0453	HMDB0033569	Syoqualdehyde	C6H8O2	M-H	111.0452	1.3
	HMDB0039778	xi-3,5-Dimethyl-2(5H)-furanone	C6H8O2	M-H	111.0452	1.3
	HMDB0031344	1,2-Cyclohexanedione	C6H8O2	M-H	111.0452	1.3
	HMDB0179337	(2Z,4E)-hexa-2,4-dienoic acid	C6H8O2	M-H	111.0452	1.3
	HMDB0179339	3-[(1E)-prop-1-en-1-yl]oxirane-2-carbaldehyde	C6H8O2	M-H	111.0452	1.3
	HMDB0179340	(2Z)-3-(3-methyloxiran-2-yl)prop-2-enal	C6H8O2	M-H	111.0452	1.3
	HMDB0179338	(2Z,4E)-6-hydroxyhexa-2,4-dienal	C6H8O2	M-H	111.0452	1.3
	HMDB0187593	1,4-Cyclohexanedione	C6H8O2	M-H	111.0452	1.3
111.0816	HMDB0061878	Cyclopentadiene	C5H6	M+FA-H	111.0452	1.3
	HMDB0031486	3-Hepten-2-one	C7H12O	M-H	111.0815	0.5
	HMDB0031540	4-Methylcyclohexanone	C7H12O	M-H	111.0815	0.5
	HMDB0033667	(R)-3-Methylcyclohexanone	C7H12O	M-H	111.0815	0.5
	HMDB0033827	(2E)-2-Heptenal	C7H12O	M-H	111.0815	0.5
	HMDB0031539	2-Methylcyclohexanone	C7H12O	M-H	111.0815	0.5
	HMDB0031487	(E)-4-Hepten-2-one	C7H12O	M-H	111.0815	0.5
	HMDB0034372	xi-3-Methyl-3-cyclohexen-1-ol	C7H12O	M-H	111.0815	0.5
	HMDB0040339	2,5-Heptadien-1-ol	C7H12O	M-H	111.0815	0.5
	HMDB0061957	(Z)-2-Heptenal	C7H12O	M-H	111.0815	0.5
	HMDB0031550	5-Methyl-3-hexen-2-one	C7H12O	M-H	111.0815	0.5
	HMDB0062028	3-Ethylcyclopentanone	C7H12O	M-H	111.0815	0.5
	HMDB0061994	2-methyl-2-hexenal	C7H12O	M-H	111.0815	0.5
	HMDB0061985	2-ethylcyclopentan-1-one	C7H12O	M-H	111.0815	0.5
	HMDB0032301	trans-2-trans-4-Heptadien-1-ol	C7H12O	M-H	111.0815	0.5
	HMDB0031551	5-Methyl-5-hexen-2-one	C7H12O	M-H	111.0815	0.5
	HMDB0031488	2-Hepten-4-one	C7H12O	M-H	111.0815	0.5
	HMDB0031483	(Z)-4-Heptenal	C7H12O	M-H	111.0815	0.5
112.0406	HMDB0006875	1-Pyrroline-2-carboxylic acid	C5H7NO2	M-H	112.0404	1.8
	HMDB0001301	(S)-1-pyrroline-5-carboxylate	C5H7NO2	M-H	112.0404	1.8
	HMDB0035924	Pyrrole	C4H5N	M+FA-H	112.0404	1.8
	HMDB0031323	3-Butenenitrile	C4H5N	M+FA-H	112.0404	1.8
112.0517	HMDB0000562	Creatinine	C4H7N3O	M-H	112.0516	0.6
113.0245	HMDB0031859	Norfuranol	C5H6O3	M-H	113.0244	0.7
	HMDB0060461	cis-Acetylacrylate	C5H6O3	M-H	113.0244	0.7
	HMDB0013785	Furan	C4H4O	M+FA-H	113.0244	0.7
	HMDB0006853	3-Butyn-1-al	C4H4O	M+FA-H	113.0244	0.7
113.0358	HMDB0000076	Dihydrouracil	C4H6N2O2	M-H	113.0357	1.3
	HMDB0003646	N-Methylhydantoin	C4H6N2O2	M-H	113.0357	1.3
	HMDB0060245	L-3-Cyanoalanine	C4H6N2O2	M-H	113.0357	1.3
	HMDB0001525	Imidazole	C3H4N2	M+FA-H	113.0356	1.3
113.0609	HMDB0163350	(Z)-hex-4-enoic acid	C6H10O2	M-H	113.0608	0.8
	HMDB0163351	(4Z)-6-hydroxyhex-4-enal	C6H10O2	M-H	113.0608	0.8
	HMDB0163353	3-(3-methyloxiran-2-yl)propanal	C6H10O2	M-H	113.0608	0.8
	HMDB0163352	(4Z)-3-hydroxyhex-4-enal	C6H10O2	M-H	113.0608	0.8
	HMDB0179351	4-Hexenoic acid	C6H10O2	M-H	113.0608	0.8
	HMDB0179346	(2Z)-3-(3-methyloxiran-2-yl)prop-2-en-1-ol	C6H10O2	M-H	113.0608	0.8
	HMDB0179345	{3-[(1E)-prop-1-en-1-yl]oxiran-2-yl}methanol	C6H10O2	M-H	113.0608	0.8
	HMDB0179341	(4E)-6-hydroxyhex-4-enal	C6H10O2	M-H	113.0608	0.8
	HMDB0179344	cis-2,4-hexadien-1,6-diol	C6H10O2	M-H	113.0608	0.8
	HMDB0179343	(4E)-2-hydroxyhex-4-enal	C6H10O2	M-H	113.0608	0.8
	HMDB0179342	(4E)-3-hydroxyhex-4-enal	C6H10O2	M-H	113.0608	0.8
	HMDB0169695	(Z)-3-methyl-2-pentenoic acid	C6H10O2	M-H	113.0608	0.8
	HMDB0169664	(E)-3-Methyl-2-pentenoic acid	C6H10O2	M-H	113.0608	0.8
	HMDB0165582	(2Z)-4-hydroxy-2-methylpent-2-enal	C6H10O2	M-H	113.0608	0.8
	HMDB0165583	2-Methyl-3-ethyloxiran-2-carbaldehyde	C6H10O2	M-H	113.0608	0.8
	HMDB0165584	(2Z)-5-hydroxy-2-methylpent-2-enal	C6H10O2	M-H	113.0608	0.8
	HMDB0165581	(2Z)-2-(hydroxymethyl)pent-2-enal	C6H10O2	M-H	113.0608	0.8
	HMDB0163703	(3Z)-5-hydroxy-3-methylpent-3-en-2-one	C6H10O2	M-H	113.0608	0.8
	HMDB0163702	Pentanal, 3-methyl-4-oxo-	C6H10O2	M-H	113.0608	0.8
	HMDB0163354	(4Z)-2-hydroxyhex-4-enal	C6H10O2	M-H	113.0608	0.8
	HMDB0000453	delta-Hexanolactone	C6H10O2	M-H	113.0608	0.8
	HMDB0031562	2-Methyl-3-pentenoic acid	C6H10O2	M-H	113.0608	0.8
	HMDB0031158	2-Methyl-4-pentenoic acid	C6H10O2	M-H	113.0608	0.8
	HMDB0039581	Ethyl crotonate	C6H10O2	M-H	113.0608	0.8
	HMDB0032490	Prenyl formate	C6H10O2	M-H	113.0608	0.8
	HMDB0060476	epsilon-Caprolactone	C6H10O2	M-H	113.0608	0.8

	HMDB0040328	Methyl 4-pentenoate	C6H10O2	M-H	113.0608	0.8
	HMDB0031559	4-Methyl-2,3-pentanedione	C6H10O2	M-H	113.0608	0.8
	HMDB0031491	2,3-Hexanedione	C6H10O2	M-H	113.0608	0.8
	HMDB0003843	Gamma-Caprolactone	C6H10O2	M-H	113.0608	0.8
	HMDB0010719	Isohydrosorbic acid	C6H10O2	M-H	113.0608	0.8
	HMDB0031561	4-Methyl-2-pentenoic acid	C6H10O2	M-H	113.0608	0.8
	HMDB0031492	3,4-Hexanedione	C6H10O2	M-H	113.0608	0.8
	HMDB0033568	5-Oxohexanal	C6H10O2	M-H	113.0608	0.8
	HMDB0029487	Allyl propionate	C6H10O2	M-H	113.0608	0.8
	HMDB0031501	3-Hexenoic acid	C6H10O2	M-H	113.0608	0.8
	HMDB0031560	2-Methyl-2-pentenoic acid	C6H10O2	M-H	113.0608	0.8
	HMDB0061929	Dihydro-4,4-dimethyl-2(3H)-furanone	C6H10O2	M-H	113.0608	0.8
	HMDB0062135	methyl (2E)-2-methylbut-2-enoate	C6H10O2	M-H	113.0608	0.8
	HMDB0061965	1-methyl-2,3-dioxabicyclo[2.2.1]heptane	C6H10O2	M-H	113.0608	0.8
	HMDB0240384	4-Hydroxyhexanal	C6H10O2	M-H	113.0608	0.8
	HMDB0061977	penta-1,4-diene	C5H8	M+FA-H	113.0608	0.9
	HMDB0062111	ethylidenecyclopropane	C5H8	M+FA-H	113.0608	0.9
	HMDB0062165	(E)-1,3-pentadiene	C5H8	M+FA-H	113.0608	0.9
113.0973	HMDB0003671	2-Heptanone	C7H14O	M-H	113.0972	1.0
	HMDB0062059	4-methylhexan-3-one	C7H14O	M-H	113.0972	1.0
	HMDB0166735	trans-2-Hepten-1-ol	C7H14O	M-H	113.0972	1.0
	HMDB0061896	2-Methyl-3-hexanone	C7H14O	M-H	113.0972	1.0
	HMDB0004814	4-Heptanone	C7H14O	M-H	113.0972	1.0
	HMDB0005841	Ethyl isobutyl ketone	C7H14O	M-H	113.0972	1.0
	HMDB0041320	(2R,4Z)-4-Hepten-2-ol	C7H14O	M-H	113.0972	1.0
	HMDB0040191	2-Methylhexanal	C7H14O	M-H	113.0972	1.0
	HMDB0031475	Heptanal	C7H14O	M-H	113.0972	1.0
	HMDB0031482	3-Heptanone	C7H14O	M-H	113.0972	1.0
	HMDB0031429	2,4-Dimethyl-3-pentanone	C7H14O	M-H	113.0972	1.0
	HMDB0031538	3-Methylcyclohexanol	C7H14O	M-H	113.0972	1.0
	HMDB0031405	(Z)-4-Hepten-1-ol	C7H14O	M-H	113.0972	1.0
	HMDB0031549	5-Methyl-2-hexanone	C7H14O	M-H	113.0972	1.0
	HMDB0038052	1-Ethoxy-3-methyl-2-butene	C7H14O	M-H	113.0972	1.0
	HMDB0032405	3-Methylhexanal	C7H14O	M-H	113.0972	1.0
	HMDB0059693	1-Methylcyclohexanol	C7H14O	M-H	113.0972	1.0
	HMDB0175178	6-Hepten-1-ol	C7H14O	M-H	113.0972	1.0
114.0200	HMDB0240339	maleamate	C4H4NO3	M-H	114.0197	2.9
114.0561	HMDB0000162	L-Proline	C5H9NO2	M-H	114.0561	0.4
	HMDB0167283	2,4-dihydroxy-2-methylbutanenitrile	C5H9NO2	M-H	114.0561	0.4
	HMDB0167281	2,3-dihydroxy-2-methylbutanenitrile	C5H9NO2	M-H	114.0561	0.4
	HMDB0167282	2-hydroxy-2-(hydroxymethyl)butanenitrile	C5H9NO2	M-H	114.0561	0.4
	HMDB0177063	1-formyl-pyrrolidin-2-ol	C5H9NO2	M-H	114.0561	0.4
	HMDB0003411	D-Proline	C5H9NO2	M-H	114.0561	0.4
	HMDB0030409	4-Amino-2-methylenebutanoic acid	C5H9NO2	M-H	114.0561	0.4
	HMDB0034208	Pterolactam	C5H9NO2	M-H	114.0561	0.4
	HMDB0179973	SCHEMBL55844	C5H9NO2	M-H	114.0561	0.4
	HMDB0012880	Acetamidopropanal	C5H9NO2	M-H	114.0561	0.4
	HMDB0012497	1-Pyrroline	C4H7N	M+FA-H	114.0561	0.4
	HMDB0060246	1-Pyrroline	C4H7N	M+FA-H	114.0561	0.4
115.0038	HMDB0000134	Fumaric acid	C4H4O4	M-H	115.0037	1.0
	HMDB0187641	SCHEMBL127359	C4H4O4	M-H	115.0037	1.0
	HMDB0000176	Maleic acid	C4H4O4	M-H	115.0037	1.0
	HMDB0006804	Propynoic acid	C3H2O2	M+FA-H	115.0037	1.0
	HMDB0038974	3,3-Dimethyl-1,2-dithiolane	C5H10S2	M-H20-H	115.0040	-1.8
	HMDB0039790	Tetrahydro-2-methyl-3-thiophenethiol	C5H10S2	M-H20-H	115.0040	-1.8
	HMDB0039789	Tetrahydro-2-methyl-2-thiophenethiol	C5H10S2	M-H20-H	115.0040	-1.8
	HMDB0003771	2-Methylacetoacetic acid	C5H8O3	M-H	115.0401	0.3
	HMDB0168839	2-HYDROXYETHYL ACRYLATE	C5H8O3	M-H	115.0401	0.3
	HMDB0132477	2-(hydroxymethyl)but-2-enoic acid	C5H8O3	M-H	115.0401	0.3
	HMDB0129097	4-hydroxy-2-methylbut-2-enoic acid	C5H8O3	M-H	115.0401	0.3
	HMDB0177210	4-hydroxytiglic acid	C5H8O3	M-H	115.0401	0.3
	HMDB0177209	2-Hydroxymethyl-trans-crotonsacure	C5H8O3	M-H	115.0401	0.3
	HMDB0169666	SCHEMBL4558754	C5H8O3	M-H	115.0401	0.3
	HMDB0168838	Ethyl 2,3-epoxypropanoate	C5H8O3	M-H	115.0401	0.3
	HMDB0129098	2,3-dimethyloxirane-2-carboxylic acid	C5H8O3	M-H	115.0401	0.3

115.0401	HMDB0129096	(2Z)-2-(hydroxymethyl)but-2-enoic acid	C5H8O3	M-H	115.0401	0.3
	HMDB0128943	(2E)-4-hydroxy-3-methylbut-2-enoic acid	C5H8O3	M-H	115.0401	0.3
	HMDB0128917	dimethyloxirane-2-carboxylic acid	C5H8O3	M-H	115.0401	0.3
	HMDB0128916	4-hydroxy-3-methylbut-2-enoic acid	C5H8O3	M-H	115.0401	0.3
	HMDB0000720	Levulinic acid	C5H8O3	M-H	115.0401	0.3
	HMDB0034466	Acetoxyacetone	C5H8O3	M-H	115.0401	0.3
	HMDB0012233	Glutarate semialdehyde	C5H8O3	M-H	115.0401	0.3
	HMDB0029172	2-Methylacetoacetic acid	C5H8O3	M-H	115.0401	0.3
	HMDB0001865	2-Oxovaleric acid	C5H8O3	M-H	115.0401	0.3
	HMDB0000310	Methylacetoacetic acid	C5H8O3	M-H	115.0401	0.3
	HMDB0031643	Ethyl pyruvate	C5H8O3	M-H	115.0401	0.3
	HMDB0000019	alpha-Ketoisovaleric acid	C5H8O3	M-H	115.0401	0.3
	HMDB0034233	Crotonaldehyde	C4H6O	M+FA-H	115.0401	0.3
	HMDB0061874	Methacrolein	C4H6O	M+FA-H	115.0401	0.3
	HMDB0061873	3-Buten-2-one	C4H6O	M+FA-H	115.0401	0.3
	HMDB0062007	Dihydrofuran I	C4H6O	M+FA-H	115.0401	0.3
115.0765	HMDB0163678	6-hydroxyhexan-2-one	C6H12O2	M-H	115.0765	0.4
	HMDB0163355	(4Z)-hex-4-ene-1,2-diol	C6H12O2	M-H	115.0765	0.4
	HMDB0163356	(2Z)-hex-2-ene-1,6-diol	C6H12O2	M-H	115.0765	0.4
	HMDB0163357	(4Z)-hex-4-ene-1,3-diol	C6H12O2	M-H	115.0765	0.4
	HMDB0185846	4-(hydroxymethyl)-2-pentanone	C6H12O2	M-H	115.0765	0.4
	HMDB0176889	SCHEMBL58684	C6H12O2	M-H	115.0765	0.4
	HMDB0176888	2-Hexene-1,4-diol	C6H12O2	M-H	115.0765	0.4
	HMDB0176891	(E)-2-Hexene-1,6-diol	C6H12O2	M-H	115.0765	0.4
	HMDB0176890	(3-propyloxiran-2-yl)methanol	C6H12O2	M-H	115.0765	0.4
	HMDB0165589	SCHEMBL63629	C6H12O2	M-H	115.0765	0.4
	HMDB0165585	(2Z)-2-methylpent-2-ene-1,4-diol	C6H12O2	M-H	115.0765	0.4
	HMDB0165586	(2Z)-2-methylpent-2-ene-1,5-diol	C6H12O2	M-H	115.0765	0.4
	HMDB0165588	2-propylidene-1,3-propanediol	C6H12O2	M-H	115.0765	0.4
	HMDB0163715	1567-93-7	C6H12O2	M-H	115.0765	0.4
	HMDB0163358	3-(3-methyloxiranyl)propan-1-ol	C6H12O2	M-H	115.0765	0.4
	HMDB0031207	Methyl pentanoate	C6H12O2	M-H	115.0765	0.4
	HMDB0030059	Propyl propionate	C6H12O2	M-H	115.0765	0.4
	HMDB0040279	2,4,5-Trimethyl-1,3-dioxolane	C6H12O2	M-H	115.0765	0.4
	HMDB0034163	3-Methylbutyl formate	C6H12O2	M-H	115.0765	0.4
	HMDB0031511	Diacetone alcohol	C6H12O2	M-H	115.0765	0.4
	HMDB0031580	2-Methylpentanoic acid	C6H12O2	M-H	115.0765	0.4
	HMDB0030027	Methyl 3-methylbutanoate	C6H12O2	M-H	115.0765	0.4
	HMDB0037266	2,2,4-Trimethyl-1,3-dioxolane	C6H12O2	M-H	115.0765	0.4
	HMDB0029762	Methyl (S)-2-Methylbutanoate	C6H12O2	M-H	115.0765	0.4
	HMDB0062131	Methyl (S)-2-Methylbutanoate	C6H12O2	M-H	115.0765	0.4
	HMDB0033774	3-Methylpentanoic acid	C6H12O2	M-H	115.0765	0.4
	HMDB0000535	Caproic acid	C6H12O2	M-H	115.0765	0.4
	HMDB0061883	Caproic acid	C6H12O2	M-H	115.0765	0.4
	HMDB0033889	Ethyl butyrate	C6H12O2	M-H	115.0765	0.4
	HMDB0031248	Ethyl 2-methylpropanoate	C6H12O2	M-H	115.0765	0.4
	HMDB0176566	3,3-dimethylbutyric acid	C6H12O2	M-H	115.0765	0.4
	HMDB0040327	Pentyl formate	C6H12O2	M-H	115.0765	0.4
	HMDB0031221	2-Ethylbutanoic acid	C6H12O2	M-H	115.0765	0.4
	HMDB0000689	Isocaproic acid	C6H12O2	M-H	115.0765	0.4
	HMDB0031325	n-Butyl acetate	C6H12O2	M-H	115.0765	0.4
	HMDB0030056	Isopropyl propionate	C6H12O2	M-H	115.0765	0.4
	HMDB0031246	2-Methylpropyl acetate	C6H12O2	M-H	115.0765	0.4
	HMDB0062097	Cyclopentane	C5H10	M+FA-H	115.0765	0.4
116.0718	HMDB0000883	L-Valine	C5H11NO2	M-H	116.0717	0.8
	HMDB0061966	1-nitropentane	C5H11NO2	M-H	116.0717	0.8
	HMDB0062141	N,N-Dimethyl-L-Alanine	C5H11NO2	M-H	116.0717	0.8
	HMDB0015550	Amyl Nitrite	C5H11NO2	M-H	116.0717	0.8
	HMDB0001382	Vaporole	C5H11NO2	M-H	116.0717	0.8
	HMDB0002141	N-Methyl-a-aminoisobutyric acid	C5H11NO2	M-H	116.0717	0.8
	HMDB0003355	5-Aminopentanoic acid	C5H11NO2	M-H	116.0717	0.8
	HMDB0013716	Norvaline	C5H11NO2	M-H	116.0717	0.8
	HMDB0031641	Pyrrolidine	C4H9N	M+FA-H	116.0717	0.9
	HMDB0062095	Cyclobutylamine	C4H9N	M+FA-H	116.0717	0.9
	HMDB0171605	2-Methylallylamine	C4H9N	M+FA-H	116.0717	0.9

117.0196	HMDB0031160	1-Pentanesulfenothioic acid	C5H12S2	M-H2O-H	117.0197	-0.4
	HMDB0033054	Ethyl isopropyl disulfide	C5H12S2	M-H2O-H	117.0197	-0.4
	HMDB0033053	Ethyl propyl disulfide	C5H12S2	M-H2O-H	117.0197	-0.4
	HMDB0000254	Succinic acid	C4H6O4	M-H	117.0193	2.3
	HMDB0130020	3-methoxy-3-oxopropanoic acid	C4H6O4	M-H	117.0193	2.3
	HMDB0157670	2-hydroxy-4-oxobutanoic acid	C4H6O4	M-H	117.0193	2.3
	HMDB0000202	Methylmalonic acid	C4H6O4	M-H	117.0193	2.3
	HMDB0000349	Erythrono-1,4-lactone	C4H6O4	M-H	117.0193	2.3
	HMDB0187640	SCHEMBL7512234	C4H6O4	M-H	117.0193	2.3
	HMDB0000940	Threonolactone	C4H6O4	M-H	117.0193	2.3
	HMDB0039324	xi-3-Hydroxy-2-oxobutanoic acid	C4H6O4	M-H	117.0193	2.3
	HMDB0031204	4-Hydroxy-2-oxobutanoic acid	C4H6O4	M-H	117.0193	2.3
	HMDB0001167	Pyruvaldehyde	C3H4O2	M+FA-H	117.0193	2.3
	HMDB0061359	Pyruvaldehyde	C3H4O2	M+FA-H	117.0193	2.3
	HMDB0006112	Malondialdehyde	C3H4O2	M+FA-H	117.0193	2.3
	HMDB0031647	Acrylic acid	C3H4O2	M+FA-H	117.0193	2.3
118.0297	HMDB0062270	1,2-Diacylglycerol-LD-PI-pool	C7H5NO	M-H	118.0298	-1.2
118.0511	HMDB0000167	L-Threonine	C4H9NO3	M-H	118.0510	1.1
	HMDB0060587	Aminoethoxyacetic acid	C4H9NO3	M-H	118.0510	1.1
	HMDB0155268	N,N-dimethylhydroxyglycine	C4H9NO3	M-H	118.0510	1.1
	HMDB0162440	3-amino-4-hydroxybutanoic acid	C4H9NO3	M-H	118.0510	1.1
	HMDB0061148	Hydroxyethyl glycine	C4H9NO3	M-H	118.0510	1.1
	HMDB0061877	4-Amino-3-hydroxybutyrate	C4H9NO3	M-H	118.0510	1.1
	HMDB0004041	L-Allothreonine	C4H9NO3	M-H	118.0510	1.1
	HMDB0159151	alpha-Amino-beta-hydroxybutyric acid	C4H9NO3	M-H	118.0510	1.1
	HMDB0240310	2-methylserine zwitterion	C4H9NO3	M-H	118.0510	1.1
	HMDB0000719	L-Homoserine	C4H9NO3	M-H	118.0510	1.1
	HMDB0159152	L-Homoserine	C4H9NO3	M-H	118.0510	1.1
	HMDB0001888	N,N-Dimethylformamide	C3H7NO	M+FA-H	118.0510	1.1
	HMDB0142435	2-(methylamino)acetaldehyde	C3H7NO	M+FA-H	118.0510	1.1
	HMDB0062210	3-ammoniopropanal	C3H8NO	M+FA-H	118.0510	1.1
	HMDB0062149	Propionamide	C3H7NO	M+FA-H	118.0510	1.1
	HMDB0001106	3-Aminopropionaldehyde	C3H7NO	M+FA-H	118.0510	1.1
	HMDB0002134	Aminoacetone	C3H7NO	M+FA-H	118.0510	1.1
119.0504	HMDB0006236	Phenylacetaldehyde	C8H8O	M-H	119.0502	1.4
	HMDB0062765	styrene oxide	C8H8O	M-H	119.0502	1.4
	HMDB0013815	2,3-Dihydrobenzofuran	C8H8O	M-H	119.0502	1.4
	HMDB0029637	3-Methylbenzaldehyde	C8H8O	M-H	119.0502	1.4
	HMDB0029638	4-Methylbenzaldehyde	C8H8O	M-H	119.0502	1.4
	HMDB0172088	2-Vinylphenol	C8H8O	M-H	119.0502	1.4
	HMDB0029636	2-Methylbenzaldehyde	C8H8O	M-H	119.0502	1.4
	HMDB0038997	Lentialexin	C8H8O	M-H	119.0502	1.4
	HMDB0004072	4-Hydroxystyrene	C8H8O	M-H	119.0502	1.4
	HMDB0033910	Acetophenone	C8H8O	M-H	119.0502	1.4
	HMDB0124943	3-ethenylphenol	C8H8O	M-H	119.0502	1.4
121.0296	HMDB0011718	4-Hydroxybenzaldehyde	C7H6O2	M-H	121.0295	0.8
	HMDB0186744	3-hydroxybenzaldehyde	C7H6O2	M-H	121.0295	0.8
	HMDB0034170	2-Hydroxybenzaldehyde	C7H6O2	M-H	121.0295	0.8
	HMDB0032918	3-(2-Furanyl)-2-propenal	C7H6O2	M-H	121.0295	0.8
	HMDB0001870	Benzoic acid	C7H6O2	M-H	121.0295	0.8
121.0660	HMDB0033944	2-Phenylethanol	C8H10O	M-H	121.0659	0.9
	HMDB0062024	2,7-Dimethyloxepine	C8H10O	M-H	121.0659	0.9
	HMDB0041609	4-Methylbenzyl alcohol	C8H10O	M-H	121.0659	0.9
	HMDB0059873	3-Ethylphenol	C8H10O	M-H	121.0659	0.9
	HMDB0032151	3,4-Dimethylphenol	C8H10O	M-H	121.0659	0.9
	HMDB0029306	4-Ethylphenol	C8H10O	M-H	121.0659	0.9
	HMDB0032148	2,3-Dimethylphenol	C8H10O	M-H	121.0659	0.9
	HMDB0032619	1-Phenylethanol	C8H10O	M-H	121.0659	0.9
	HMDB0032076	1-Methoxy-4-methylbenzene	C8H10O	M-H	121.0659	0.9
	HMDB0032074	1-Methoxy-2-methylbenzene	C8H10O	M-H	121.0659	0.9
	HMDB0032150	2,6-Dimethylphenol	C8H10O	M-H	121.0659	0.9
	HMDB0030540	2,5-Dimethylphenol	C8H10O	M-H	121.0659	0.9
122.9856	HMDB0172018	(1Z)-3-chloroprop-1-ene-1,2,3-triol	C3H5ClO3	M-H	122.9854	1.3
	HMDB0013860	Chloroacetaldehyde	C2H3ClO	M+FA-H	122.9854	1.3
123.0089	HMDB0187590	7-oxabicyclo[4.1]hept-3-ene-2,5-dione	C6H4O3	M-H	123.0088	1.1

123.0452	HMDB0059712	3-Hydroxybenzyl alcohol	C7H8O2	M-H	123.0452	0.4
	HMDB0059709	2-Hydroxybenzyl alcohol	C7H8O2	M-H	123.0452	0.4
	HMDB0040280	1-(2-Furanyl)-1-propanone	C7H8O2	M-H	123.0452	0.4
	HMDB0032917	1-(2-Furanyl)-2-propanone	C7H8O2	M-H	123.0452	0.4
	HMDB0034877	2-Acetyl-3-methylfuran	C7H8O2	M-H	123.0452	0.4
	HMDB0029696	Mequinol	C7H8O2	M-H	123.0452	0.4
	HMDB0035226	2-Acetyl-5-methylfuran	C7H8O2	M-H	123.0452	0.4
	HMDB0038963	4,6-Heptadiyne-1,3-diol	C7H8O2	M-H	123.0452	0.4
	HMDB0011724	4-Hydroxybenzyl alcohol	C7H8O2	M-H	123.0452	0.4
	HMDB0000873	4-Methylcatechol	C7H8O2	M-H	123.0452	0.4
	HMDB0135619	3-methoxyphenol	C7H8O2	M-H	123.0452	0.4
	HMDB0001398	Guaiacol	C7H8O2	M-H	123.0452	0.4
123.0816	HMDB0001505	Benzene	C6H6	M+FA-H	123.0452	0.4
	HMDB0031686	(E,E)-2,4-Octadienal	C8H12O	M-H	123.0815	0.5
	HMDB0039844	(E,E)-2,6-Octadienal	C8H12O	M-H	123.0815	0.5
	HMDB0031582	6-Methyl-3,5-heptadien-2-one	C8H12O	M-H	123.0815	0.5
	HMDB0040272	2-Butylfuran	C8H12O	M-H	123.0815	0.5
	HMDB0033238	2-Isopropyl-5-methylfuran	C8H12O	M-H	123.0815	0.5
	HMDB0031414	2,3-Dimethyl-2-cyclohexen-1-one	C8H12O	M-H	123.0815	0.5
	HMDB0040246	3,5,5-Trimethyl-2-cyclopenten-1-one	C8H12O	M-H	123.0815	0.5
	HMDB0032446	trans, trans-3,5-Octadien-2-one	C8H12O	M-H	123.0815	0.5
	HMDB0032447	1,5-Octadien-3-one	C8H12O	M-H	123.0815	0.5
	HMDB0061898	Methyl-1-cyclopenten-1-yl)-ethanone	C8H12O	M-H	123.0815	0.5
	HMDB0062073	5-Octen-2-yn-4-ol	C8H12O	M-H	123.0815	0.5
124.0076	HMDB0000251	Taurine	C2H7NO3S	M-H	124.0074	1.7
124.9644	HMDB0014670	Foscarnet	CH3O5P	M-H	124.9645	-1.1
125.0245	HMDB0187591	7-Oxabicyclo[4.1]heptane-2,5-dione	C6H6O3	M-H	125.0244	0.7
	HMDB0187592	5-hydroxycyclohex-2-ene-1,4-dione	C6H6O3	M-H	125.0244	0.7
	HMDB0031256	4-Hydroxy-2H-pyran-3-carboxaldehyde	C6H6O3	M-H	125.0244	0.7
	HMDB0032651	(Z)-Tamarindial	C6H6O3	M-H	125.0244	0.7
	HMDB0029750	Methyl 2-furoate	C6H6O3	M-H	125.0244	0.7
	HMDB0030776	Maltol	C6H6O3	M-H	125.0244	0.7
	HMDB0013674	1,2,3-Trihydroxybenzene	C6H6O3	M-H	125.0244	0.7
	HMDB0013675	1,3,5-Trihydroxybenzene	C6H6O3	M-H	125.0244	0.7
	HMDB0059735	5-Methylfuran-2-carboxylic acid	C6H6O3	M-H	125.0244	0.7
	HMDB0124831	benzene-1,2,4-triol	C6H6O3	M-H	125.0244	0.7
	HMDB0034355	5-Hydroxymethyl-2-furancarboxaldehyde	C6H6O3	M-H	125.0244	0.7
	HMDB0000262	Thymine	C5H6N2O2	M-H	125.0357	1.2
125.0358	HMDB0029736	1H-Imidazole-1-acetic acid	C5H6N2O2	M-H	125.0357	1.2
	HMDB0002024	Imidazoleacetic acid	C5H6N2O2	M-H	125.0357	1.2
	HMDB0060261	Imidazoleacetic acid	C5H6N2O2	M-H	125.0357	1.2
	HMDB0034176	Pyrazine	C4H4N2	M+FA-H	125.0356	1.2
	HMDB0003361	Pyrimidine	C4H4N2	M+FA-H	125.0356	1.2
	HMDB0033629	xi-4-Hydroxy-4-methyl-2-cyclohexen-1-one	C7H10O2	M-H	125.0608	0.8
125.0609	HMDB0041474	xi-5-Isopropyl-2(5H)-furanone	C7H10O2	M-H	125.0608	0.8
	HMDB0031222	3-Ethyl-1,2-cyclopentanedione	C7H10O2	M-H	125.0608	0.8
	HMDB0034835	3-(3-Ethylloxiranyl)-2-propenal	C7H10O2	M-H	125.0608	0.8
	HMDB0031223	Enol-3-Ethyl-1,2-cyclopentanedione	C7H10O2	M-H	125.0608	0.8
	HMDB0040445	2-(Ethoxymethyl)furan	C7H10O2	M-H	125.0608	0.8
	HMDB0037026	3,4-Dimethyl-1,2-cyclopentanedione	C7H10O2	M-H	125.0608	0.8
	HMDB0037027	3,5-Dimethyl-1,2-cyclopentanedione	C7H10O2	M-H	125.0608	0.8
	HMDB0034080	3-Methyl-1,2-cyclohexanedione	C7H10O2	M-H	125.0608	0.8
	HMDB0029582	Methyl sorbate	C7H10O2	M-H	125.0608	0.8
	HMDB0032067	Allyl crotonate	C7H10O2	M-H	125.0608	0.8
	HMDB0032333	4-Hydroxy-4-methyl-5-hexenoic acid gamma lactone	C7H10O2	M-H	125.0608	0.8
	HMDB0181106	7-Octen-3-one	C8H14O	M-H	125.0972	0.1
	HMDB0062529	3,5-Dimethyl-1-hexyn-3-ol	C8H14O	M-H	125.0972	0.1
	HMDB0040151	(2E,4E)-2,4-Octadien-1-ol	C8H14O	M-H	125.0972	0.1
	HMDB0031197	2,4,4-Trimethylcyclopentanone	C8H14O	M-H	125.0972	0.1
	HMDB0039769	6-Octenal	C8H14O	M-H	125.0972	0.1
	HMDB0031301	2-Octen-4-one	C8H14O	M-H	125.0972	0.1
	HMDB0031591	5-Methyl-5-hepten-2-one	C8H14O	M-H	125.0972	0.1
	HMDB0030966	(3xi,5Z)-1,5-Octadien-3-ol	C8H14O	M-H	125.0972	0.1
	HMDB0030961	2-Octenal	C8H14O	M-H	125.0972	0.1
	HMDB0035915	Sulcatone	C8H14O	M-H	125.0972	0.1

125.0972	HMDB0031309	1-Octen-3-one	C8H14O	M-H	125.0972	0.1
	HMDB0035242	(S,E)-Filbertone	C8H14O	M-H	125.0972	0.1
	HMDB0040149	(3E,5Z)-3,5-Octadien-1-ol	C8H14O	M-H	125.0972	0.1
	HMDB0033547	3-Octen-2-one	C8H14O	M-H	125.0972	0.1
	HMDB0037152	2-Ethylidenehexanal	C8H14O	M-H	125.0972	0.1
	HMDB0031590	3-Methyl-3-hepten-2-one	C8H14O	M-H	125.0972	0.1
	HMDB0163322	7-octen-2-one	C8H14O	M-H	125.0972	0.1
	HMDB0061945	2-Ethyl-2-hexenal	C8H14O	M-H	125.0972	0.1
	HMDB0013809	(E)-2-octenal	C8H14O	M-H	125.0972	0.1
	HMDB0032451	4-Octen-3-one	C8H14O	M-H	125.0972	0.1
	HMDB0032403	6-Methyl-3-hepten-2-one, trans-	C8H14O	M-H	125.0972	0.1
	HMDB0039770	(Z)-5-Octenal	C8H14O	M-H	125.0972	0.1
	HMDB0040146	2,5-Octadien-1-ol	C8H14O	M-H	125.0972	0.1
	HMDB0035390	5-Octen-2-one	C8H14O	M-H	125.0972	0.1
126.0197	HMDB0034368	Hydroxyminaline	C5H5NO3	M-H	126.0197	0.3
127.0039	HMDB0041390	(E,E)-Di-1-propenyl disulfide	C6H10S2	M-H2O-H	127.0040	-0.8
	HMDB0033966	Di-2-propenyl disulfide, 9CI	C6H10S2	M-H2O-H	127.0040	-0.8
	HMDB0041393	(E)-1-Propenyl 2-propenyl disulfide	C6H10S2	M-H2O-H	127.0040	-0.8
	HMDB0059784	5-Hydroxy-2-furoic acid	C5H4O4	M-H	127.0037	1.7
127.0151	HMDB0041833	Barbituric acid	C4H4N2O3	M-H	127.0149	1.4
127.0402	HMDB0173548	2,5-furandimethanol	C6H8O3	M-H	127.0401	1.0
	HMDB0163704	SCHEMBL144397	C6H8O3	M-H	127.0401	1.0
	HMDB0179348	3-[(1E)-prop-1-en-1-yl]oxirane-2-carboxylic acid	C6H8O3	M-H	127.0401	1.0
	HMDB0179347	(2Z)-6-hydroxyhexa-2,4-dienoic acid	C6H8O3	M-H	127.0401	1.0
	HMDB0062047	3,4-dimethyloxolane-2,5-dione	C6H8O3	M-H	127.0401	1.0
	HMDB0033285	L-erythro-5-(1-Hydroxyethyl)-2(5H)-furanone	C6H8O3	M-H	127.0401	1.0
	HMDB0038072	xi-5-Acetyltetrahydro-2(3H)-furanone	C6H8O3	M-H	127.0401	1.0
	HMDB0031303	Osmundalactone	C6H8O3	M-H	127.0401	1.0
	HMDB0040594	Furaneol	C6H8O3	M-H	127.0401	1.0
	HMDB0031306	3-Hydroxy-4,5-dimethyl-2(5H)-furanone	C6H8O3	M-H	127.0401	1.0
	HMDB0033517	5,6-Dihydro-4-methoxy-2H-pyran-2-one	C6H8O3	M-H	127.0401	1.0
	HMDB0040732	2,7-Oxepanedione	C6H8O3	M-H	127.0401	1.0
	HMDB0031847	2-Ethyl-3,4-dihydroxyfuran	C6H8O3	M-H	127.0401	1.0
	HMDB0179349	(2Z)-3-(3-methyloxiran-2-yl)prop-2-enoic acid	C6H8O3	M-H	127.0401	1.0
	HMDB0013749	2-Methylfuran	C5H6O	M+FA-H	127.0401	1.1
	HMDB0031597	2,4-Pentadienal	C5H6O	M+FA-H	127.0401	1.1
	HMDB0061999	Cyclopropanecarboxaldehyde, methylene-	C5H6O	M+FA-H	127.0401	1.1
	HMDB0062137	Cyclopropanecarboxaldehyde, methylene-	C5H6O	M+FA-H	127.0401	1.1
	HMDB0062036	3-Methylfuran	C5H6O	M+FA-H	127.0401	1.1
127.0514	HMDB0000079	(5s)-dihydrothymine	C5H8N2O2	M-H	127.0513	0.8
	HMDB0062558	2,6-Piperidinedione, 3-amino-, (3S)-	C5H8N2O2	M-H	127.0513	0.8
	HMDB0029874	Squamolone	C5H8N2O2	M-H	127.0513	0.8
	HMDB0031547	L-Cyclo(alanylglycyl)	C5H8N2O2	M-H	127.0513	0.8
	HMDB0062037	3-methyl-1H-pyrazole	C4H6N2	M+FA-H	127.0513	0.8
	HMDB0015344	Fomepizole	C4H6N2	M+FA-H	127.0513	0.8
127.0765	HMDB0180322	3-(3-ethyloxiran-2-yl)propanal	C7H12O2	M-H	127.0765	0.4
	HMDB0059876	Pantolactone	C7H12O2	M-H	127.0765	0.4
	HMDB0180323	(2E)-3-(3-ethyloxiran-2-yl)prop-2-en-1-ol	C7H12O2	M-H	127.0765	0.4
	HMDB0173762	5-methylcyclohex-4-ene-1,3-diol	C7H12O2	M-H	127.0765	0.4
	HMDB0173763	1-methyl-7-oxabicyclo[4.1]heptan-3-ol	C7H12O2	M-H	127.0765	0.4
	HMDB0173761	3-methylcyclohex-3-ene-1,2-diol	C7H12O2	M-H	127.0765	0.4
	HMDB0173760	SCHEMBL14734478	C7H12O2	M-H	127.0765	0.4
	HMDB0166736	4-Hydroxyheptenal	C7H12O2	M-H	127.0765	0.4
	HMDB0166737	6-Hydroxy-2-heptenal	C7H12O2	M-H	127.0765	0.4
	HMDB0166739	(2E)-7-hydroxyhept-2-enal	C7H12O2	M-H	127.0765	0.4
	HMDB0165097	SCHEMBL132855	C7H12O2	M-H	127.0765	0.4
	HMDB0165095	3-Hydroxy-3-methylcyclohexan-1-one	C7H12O2	M-H	127.0765	0.4
	HMDB0165096	SCHEMBL443446	C7H12O2	M-H	127.0765	0.4
	HMDB0165094	3-(Hydroxymethyl)cyclohexanone	C7H12O2	M-H	127.0765	0.4
	HMDB0164724	4-Hydroxy-4-methylcyclohexanone	C7H12O2	M-H	127.0765	0.4
	HMDB0166738	3-butyloxirane-2-carbaldehyde	C7H12O2	M-H	127.0765	0.4
	HMDB0032391	3-Methyl-3-butenyl acetate	C7H12O2	M-H	127.0765	0.4
	HMDB0032460	4-Pentenyl acetate	C7H12O2	M-H	127.0765	0.4
	HMDB0031603	Ethyl 4-pentenoate	C7H12O2	M-H	127.0765	0.4
	HMDB0031504	Methyl (Z)-3-hexenoate	C7H12O2	M-H	127.0765	0.4

	HMDB0040591	Allyl butyrate	C7H12O2	M-H	127.0765	0.4
	HMDB0031351	Cyclohexyl formate	C7H12O2	M-H	127.0765	0.4
	HMDB0030330	1-Methoxy-3-methylene-2-pentanone	C7H12O2	M-H	127.0765	0.4
	HMDB0039819	2,4-Dimethyl-2-pentenoic acid	C7H12O2	M-H	127.0765	0.4
	HMDB0031476	2,3-Heptanedione	C7H12O2	M-H	127.0765	0.4
	HMDB0033793	4-Heptenoic acid	C7H12O2	M-H	127.0765	0.4
	HMDB0031477	3,4-Heptanedione	C7H12O2	M-H	127.0765	0.4
	HMDB0038962	Ethyl tiglate	C7H12O2	M-H	127.0765	0.4
	HMDB0031500	Methyl 2E-hexenoate	C7H12O2	M-H	127.0765	0.4
	HMDB0031484	2-Heptenoic acid	C7H12O2	M-H	127.0765	0.4
	HMDB0029314	Isopentenyl acetate	C7H12O2	M-H	127.0765	0.4
	HMDB0029165	1,3-Diacetylpropane	C7H12O2	M-H	127.0765	0.4
	HMDB0031681	Dihydro-5-propyl-2(3H)-furanone	C7H12O2	M-H	127.0765	0.4
	HMDB0031593	5-Methyl-2,3-hexanedione	C7H12O2	M-H	127.0765	0.4
	HMDB0031174	4-Methyl-5-hexanolide	C7H12O2	M-H	127.0765	0.4
	HMDB0038271	2-Hexenyl formate	C7H12O2	M-H	127.0765	0.4
	HMDB0031342	Cyclohexanecarboxylic acid	C7H12O2	M-H	127.0765	0.4
	HMDB0040214	cis-3-Hexenyl formate	C7H12O2	M-H	127.0765	0.4
	HMDB0031544	3-Methylcyclopentene	C6H10	M+FA-H	127.0765	0.4
127.1129	HMDB0062076	6-Methylheptan-2-one	C8H16O	M-H	127.1128	0.5
	HMDB0062072	5-methylheptan-2-one	C8H16O	M-H	127.1128	0.5
	HMDB0013821	2-Methyl-4-heptanone	C8H16O	M-H	127.1128	0.5
	HMDB0172314	1-OCTEN-2-OL	C8H16O	M-H	127.1128	0.5
	HMDB0170962	7-Octen-1-ol	C8H16O	M-H	127.1128	0.5
	HMDB0061986	2-ethylhexanal	C8H16O	M-H	127.1128	0.5
	HMDB0061912	3,4-Dimethylcyclohexanol	C8H16O	M-H	127.1128	0.5
	HMDB0061913	3,5-Dimethylcyclohexanol	C8H16O	M-H	127.1128	0.5
	HMDB0031298	(Z)-5-Octen-1-ol	C8H16O	M-H	127.1128	0.5
	HMDB0031295	Ethyl pentyl ketone	C8H16O	M-H	127.1128	0.5
	HMDB0032450	trans-3-Octen-2-ol	C8H16O	M-H	127.1128	0.5
	HMDB0030030	(R)-Sulcatol	C8H16O	M-H	127.1128	0.5
	HMDB0031299	(R)-1-Octen-3-ol	C8H16O	M-H	127.1128	0.5
	HMDB0037181	xi-7-Octen-2-ol	C8H16O	M-H	127.1128	0.5
	HMDB0029574	2,5-Diethyltetrahydrofuran	C8H16O	M-H	127.1128	0.5
	HMDB0001140	Octanal	C8H16O	M-H	127.1128	0.5
	HMDB0035768	(E)-3-Octen-1-ol	C8H16O	M-H	127.1128	0.5
	HMDB0035231	(Z)-3-Octen-1-ol	C8H16O	M-H	127.1128	0.5
	HMDB0032402	2-Methyl-3-heptanone	C8H16O	M-H	127.1128	0.5
	HMDB0031294	2-Octanone	C8H16O	M-H	127.1128	0.5
128.0354	HMDB0031300	(E)-2-Octen-4-ol	C8H16O	M-H	127.1128	0.5
	HMDB0031296	(E)-2-Octen-1-ol	C8H16O	M-H	127.1128	0.5
	HMDB0062585	(3R,5S)-1-pyrroline-3-hydroxy-5-carboxylic acid	C5H7NO3	M-H	128.0353	0.6
	HMDB0061093	dimethadione	C5H7NO3	M-H	128.0353	0.6
	HMDB0000267	Pyroglutamic acid	C5H7NO3	M-H	128.0353	0.6
	HMDB0002234	1-Pyrroline-4-hydroxy-2-carboxylate	C5H7NO3	M-H	128.0353	0.6
	HMDB0001843	N-Acryloylglycine	C5H7NO3	M-H	128.0353	0.6
	HMDB0001369	Pyrroline hydroxycarboxylic acid	C5H7NO3	M-H	128.0353	0.6
128.0718	HMDB0000805	Pyrrolidonecarboxylic acid	C5H7NO3	M-H	128.0353	0.6
	HMDB0060262	Pyrrolidonecarboxylic acid	C5H7NO3	M-H	128.0353	0.6
	HMDB0094697	piperidine-1-carboxylic acid	C6H11NO2	M-H	128.0717	0.8
	HMDB0029444	56633-75-1	C6H11NO2	M-H	128.0717	0.8
	HMDB0059649	3-Acetamidobutanal	C6H11NO2	M-H	128.0717	0.8
	HMDB0062225	(2E)-Decenoyl-ACP	C6H11NO2	M-H	128.0717	0.8
	HMDB0029435	L-trans-4-Methyl-2-pyrrolidinecarboxylic acid	C6H11NO2	M-H	128.0717	0.8
	HMDB0000070	Pipecolic acid	C6H11NO2	M-H	128.0717	0.8
	HMDB0062767	Pipecolic acid	C6H11NO2	M-H	128.0717	0.8
	HMDB0005960	D-Pipecolic acid	C6H11NO2	M-H	128.0717	0.8
	HMDB0004226	N4-Acetylaminobutanal	C6H11NO2	M-H	128.0717	0.8
	HMDB0094696	N-Methyl-L-proline	C6H11NO2	M-H	128.0717	0.8
	HMDB0015212	Vigabatrin	C6H11NO2	M-H	128.0717	0.8
	HMDB0000716	L-Pipecolic acid	C6H11NO2	M-H	128.0717	0.8
	HMDB0033529	(+)-2,3-Dihydro-3-methyl-1H-pyrrole	C5H9N	M+FA-H	128.0717	0.8
	HMDB0040173	Pentanenitrile	C5H9N	M+FA-H	128.0717	0.8
	HMDB0038890	Methyl 3-methyl-1-butenyl disulfide	C6H12S2	M-H2O-H	129.0197	-0.4
	HMDB0041392	1-Propenyl propyl disulfide	C6H12S2	M-H2O-H	129.0197	-0.4

129.0196	HMDB0033912	2-Propenyl propyl disulfide	C6H12S2	M-H2O-H	129.0197	-0.4
	HMDB0000634	Citraconic acid	C5H6O4	M-H	129.0193	2.1
	HMDB0060365	2,5-Dioxopentanoate	C5H6O4	M-H	129.0193	2.1
	HMDB0059743	2-Hydroxyglutaric acid lactone	C5H6O4	M-H	129.0193	2.1
	HMDB0000620	Glutaconic acid	C5H6O4	M-H	129.0193	2.1
	HMDB0061185	Glutaconic acid	C5H6O4	M-H	129.0193	2.1
	HMDB0000749	Mesaconic acid	C5H6O4	M-H	129.0193	2.1
	HMDB0002092	Itaconic acid	C5H6O4	M-H	129.0193	2.1
	HMDB0033809	Methyl hydrogen fumarate	C5H6O4	M-H	129.0193	2.1
	HMDB0013233	Gamma-delta-Dioxovaleric acid	C5H6O4	M-H	129.0193	2.1
	HMDB0062133	methyl prop-2-ynoate	C4H4O2	M+FA-H	129.0193	2.1
	HMDB0032330	4-Hydroxy-2-butenic acid gamma-lactone	C4H4O2	M+FA-H	129.0193	2.1
	HMDB0094691	but-3-en-4-olide	C4H4O2	M+FA-H	129.0193	2.1
	HMDB0041602	Methyl levulinate	C6H10O3	M-H	129.0557	0.6
129.0558	HMDB0163716	3-Methyl-4-oxopentanoic acid	C6H10O3	M-H	129.0557	0.6
	HMDB0169669	3-ethyl-3-methyl-oxiranecarboxylic acid	C6H10O3	M-H	129.0557	0.6
	HMDB0162571	SCHEMBL13481223	C6H10O3	M-H	129.0557	0.6
	HMDB0165590	(2Z)-2-(hydroxymethyl)pent-2-enoic acid	C6H10O3	M-H	129.0557	0.6
	HMDB0165593	(2Z)-5-hydroxy-2-methylpent-2-enoic acid	C6H10O3	M-H	129.0557	0.6
	HMDB0169668	AKO238761	C6H10O3	M-H	129.0557	0.6
	HMDB0169667	SCHEMBL159549	C6H10O3	M-H	129.0557	0.6
	HMDB0169670	SCHEMBL1645858	C6H10O3	M-H	129.0557	0.6
	HMDB0169696	(2Z)-4-hydroxy-3-methylpent-2-enoic acid	C6H10O3	M-H	129.0557	0.6
	HMDB0169697	(2E)-3-(hydroxymethyl)pent-2-enoic acid	C6H10O3	M-H	129.0557	0.6
	HMDB0169698	SCHEMBL6488	C6H10O3	M-H	129.0557	0.6
	HMDB0165592	SCHEMBL2684392	C6H10O3	M-H	129.0557	0.6
	HMDB0165591	(2Z)-4-hydroxy-2-methylpent-2-enoic acid	C6H10O3	M-H	129.0557	0.6
	HMDB0163359	(4Z)-6-hydroxyhex-4-enoic acid	C6H10O3	M-H	129.0557	0.6
	HMDB0163360	SCHEMBL667341	C6H10O3	M-H	129.0557	0.6
	HMDB0163362	AKO06375916	C6H10O3	M-H	129.0557	0.6
	HMDB0163361	3-(3-methyloxiran-2-yl)propanoic acid	C6H10O3	M-H	129.0557	0.6
	HMDB0163707	1-[3-(hydroxymethyl)-2-methyloxiran-2-yl]ethan-1-one	C6H10O3	M-H	129.0557	0.6
	HMDB0163705	3-(hydroxymethyl)-4-oxopentanal	C6H10O3	M-H	129.0557	0.6
	HMDB0163706	(3Z)-5-hydroxy-3-(hydroxymethyl)pent-3-en-2-one	C6H10O3	M-H	129.0557	0.6
	HMDB0163708	(3Z)-1,5-dihydroxy-3-methylpent-3-en-2-one	C6H10O3	M-H	129.0557	0.6
	HMDB0000408	2-Methyl-3-ketovaleric acid	C6H10O3	M-H	129.0557	0.6
	HMDB0012882	Adipate semialdehyde	C6H10O3	M-H	129.0557	0.6
	HMDB0000695	Ketoleucine	C6H10O3	M-H	129.0557	0.6
	HMDB0031214	5-Ethoxy-4,5-dihydro-2(3H)furanone	C6H10O3	M-H	129.0557	0.6
	HMDB0033698	Acetoin acetate	C6H10O3	M-H	129.0557	0.6
	HMDB0000491	(S)-3-methyl-2-oxopentanoate	C6H10O3	M-H	129.0557	0.6
	HMDB0031216	Ethyl acetoacetate	C6H10O3	M-H	129.0557	0.6
	HMDB0031218	Ethyl acetoacetate	C6H10O3	M-H	129.0557	0.6
	HMDB0033286	Sherry lactone	C6H10O3	M-H	129.0557	0.6
	HMDB0033302	(4S,6S)-3,4,5,6-Tetrahydro-4-hydroxy-6-methyl-2H-pyran-2-one	C6H10O3	M-H	129.0557	0.6
	HMDB0010717	3-Oxohexanoic acid	C6H10O3	M-H	129.0557	0.6
	HMDB0006024	Mevalonolactone	C6H10O3	M-H	129.0557	0.6
	HMDB0001864	2-Ketohexanoic acid	C6H10O3	M-H	129.0557	0.6
	HMDB0061881	4-Acetylbutyrate	C6H10O3	M-H	129.0557	0.6
	HMDB0031407	Cyclopentanone	C5H8O	M+FA-H	129.0557	0.7
	HMDB0037788	xi-2,3-Dihydro-3-methylfuran	C5H8O	M+FA-H	129.0557	0.7
	HMDB0012157	3-Methyl-2-butenal	C5H8O	M+FA-H	129.0557	0.7
	HMDB0001184	Methyl propenyl ketone	C5H8O	M+FA-H	129.0557	0.7
	HMDB0040584	2,3-Dihydro-4-methylfuran	C5H8O	M+FA-H	129.0557	0.7
	HMDB0032458	4-Pentenol	C5H8O	M+FA-H	129.0557	0.7
	HMDB0031512	Tiglic aldehyde	C5H8O	M+FA-H	129.0557	0.7
	HMDB0175216	2-Methylbut-2-en-1-al	C5H8O	M+FA-H	129.0557	0.7
	HMDB0031530	3-Methyl-3-buten-2-one	C5H8O	M+FA-H	129.0557	0.7
	HMDB0031607	1-Penten-3-one	C5H8O	M+FA-H	129.0557	0.7
	HMDB0031601	2-Pentenol	C5H8O	M+FA-H	129.0557	0.7
	HMDB0031606	4-Penten-2-one	C5H8O	M+FA-H	129.0557	0.7
	HMDB0166743	(2E)-hept-2-ene-1,7-diol	C7H14O2	M-H	129.0921	0.7
	HMDB0166741	(2E)-hept-2-ene-1,6-diol	C7H14O2	M-H	129.0921	0.7
	HMDB0166742	3-Butyloxirane-2-methanol	C7H14O2	M-H	129.0921	0.7

129.0922	HMDB0166740	SCHEMBL32814	C7H14O2	M-H	129.0921	0.7
	HMDB0032204	cis- and trans-2-Isopropyl-4-methyl-1,3-dioxolane	C7H14O2	M-H	129.0921	0.7
	HMDB0034239	2-Methylpropyl propanoate	C7H14O2	M-H	129.0921	0.7
	HMDB0038227	Isopropyl 2-methylpropanoate	C7H14O2	M-H	129.0921	0.7
	HMDB0030028	Ethyl isovalerate	C7H14O2	M-H	129.0921	0.7
	HMDB0039618	Propyl butyrate	C7H14O2	M-H	129.0921	0.7
	HMDB0035238	Methyl hexanoate	C7H14O2	M-H	129.0921	0.7
	HMDB0036237	Methyl 2-methylpentanoate	C7H14O2	M-H	129.0921	0.7
	HMDB0030052	Butyl propionate	C7H14O2	M-H	129.0921	0.7
	HMDB0031600	2-Pentanol acetate	C7H14O2	M-H	129.0921	0.7
	HMDB0036238	Methyl 4-methylpentanoate	C7H14O2	M-H	129.0921	0.7
	HMDB0031594	2-Methylhexanoic acid	C7H14O2	M-H	129.0921	0.7
	HMDB0031528	Isopentyl acetate	C7H14O2	M-H	129.0921	0.7
	HMDB0033745	Ethyl 2-methylbutyrate	C7H14O2	M-H	129.0921	0.7
	HMDB0034166	2-Methylbutyl acetate	C7H14O2	M-H	129.0921	0.7
	HMDB0031595	5-Methylhexanoic acid	C7H14O2	M-H	129.0921	0.7
	HMDB0032874	Hexyl formate	C7H14O2	M-H	129.0921	0.7
	HMDB0000666	Heptanoic acid	C7H14O2	M-H	129.0921	0.7
	HMDB0040297	Ethyl pentanoate	C7H14O2	M-H	129.0921	0.7
	HMDB0039619	Isopropyl butyrate	C7H14O2	M-H	129.0921	0.7
	HMDB0039095	Pentyl acetate	C7H14O2	M-H	129.0921	0.7
	HMDB0036209	Propyl 2-methylpropanoate	C7H14O2	M-H	129.0921	0.7
	HMDB0029597	Cyclohexane	C6H12	M+FA-H	129.0921	0.8
	HMDB0062035	3-Methyl-2-pentene	C6H12	M+FA-H	129.0921	0.8
	HMDB0031542	Methylcyclopentane	C6H12	M+FA-H	129.0921	0.8
	HMDB0061958	(2Z)-4-methylpent-2-ene	C6H12	M+FA-H	129.0921	0.8
	HMDB0062011	2,3-DIMETHYL-2-BUTENE	C6H12	M+FA-H	129.0921	0.8
	HMDB0062010	2,3-DIMETHYL-1-BUTENE	C6H12	M+FA-H	129.0921	0.8
130.0874	HMDB0240479	Alanine betaine	C6H13NO2	M-H	130.0874	0.4
	HMDB0171681	SCHEMBL1266	C6H13NO2	M-H	130.0874	0.4
	HMDB0171682	N-(2-methylpropyl)glycolamide	C6H13NO2	M-H	130.0874	0.4
	HMDB0171680	SCHEMBL311743	C6H13NO2	M-H	130.0874	0.4
	HMDB0168722	N,N-diethyl-2-oxoethanamine oxide	C6H13NO2	M-H	130.0874	0.4
	HMDB0168721	SCHEMBL124646	C6H13NO2	M-H	130.0874	0.4
	HMDB0168720	2-[ethyl(1-hydroxyethyl)amino]acetaldehyde	C6H13NO2	M-H	130.0874	0.4
	HMDB0168719	SCHEMBL63485	C6H13NO2	M-H	130.0874	0.4
	HMDB0145163	2-hydroxy-3-(propylamino)propanal	C6H13NO2	M-H	130.0874	0.4
	HMDB0144645	N,N-Diethylglycine	C6H13NO2	M-H	130.0874	0.4
	HMDB0062052	4-(dimethylamino)butanoic acid	C6H13NO2	M-H	130.0874	0.4
	HMDB0036382	6-Deoxyfagomine	C6H13NO2	M-H	130.0874	0.4
	HMDB0033923	erythro-Isoleucine	C6H13NO2	M-H	130.0874	0.4
	HMDB0003640	Beta-Leucine	C6H13NO2	M-H	130.0874	0.4
	HMDB0001645	L-Norleucine	C6H13NO2	M-H	130.0874	0.4
	HMDB0000557	L-Alloisoleucine	C6H13NO2	M-H	130.0874	0.4
	HMDB0001901	Aminocaproic acid	C6H13NO2	M-H	130.0874	0.4
	HMDB0000172	L-Isoleucine	C6H13NO2	M-H	130.0874	0.4
	HMDB0013773	D-Leucine	C6H13NO2	M-H	130.0874	0.4
	HMDB0029168	3-Aminocaproic acid	C6H13NO2	M-H	130.0874	0.4
	HMDB0061716	N-methylvaline	C6H13NO2	M-H	130.0874	0.4
	HMDB0060650	N-(2-Hydroxyethyl)-morpholine	C6H13NO2	M-H	130.0874	0.4
	HMDB0000687	L-Leucine	C6H13NO2	M-H	130.0874	0.4
	HMDB0062203	L-Leucine	C6H13NO2	M-H	130.0874	0.4
	HMDB0034301	Piperidine	C5H11N	M+FA-H	130.0874	0.4
	HMDB0040056	xi-1-(Propylthio)-1-propanethiol	C6H14S2	M-H20-H	131.0353	0.0
	HMDB0029578	Diisopropyl disulfide	C6H14S2	M-H20-H	131.0353	0.0
	HMDB0031161	Methyl pentyl disulfide	C6H14S2	M-H20-H	131.0353	0.0
	HMDB0031709	1,6-Hexanedithiol	C6H14S2	M-H20-H	131.0353	0.0
	HMDB0031472	Dipropyl disulfide	C6H14S2	M-H20-H	131.0353	0.0
	HMDB0032180	Butyl ethyl disulfide	C6H14S2	M-H20-H	131.0353	0.0
	HMDB0032408	Methyl isopentyl disulfide	C6H14S2	M-H20-H	131.0353	0.0
	HMDB0154760	alpha-keto-beta-methyl-gamma-hydroxy-butyric acid	C5H8O4	M-H	131.0350	2.4
	HMDB0145654	SCHEMBL17123851	C5H8O4	M-H	131.0350	2.4
	HMDB0001844	(S)-methylsuccinic acid	C5H8O4	M-H	131.0350	2.4
	HMDB0002001	Dimethylmalonic acid	C5H8O4	M-H	131.0350	2.4
	HMDB0006833	2-Acetolactate	C5H8O4	M-H	131.0350	2.4

131.0353	HMDB0006855	(S)-2-Acetolactate	C5H8O4	M-H	131.0350	2.4
	HMDB0000576	Monoethyl malonic acid	C5H8O4	M-H	131.0350	2.4
	HMDB0154759	3-Hydroxy-3-methyl-2-oxobutanoic acid	C5H8O4	M-H	131.0350	2.4
	HMDB0000622	Ethylmalonic acid	C5H8O4	M-H	131.0350	2.4
	HMDB0033958	2-Deoxy-L-ribono-1,4-lactone	C5H8O4	M-H	131.0350	2.4
	HMDB0040531	2-Hydroxy-4-oxopentanoic acid	C5H8O4	M-H	131.0350	2.4
	HMDB0000661	Glutaric acid	C5H8O4	M-H	131.0350	2.4
	HMDB0029884	2-C-Methyl-1,4-erythrono-D-lactone	C5H8O4	M-H	131.0350	2.4
	HMDB0002523	Oxolan-3-one	C4H6O2	M+FA-H	131.0350	2.4
	HMDB0000549	gamma-Butyrolactone	C4H6O2	M+FA-H	131.0350	2.4
	HMDB0167138	(2Z)-4-hydroxybut-2-enal	C4H6O2	M+FA-H	131.0350	2.4
	HMDB0167139	3-Methyloxirane-2-carbaldehyde	C4H6O2	M+FA-H	131.0350	2.4
	HMDB0033977	Methyl acrylate	C4H6O2	M+FA-H	131.0350	2.4
	HMDB0034439	Isocrotonic acid	C4H6O2	M+FA-H	131.0350	2.4
	HMDB0010720	But-2-enoic acid	C4H6O2	M+FA-H	131.0350	2.4
	HMDB0031209	Ethenyl acetate	C4H6O2	M+FA-H	131.0350	2.4
	HMDB0174868	but-3-enoic acid	C4H6O2	M+FA-H	131.0350	2.4
	HMDB0003407	Diacetyl	C4H6O2	M+FA-H	131.0350	2.4
131.0716	HMDB0059770	Threo-3-Hydroxy-2-methylbutyric acid	C6H12O3	M-H	131.0714	1.8
	HMDB0041844	Butoxyacetic acid	C6H12O3	M-H	131.0714	1.8
	HMDB0061652	(S)-3-hydroxyhexanoic acid	C6H12O3	M-H	131.0714	1.8
	HMDB0171222	4-hydroxy-3-methylbutyl formate	C6H12O3	M-H	131.0714	1.8
	HMDB0165041	4-hydroxy-3-methyl-valeric acid	C6H12O3	M-H	131.0714	1.8
	HMDB0165042	3-hydroxymethyl-valeric acid	C6H12O3	M-H	131.0714	1.8
	HMDB0165043	5-hydroxy-3-methylpentanoic acid	C6H12O3	M-H	131.0714	1.8
	HMDB0163680	SCHEMBL5464	C6H12O3	M-H	131.0714	1.8
	HMDB0163681	3,6-dihydroxyhexan-2-one	C6H12O3	M-H	131.0714	1.8
	HMDB0163679	5,6-dihydroxyhexan-2-one	C6H12O3	M-H	131.0714	1.8
	HMDB0161115	4-hydroxy-4-methylpentanoic acid	C6H12O3	M-H	131.0714	1.8
	HMDB0161116	5-hydroxy-4-methylpentanoic acid	C6H12O3	M-H	131.0714	1.8
	HMDB0029166	2-Methyl-3-hydroxyvaleric acid	C6H12O3	M-H	131.0714	1.8
	HMDB0040409	Ethyl 3-hydroxybutyrate	C6H12O3	M-H	131.0714	1.8
	HMDB0000317	2-Hydroxy-3-methylpentanoic acid	C6H12O3	M-H	131.0714	1.8
	HMDB0033851	4,4-Dimethoxy-2-butanone	C6H12O3	M-H	131.0714	1.8
	HMDB0010718	(R)-3-Hydroxyhexanoic acid	C6H12O3	M-H	131.0714	1.8
	HMDB0163682	1,6-dihydroxy-2-hexanone	C6H12O3	M-H	131.0714	1.8
	HMDB0001975	2-Ethyl-2-Hydroxybutyric acid	C6H12O3	M-H	131.0714	1.8
	HMDB0001624	2-Hydroxycaproic acid	C6H12O3	M-H	131.0714	1.8
	HMDB0000746	Hydroxyisocaproic acid	C6H12O3	M-H	131.0714	1.8
	HMDB0000665	Leucinic acid	C6H12O3	M-H	131.0714	1.8
	HMDB0000624	D-Leucic acid	C6H12O3	M-H	131.0714	1.8
	HMDB0000525	5-Hydroxyhexanoic acid	C6H12O3	M-H	131.0714	1.8
	HMDB0000409	(5R)-5-Hydroxyhexanoic acid	C6H12O3	M-H	131.0714	1.8
	HMDB0165040	3-hydroxy-3-methylpentanoic acid	C6H12O3	M-H	131.0714	1.8
	HMDB0032158	(+/-)-1-Acetoxy-1-ethoxyethane	C6H12O3	M-H	131.0714	1.8
	HMDB0012843	6-Hydroxyhexanoic acid	C6H12O3	M-H	131.0714	1.8
	HMDB0032456	Paraldehyde	C6H12O3	M-H	131.0714	1.8
	HMDB0180842	Pentenol	C5H10O	M+FA-H	131.0714	1.8
	HMDB0062042	3,3-Dimethyloxetane	C5H10O	M+FA-H	131.0714	1.8
	HMDB0163717	Methylisopropyl ketone	C5H10O	M+FA-H	131.0714	1.8
	HMDB0006478	Iso-Valeraldehyde	C5H10O	M+FA-H	131.0714	1.8
	HMDB0240630	Iso-Valeraldehyde	C5H10O	M+FA-H	131.0714	1.8
	HMDB0031206	Pentanal	C5H10O	M+FA-H	131.0714	1.8
	HMDB0171227	2-Methyl-3-buten-1-ol	C5H10O	M+FA-H	131.0714	1.8
	HMDB0171226	2-methylidenebutan-1-ol	C5H10O	M+FA-H	131.0714	1.8
	HMDB0039779	xi-3-Methyl-3-buten-2-ol	C5H10O	M+FA-H	131.0714	1.8
	HMDB0031526	2-Methylbutanal	C5H10O	M+FA-H	131.0714	1.8
	HMDB0033854	Isoprenyl alcohol	C5H10O	M+FA-H	131.0714	1.8
	HMDB0031605	1-Penten-3-ol	C5H10O	M+FA-H	131.0714	1.8
	HMDB0034465	2-Methyl-2-buten-1-ol	C5H10O	M+FA-H	131.0714	1.8
	HMDB0034235	2-Pentanone	C5H10O	M+FA-H	131.0714	1.8
	HMDB0166255	79144-27-7	C5H10O	M+FA-H	131.0714	1.8
	HMDB0031525	(S)-2-Methylbutanal	C5H10O	M+FA-H	131.0714	1.8
	HMDB0062040	3-Pentanone	C5H10O	M+FA-H	131.0714	1.8
	HMDB0031604	(E)-2-Penten-1-ol	C5H10O	M+FA-H	131.0714	1.8

	HMDB0030126	3-Methyl-3-buten-1-ol	C5H10O	M+FA-H	131.0714	1.8
	HMDB0030124	Prenol	C5H10O	M+FA-H	131.0714	1.8
132.0304	HMDB0000191	L-Aspartic acid	C4H7NO4	M-H	132.0302	1.3
	HMDB0011753	Iminodiacetic acid	C4H7NO4	M-H	132.0302	1.3
	HMDB0159995	SCHEMBL51875	C4H7NO4	M-H	132.0302	1.3
	HMDB0006483	D-Aspartic acid	C4H7NO4	M-H	132.0302	1.3
	HMDB0161155	AC1N37K4	C4H6NO4	M-H	132.0302	1.3
	HMDB0003609	2-Aminoacrylic acid	C3H5NO2	M+FA-H	132.0302	1.3
	HMDB0039426	3-Isoxazolidinone	C3H5NO2	M+FA-H	132.0302	1.3
133.0145	HMDB0000156	L-Malic acid	C4H6O5	M-H	133.0142	1.9
	HMDB0000744	Malic acid	C4H6O5	M-H	133.0142	1.9
	HMDB0031518	D-Malic acid	C4H6O5	M-H	133.0142	1.9
	HMDB0032872	Velcorin	C4H6O5	M-H	133.0142	1.9
	HMDB0040261	Glucosereductone	C3H4O3	M+FA-H	133.0142	1.9
	HMDB0011111	Malonic semialdehyde	C3H4O3	M+FA-H	133.0142	1.9
	HMDB0062676	2-hydroxyacrylic acid	C3H4O3	M+FA-H	133.0142	1.9
	HMDB0168832	Oxirane-2-carboxylic acid	C3H4O3	M+FA-H	133.0142	1.9
133.0658	HMDB0000243	Pyruvic acid	C3H4O3	M+FA-H	133.0142	1.9
	HMDB0061984	2-ethylbenzaldehyde	C9H10O	M-H	133.0659	-0.7
	HMDB0062048	3,5-Dimethylbenzaldehyde	C9H10O	M-H	133.0659	-0.7
	HMDB0032386	1-(2-methylphenyl)ethan-1-one	C9H10O	M-H	133.0659	-0.7
	HMDB0173827	Benzenemethanol,4-methyl-a-methylene-	C9H10O	M-H	133.0659	-0.7
	HMDB0175242	beta-Methylenephenethyl alcohol	C9H10O	M-H	133.0659	-0.7
	HMDB0061970	phenylacetone	C9H10O	M-H	133.0659	-0.7
	HMDB0061961	1-ethenyl-3-methoxybenzene	C9H10O	M-H	133.0659	-0.7
	HMDB0030839	(Z)-4-(1-Propenyl)phenol	C9H10O	M-H	133.0659	-0.7
	HMDB0034563	7-Nonene-3,5-diyn-1-ol	C9H10O	M-H	133.0659	-0.7
	HMDB0033716	3-Phenylpropanal	C9H10O	M-H	133.0659	-0.7
	HMDB0034107	Chavicol	C9H10O	M-H	133.0659	-0.7
	HMDB0029639	(4-Methylphenyl)acetaldehyde	C9H10O	M-H	133.0659	-0.7
	HMDB0029697	Cinnamyl alcohol	C9H10O	M-H	133.0659	-0.7
	HMDB0036441	o-Vinylanisole	C9H10O	M-H	133.0659	-0.7
	HMDB0032024	4-Ethylbenzaldehyde	C9H10O	M-H	133.0659	-0.7
	HMDB0031626	2-Phenylpropanal	C9H10O	M-H	133.0659	-0.7
	HMDB0029698	trans-Cinnamyl alcohol	C9H10O	M-H	133.0659	-0.7
	HMDB0032142	2,4-Dimethylbenzaldehyde	C9H10O	M-H	133.0659	-0.7
	HMDB0032608	4'-Methylacetophenone	C9H10O	M-H	133.0659	-0.7
	HMDB0032623	1-Phenyl-1-propanone	C9H10O	M-H	133.0659	-0.7
	HMDB0059601	Indan-1-ol	C9H10O	M-H	133.0659	-0.7
	HMDB0059895	m-Methylacetophenone	C9H10O	M-H	133.0659	-0.7
134.0473	HMDB0000034	Adenine	C5H5N5	M-H	134.0472	0.6
134.0613	HMDB0170598	p-hydroxystyrylamine	C8H9NO	M-H	134.0611	1.2
	HMDB0001250	N-Acetylarlyamine	C8H9NO	M-H	134.0611	1.2
	HMDB0010715	2-Phenylacetamide	C8H9NO	M-H	134.0611	1.2
	HMDB0037071	2-Acetyl-4-methylpyridine	C8H9NO	M-H	134.0611	1.2
	HMDB0040223	4-Acetyl-2-methylpyridine	C8H9NO	M-H	134.0611	1.2
	HMDB0040222	2-Acetyl-5-methylpyridine	C8H9NO	M-H	134.0611	1.2
	HMDB0040224	4-Acetyl-3-methylpyridine	C8H9NO	M-H	134.0611	1.2
	HMDB0037072	2-Acetyl-6-methylpyridine	C8H9NO	M-H	134.0611	1.2
	HMDB0032628	2-Aminoacetophenone	C8H9NO	M-H	134.0611	1.2
	HMDB0032630	2'-Aminoacetophenone	C8H9NO	M-H	134.0611	1.2
	HMDB0040013	5-(2-Furanyl)-3,4-dihydro-2H-pyrrole	C8H9NO	M-H	134.0611	1.2
	HMDB0040008	2,3-Dihydro-1H-pyrrolizine-5-carboxaldehyde	C8H9NO	M-H	134.0611	1.2
	HMDB0062068	5-Acetyl-2-methylpyridine	C8H9NO	M-H	134.0611	1.2
	HMDB0041485	Benzyl formate	C8H8O2	M-H	135.0452	0.3
	HMDB0002340	2-Methylbenzoic acid	C8H8O2	M-H	135.0452	0.3
	HMDB0031459	3-Methoxybenzaldehyde	C8H8O2	M-H	135.0452	0.3
	HMDB0032400	3-(5-Methyl-2-furyl)prop-2-enal	C8H8O2	M-H	135.0452	0.3
	HMDB0032603	2-Hydroxy-4-methylbenzaldehyde	C8H8O2	M-H	135.0452	0.3
	HMDB0029686	4-Methoxybenzaldehyde	C8H8O2	M-H	135.0452	0.3
	HMDB0032568	2'-Hydroxyacetophenone	C8H8O2	M-H	135.0452	0.3
	HMDB0040638	3-(3-Furanyl)-2-methyl-2-propenal	C8H8O2	M-H	135.0452	0.3
	HMDB0033766	2-Methoxybenzaldehyde	C8H8O2	M-H	135.0452	0.3
	HMDB0033128	4-(2-Furanyl)-3-buten-2-one	C8H8O2	M-H	135.0452	0.3
	HMDB0000209	Phenylacetic acid	C8H8O2	M-H	135.0452	0.3

135.0452	HMDB0003767	4-Hydroxyphenylacetaldehyde	C8H8O2	M-H	135.0452	0.3
	HMDB0040733	Phenyl acetate	C8H8O2	M-H	135.0452	0.3
	HMDB0167830	4'-Hydroxyacetophenone	C8H8O2	M-H	135.0452	0.3
	HMDB0038176	alpha-Methyl-2-furanacrolein	C8H8O2	M-H	135.0452	0.3
	HMDB0033968	Methyl benzoate	C8H8O2	M-H	135.0452	0.3
	HMDB0029635	4-Methylbenzoic acid	C8H8O2	M-H	135.0452	0.3
	HMDB0126385	4-ethenylbenzene-1,3-diol	C8H8O2	M-H	135.0452	0.3
	HMDB0183895	phenylacetate	C8H7O2	M-H	135.0452	0.3
	HMDB0125535	5-ethenylbenzene-1,3-diol	C8H8O2	M-H	135.0452	0.3
	HMDB0062810	m-toluic acid	C8H8O2	M-H	135.0452	0.3
	HMDB0167829	1-(3-hydroxyphenyl)ethan-1-one	C8H8O2	M-H	135.0452	0.3
135.0817	HMDB0124942	4-ethenylbenzene-1,2-diol	C8H8O2	M-H	135.0452	0.3
	HMDB0125105	1-ethyl-3-methoxybenzene	C9H12O	M-H	135.0815	1.2
	HMDB0169117	alpha, alpha-Dimethylbenzyl alcohol	C9H12O	M-H	135.0815	1.2
	HMDB0169118	3-(propan-2-yl)phenol	C9H12O	M-H	135.0815	1.2
	HMDB0038986	3-Ethyl-4-methylphenol	C9H12O	M-H	135.0815	1.2
	HMDB0032624	2-Propylphenol	C9H12O	M-H	135.0815	1.2
	HMDB0038988	2-Ethyl-4-methylphenol	C9H12O	M-H	135.0815	1.2
	HMDB0032621	(2-Methoxyethyl)benzene	C9H12O	M-H	135.0815	1.2
	HMDB0038985	3-Ethyl-5-methylphenol	C9H12O	M-H	135.0815	1.2
	HMDB0031312	Benzyl ethyl ether	C9H12O	M-H	135.0815	1.2
	HMDB0033962	3-Phenyl-1-propanol	C9H12O	M-H	135.0815	1.2
	HMDB0031627	1-Phenyl-1-propanol	C9H12O	M-H	135.0815	1.2
	HMDB0034378	1-(4-Methylphenyl)ethanol	C9H12O	M-H	135.0815	1.2
	HMDB0039782	2-(1-Pentenyl)furan	C9H12O	M-H	135.0815	1.2
	HMDB0029667	2,3,6-Trimethylphenol	C9H12O	M-H	135.0815	1.2
	HMDB0032625	4-Propylphenol	C9H12O	M-H	135.0815	1.2
	HMDB0059896	6-Ethyl-o-cresol	C9H12O	M-H	135.0815	1.2
	HMDB0032441	Nona-2,4,6-trienal	C9H12O	M-H	135.0815	1.2
	HMDB0031446	p-Isopropylphenol	C9H12O	M-H	135.0815	1.2
	HMDB0032544	2,4,6-Trimethylphenol	C9H12O	M-H	135.0815	1.2
	HMDB0038984	4-Ethyl-2-methylphenol	C9H12O	M-H	135.0815	1.2
	HMDB0038987	2-Ethyl-5-methylphenol	C9H12O	M-H	135.0815	1.2
	HMDB0032029	2-Isopropylphenol	C9H12O	M-H	135.0815	1.2
	HMDB0032149	1-Methoxy-2,4-dimethylbenzene	C9H12O	M-H	135.0815	1.2
	HMDB0031628	2-Phenyl-1-propanol	C9H12O	M-H	135.0815	1.2
137.0245	HMDB0001895	Salicylic acid	C7H6O3	M-H	137.0244	0.6
	HMDB0062484	keratan sulfate II (core 2-linked), degradation product 1	C7H6O3	M-H	137.0244	0.6
	HMDB0171080	2,3-dihydroxybenzaldehyde	C7H6O3	M-H	137.0244	0.6
	HMDB0032920	alpha-Furyl methyl diketone	C7H6O3	M-H	137.0244	0.6
	HMDB0059965	3,4-Dihydroxybenzaldehyde	C7H6O3	M-H	137.0244	0.6
	HMDB0171081	2,6-dihydroxybenzaldehyde	C7H6O3	M-H	137.0244	0.6
	HMDB0000500	4-Hydroxybenzoic acid	C7H6O3	M-H	137.0244	0.6
	HMDB0002466	3-Hydroxybenzoic acid	C7H6O3	M-H	137.0244	0.6
	HMDB0004062	Gentisate aldehyde	C7H6O3	M-H	137.0244	0.6
	HMDB0032576	2-Methoxy-1,4-benzoquinone	C7H6O3	M-H	137.0244	0.6
	HMDB0033812	Sesamol	C7H6O3	M-H	137.0244	0.6
137.0609	HMDB0126388	4-ethylbenzene-1,3-diol	C8H10O2	M-H	137.0608	0.7
	HMDB0041607	2-Phenoxyethanol	C8H10O2	M-H	137.0608	0.7
	HMDB0168418	3-(2-Hydroxyethyl)phenol	C8H10O2	M-H	137.0608	0.7
	HMDB0166105	2-Methoxybenzyl alcohol	C8H10O2	M-H	137.0608	0.7
	HMDB0125590	5-ethylbenzene-1,3-diol	C8H10O2	M-H	137.0608	0.7
	HMDB0168417	1-phenylethane-1,2-diol	C8H10O2	M-H	137.0608	0.7
	HMDB0029563	3-Acetyl-2,5-dimethylfuran	C8H10O2	M-H	137.0608	0.7
	HMDB0032136	2-Methoxy-4-methylphenol	C8H10O2	M-H	137.0608	0.7
	HMDB0034241	4-Methoxybenzyl alcohol	C8H10O2	M-H	137.0608	0.7
	HMDB0029672	1,3-Dimethoxybenzene	C8H10O2	M-H	137.0608	0.7
	HMDB0029671	1,4-Dimethoxybenzene	C8H10O2	M-H	137.0608	0.7
	HMDB0039802	1-(2-Furanyl)-1-butanone	C8H10O2	M-H	137.0608	0.7
	HMDB0032036	4-Ethoxyphenol	C8H10O2	M-H	137.0608	0.7
	HMDB0032139	1,2-Dimethoxybenzene	C8H10O2	M-H	137.0608	0.7
	HMDB0040177	3-Ethyl-1,2-benzenediol	C8H10O2	M-H	137.0608	0.7
	HMDB0040174	4-Ethyl-1,2-benzenediol	C8H10O2	M-H	137.0608	0.7
	HMDB0032137	2,6-Dimethyl-1,4-benzenediol	C8H10O2	M-H	137.0608	0.7
	HMDB0004284	Tyrosol	C8H10O2	M-H	137.0608	0.7

	HMDB0032159	2-Acetyl-3,5-dimethylfuran	C8H10O2	M-H	137.0608	0.7
	HMDB0032290	1-(2-Furyl)butan-3-one	C8H10O2	M-H	137.0608	0.7
	HMDB0168448	2-hydroxyphenylethanol	C8H10O2	M-H	137.0608	0.7
	HMDB0062096	cyclohepta-1,3,5-triene	C7H8	M+FA-H	137.0608	0.7
	HMDB0061953	597-85-5	C7H8	M+FA-H	137.0608	0.7
	HMDB0034168	Toluene	C7H8	M+FA-H	137.0608	0.7
137.0972	HMDB0036092	exo-2-Methyl-3-methylenebicyclo[2.2.1]heptan-2-ol	C9H14O	M-H	137.0972	0.1
	HMDB0167046	SCHEMBL19577743	C9H14O	M-H	137.0972	0.1
	HMDB0036091	exo-5,6-Dimethylbicyclo[2.2.1]hept-5-en-2-ol	C9H14O	M-H	137.0972	0.1
	HMDB0036069	Pulegone	C9H14O	M-H	137.0972	0.1
	HMDB0035929	(R)-Cryptone	C9H14O	M-H	137.0972	0.1
	HMDB0031685	2,4-Nonadienal	C9H14O	M-H	137.0972	0.1
	HMDB0013824	2-Pentylfuran	C9H14O	M-H	137.0972	0.1
	HMDB0031084	2-Pentylfuran	C9H14O	M-H	137.0972	0.1
	HMDB0033434	4-Acetyl-1-methylcyclohexene	C9H14O	M-H	137.0972	0.1
	HMDB0040338	3,5,5-Trimethyl-3-cyclohexen-1-one	C9H14O	M-H	137.0972	0.1
	HMDB0031195	3,5,5-Trimethyl-2-cyclohexen-1-one	C9H14O	M-H	137.0972	0.1
	HMDB0035229	5-Isopropylbicyclo[3.1]hexan-2-one	C9H14O	M-H	137.0972	0.1
	HMDB0031261	(2E,6E)-2,6-Nonadienal	C9H14O	M-H	137.0972	0.1
	HMDB0033857	Violet-leaf aldehyde	C9H14O	M-H	137.0972	0.1
	HMDB0031152	(3Z,6Z)-3,6-Nonadienal	C9H14O	M-H	137.0972	0.1
	HMDB0180424	Nona-trans-2-trans-4-dien-1-al	C9H14O	M-H	137.0972	0.1
138.0197	HMDB0059710	2-Hydroxynicotinic acid	C6H5NO3	M-H	138.0197	0.2
	HMDB0013188	3-Hydroxypicolinic acid	C6H5NO3	M-H	138.0197	0.2
	HMDB0002658	6-Hydroxynicotinic acid	C6H5NO3	M-H	138.0197	0.2
	HMDB0001232	4-Nitrophenol	C6H5NO3	M-H	138.0197	0.2
	HMDB0062627	4-Nitrophenol	C6H5NO3	M-H	138.0197	0.2
138.9804	HMDB0031331	Chloroacetic acid	C2H3ClO2	M+FA-H	138.9804	0.3
	HMDB0004110	Phosphonoacetate	C2H5O5P	M-H	138.9802	1.6
	HMDB0001494	Acetylphosphate	C2H5O5P	M-H	138.9802	1.6
139.0402	HMDB0181055	1-[3-(hydroxymethyl)furan-2-yl]ethan-1-one	C7H8O3	M-H	139.0401	0.9
	HMDB0137138	2-methoxybenzene-1,4-diol	C7H8O3	M-H	139.0401	0.9
	HMDB0169073	3-(Hydroxymethyl)pyrocatechol	C7H8O3	M-H	139.0401	0.9
	HMDB0125538	3-methoxybenzene-1,2-diol	C7H8O3	M-H	139.0401	0.9
	HMDB0137137	4-methoxybenzene-1,2-diol	C7H8O3	M-H	139.0401	0.9
	HMDB0172014	4-methoxy-5-methyl-2-methylidene-2,3-dihydrofuran-3-one	C7H8O3	M-H	139.0401	0.9
	HMDB0125014	4-methoxybenzene-1,3-diol	C7H8O3	M-H	139.0401	0.9
	HMDB0133970	2-methoxybenzene-1,3-diol	C7H8O3	M-H	139.0401	0.9
	HMDB0031735	Ethyl maltol	C7H8O3	M-H	139.0401	0.9
	HMDB0169074	Gentisyl alcohol	C7H8O3	M-H	139.0401	0.9
	HMDB0059880	Ethyl 3-furoate	C7H8O3	M-H	139.0401	0.9
	HMDB0034246	Furfuryl acetate	C7H8O3	M-H	139.0401	0.9
	HMDB0059862	Ethyl furoate	C7H8O3	M-H	139.0401	0.9
	HMDB0132905	5-methoxybenzene-1,3-diol	C7H8O3	M-H	139.0401	0.9
	HMDB0151713	2,4,6-trihydroxytoluene	C7H8O3	M-H	139.0401	0.9
	HMDB0179995	4-(hydroxymethyl)benzene-1,2-diol	C7H8O3	M-H	139.0401	0.9
	HMDB0062167	2-VINYLFURAN	C6H6O	M+FA-H	139.0401	1.0
	HMDB0000228	Phenol	C6H6O	M+FA-H	139.0401	1.0
139.0765	HMDB0037196	Ethyl 2-methyl-3,4-pentadienoate	C8H12O2	M-H	139.0765	0.3
	HMDB0040526	3,4,4-Trimethyl-1,2-cyclopentanedione	C8H12O2	M-H	139.0765	0.3
	HMDB0037625	Allyl tiglate	C8H12O2	M-H	139.0765	0.3
	HMDB0036176	3-Ethyl-2-hydroxy-4-methyl-2-cyclopenten-1-one	C8H12O2	M-H	139.0765	0.3
	HMDB0039652	2-Hydroxy-3,4,5-trimethyl-2-cyclopenten-1-one	C8H12O2	M-H	139.0765	0.3
	HMDB0039680	3,5,5-Trimethyl-1,2-cyclopentanedione	C8H12O2	M-H	139.0765	0.3
	HMDB0039651	3-Propyl-1,2-cyclopentanedione	C8H12O2	M-H	139.0765	0.3
	HMDB0039673	4-Ethyl-2-hydroxy-3-methyl-2-cyclopenten-1-one	C8H12O2	M-H	139.0765	0.3
	HMDB0040463	Ethyl sorbate	C8H12O2	M-H	139.0765	0.3
	HMDB0039681	3-Isopropyl-1,2-cyclopentanedione	C8H12O2	M-H	139.0765	0.3
	HMDB0037167	3-Ethyl-5-methyl-1,2-cyclopentanedione	C8H12O2	M-H	139.0765	0.3
	HMDB0032311	2,4-Hexadienyl acetate	C8H12O2	M-H	139.0765	0.3
	HMDB0060682	2-Propyl-2,4-pentadienoic acid	C8H12O2	M-H	139.0765	0.3
	HMDB0031532	1-Methyl-1,3-cyclohexadiene	C7H10	M+FA-H	139.0765	0.4
	HMDB0061889	(3E,5Z)-1,3,5-Heptatriene	C7H10	M+FA-H	139.0765	0.4
	HMDB0032395	2-Methyl-1,3-cyclohexadiene	C7H10	M+FA-H	139.0765	0.4

139.1129	HMDB0062671	(3E)-2,3,4-trimethylhex-3-enal	C9H16O	M-H	139.1128	0.4
	HMDB0167031	Violet alcohol	C9H16O	M-H	139.1128	0.4
	HMDB0037170	3-Methylene-2-octanone	C9H16O	M-H	139.1128	0.4
	HMDB0035927	1-Nonen-4-one	C9H16O	M-H	139.1128	0.4
	HMDB0030957	(3Z,6Z)-3,6-Nonadien-1-ol	C9H16O	M-H	139.1128	0.4
	HMDB0035926	8-Nonen-2-one	C9H16O	M-H	139.1128	0.4
	HMDB0031269	2-Nonenal	C9H16O	M-H	139.1128	0.4
	HMDB0034764	3-Nonen-2-one	C9H16O	M-H	139.1128	0.4
	HMDB0034761	5-Nonen-2-one	C9H16O	M-H	139.1128	0.4
	HMDB0033554	2-Methyl-2-octenal	C9H16O	M-H	139.1128	0.4
	HMDB0035916	(E)-2-Nonen-4-one	C9H16O	M-H	139.1128	0.4
	HMDB0038400	(2xi,4xi)-2,4-Nonadien-1-ol	C9H16O	M-H	139.1128	0.4
	HMDB0031834	2,6-Dimethyl-5-heptenal	C9H16O	M-H	139.1128	0.4
	HMDB0034758	8-Nonen-3-one	C9H16O	M-H	139.1128	0.4
	HMDB0031262	2,6-Nonadien-1-ol	C9H16O	M-H	139.1128	0.4
	HMDB0038067	(3E,6Z)-3,6-Nonadien-1-ol	C9H16O	M-H	139.1128	0.4
	HMDB0034845	2,4-Nonadien-1-ol	C9H16O	M-H	139.1128	0.4
	HMDB0059828	3-Nonen-5-one	C9H16O	M-H	139.1128	0.4
	HMDB0032535	trans-4-Nonenal	C9H16O	M-H	139.1128	0.4
	HMDB0039461	7-Methyl-3-octen-2-one	C9H16O	M-H	139.1128	0.4
	HMDB0030958	(Z)-6-Nonenal	C9H16O	M-H	139.1128	0.4
	HMDB0037001	Santene hydrate	C9H16O	M-H	139.1128	0.4
	HMDB0037150	2-Ethyl-2-heptenal	C9H16O	M-H	139.1128	0.4
	HMDB0033794	2,2,6-Trimethylcyclohexanone	C9H16O	M-H	139.1128	0.4
140.0120	HMDB0000224	O-Phosphoethanolamine	C2H8NO4P	M-H	140.0118	1.3
	HMDB0060151	O-Phosphoethanolamine	C2H8NO4P	M-H	140.0118	1.3
	HMDB0060152	O-Phosphoethanolamine	C2H8NO4P	M-H	140.0118	1.3
	HMDB0062270	1,2-Diacylglycerol-LD-PI-pool	C7H5NO	M+Na-2H	140.0118	1.6
141.0192	HMDB0032914	2-Furancarboxaldehyde	C5H4O2	M+FA-H	141.0193	-0.9
	HMDB0062029	3-furaldehyde	C5H4O2	M+FA-H	141.0193	-0.9
	HMDB0060503	Protoanemonin	C5H4O2	M+FA-H	141.0193	-0.9
	HMDB0125218	benzene-1,2,3,5-tetrol	C6H6O4	M-H	141.0193	-0.9
	HMDB0134002	benzene-1,2,3,4-tetrol	C6H6O4	M-H	141.0193	-0.9
	HMDB0062661	muconic acid	C6H6O4	M-H	141.0193	-0.9
	HMDB0062704	muconic acid	C6H6O4	M-H	141.0193	-0.9
	HMDB0032923	Kojic acid	C6H6O4	M-H	141.0193	-0.9
	HMDB0002349	trans-trans-Muconic acid	C6H6O4	M-H	141.0193	-0.9
	HMDB0002432	Sumiki's acid	C6H6O4	M-H	141.0193	-0.9
	HMDB0029188	Sumiki's acid	C6H6O4	M-H	141.0193	-0.9
	HMDB0006331	cis,cis-Muconic acid	C6H6O4	M-H	141.0193	-0.9
	HMDB0032988	5-Hydroxymaltol	C6H6O4	M-H	141.0193	-0.9
	HMDB0059762	2,3-Methylenesuccinic acid	C6H6O4	M-H	141.0193	-0.9
	HMDB0180629	SCHEMBL16585474	C6H8O5	M-H2O-H	141.0188	3.0
	HMDB0180630	3-hydroxy-2,4-dioxohexanoic acid	C6H8O5	M-H2O-H	141.0188	3.0
	HMDB0180628	Lactyl- Brenztraubensaure	C6H8O5	M-H2O-H	141.0188	3.0
	HMDB0039447	2-Methyl-4-oxopentanedioic acid	C6H8O5	M-H2O-H	141.0188	3.0
	HMDB0000398	3-Oxoadipic acid	C6H8O5	M-H2O-H	141.0188	3.0
	HMDB0000225	Oxoadipic acid	C6H8O5	M-H2O-H	141.0188	3.0
	HMDB0159825	(2Z)-3-(hydroxymethyl)pent-2-enedioic acid	C6H8O5	M-H2O-H	141.0188	3.0
	HMDB0159827	(2E)-4-hydroxy-3-methylpent-2-enedioic acid	C6H8O5	M-H2O-H	141.0188	3.0
	HMDB0158423	SCHEMBL6765	C6H8O5	M-H2O-H	141.0188	3.0
	HMDB0158424	(3E)-2-hydroxyhex-3-enedioic acid	C6H8O5	M-H2O-H	141.0188	3.0
	HMDB0159826	3-(carboxymethyl)-3-methyloxirane-2-carboxylic acid	C6H8O5	M-H2O-H	141.0188	3.0
141.0557	HMDB0031545	2-Methyl-2-cyclopenten-1-one	C6H8O	M+FA-H	141.0557	-0.1
	HMDB0032965	2,4-Dimethylfuran	C6H8O	M+FA-H	141.0557	-0.1
	HMDB0040588	3-Ethylfuran	C6H8O	M+FA-H	141.0557	-0.1
	HMDB0040587	2-Ethylfuran	C6H8O	M+FA-H	141.0557	-0.1
	HMDB0033182	2,5-Dimethylfuran	C6H8O	M+FA-H	141.0557	-0.1
	HMDB0031546	3-Methyl-2-cyclopenten-1-one	C6H8O	M+FA-H	141.0557	-0.1
	HMDB0034729	(E,E)-2,4-Hexadienal	C6H8O	M+FA-H	141.0557	-0.1
	HMDB0180324	(2E)-3-(3-ethyloxiran-2-yl)prop-2-enoic acid	C7H10O3	M-H	141.0557	-0.1
	HMDB0180325	(2E)-4,5-dihydroxyhepta-2,4-dienal	C7H10O3	M-H	141.0557	-0.1
	HMDB0165787	2-ethyl-5-methyloxolane-3,4-dione	C7H10O3	M-H	141.0557	-0.1
	HMDB0164727	4,6-dihydroxy-4-methylcyclohex-2-en-1-one	C7H10O3	M-H	141.0557	-0.1
	HMDB0164726	5-hydroxy-5-methyl-7-oxabicyclo[4.1]heptan-2-one	C7H10O3	M-H	141.0557	-0.1

	HMDB0164725	4-hydroxy-4-(hydroxymethyl)cyclohex-2-en-1-one	C7H10O3	M-H	141.0557	-0.1
	HMDB0163404	5-ethyl-4-methyloxolane-2,3-dione	C7H10O3	M-H	141.0557	-0.1
	HMDB0172015	4-methoxy-5-methyl-2-methylideneoxolan-3-one	C7H10O3	M-H	141.0557	-0.1
	HMDB0034230	Mesifurane	C7H10O3	M-H	141.0557	-0.1
	HMDB0041426	Erinapyrone A	C7H10O3	M-H	141.0557	-0.1
	HMDB0041427	Erinapyrone B	C7H10O3	M-H	141.0557	-0.1
	HMDB0033551	5-Ethyl-3-hydroxy-4-methyl-2(5H)-furanone	C7H10O3	M-H	141.0557	-0.1
141.0670	HMDB0033736	Homofureanol	C7H10O3	M-H	141.0557	-0.1
	HMDB0145363	1-[(carboxyamino)methyl]-3,4-dihydro-2H-pyrrol-1-ium	C6H11N2O2	M-H	141.0670	0.3
141.0921	HMDB0240650	ectoine	C6H10N2O2	M-H	141.0670	0.3
	HMDB0163318	(E)-8-Hydroxy-3-octene-2-one	C8H14O2	M-H	141.0921	0.0
	HMDB0163317	Ethanone, 1-(3-butyloxiranyl)-	C8H14O2	M-H	141.0921	0.0
	HMDB0163316	(3E)-7-hydroxyoct-3-en-2-one	C8H14O2	M-H	141.0921	0.0
	HMDB0163315	SCHEMBL17867	C8H14O2	M-H	141.0921	0.0
	HMDB0163319	(3E)-1-hydroxyoct-3-en-2-one	C8H14O2	M-H	141.0921	0.0
	HMDB0000392	2-Octenoic acid	C8H14O2	M-H	141.0921	0.0
	HMDB0032266	Ethyl (E)-3-hexenoate	C8H14O2	M-H	141.0921	0.0
	HMDB0037624	Isopropyl tiglate	C8H14O2	M-H	141.0921	0.0
	HMDB0031293	2,3-Octanedione	C8H14O2	M-H	141.0921	0.0
	HMDB0029761	Ethyl 2-methyl-4-pentenoate	C8H14O2	M-H	141.0921	0.0
	HMDB0031403	Cyclohexanecetic acid	C8H14O2	M-H	141.0921	0.0
	HMDB0035422	4-Butyl-gamma-butyrolactone	C8H14O2	M-H	141.0921	0.0
	HMDB0031352	Cyclohexyl acetate	C8H14O2	M-H	141.0921	0.0
	HMDB0031343	Methyl cyclohexanecarboxylate	C8H14O2	M-H	141.0921	0.0
	HMDB0036212	2-Methylpropyl (2E)-butenoate	C8H14O2	M-H	141.0921	0.0
	HMDB0036236	2-Methylallyl butyrate	C8H14O2	M-H	141.0921	0.0
	HMDB0032268	Ethyl 2E-hexenoate	C8H14O2	M-H	141.0921	0.0
	HMDB0001568	trans-2-Octenoic acid	C8H14O2	M-H	141.0921	0.0
	HMDB0038036	2-Propenyl 3-methylbutanoate	C8H14O2	M-H	141.0921	0.0
	HMDB0039793	(E)-4-Octenoic acid	C8H14O2	M-H	141.0921	0.0
	HMDB0037630	xi-Tetrahydro-3-propyl-2H-pyran-2-one	C8H14O2	M-H	141.0921	0.0
	HMDB0038310	xi-Tetrahydro-6-propyl-2H-pyran-2-one	C8H14O2	M-H	141.0921	0.0
	HMDB0039872	Methyl 2-heptenoate	C8H14O2	M-H	141.0921	0.0
	HMDB0037622	Ethyl 2-methyl-3-pentenoate	C8H14O2	M-H	141.0921	0.0
	HMDB0040215	cis-3-Hexenyl acetate	C8H14O2	M-H	141.0921	0.0
	HMDB0040212	2-Hexenyl acetate	C8H14O2	M-H	141.0921	0.0
	HMDB0032533	trans-3-Hexenyl acetate	C8H14O2	M-H	141.0921	0.0
	HMDB0240301	3-Octenoic acid	C8H14O2	M-H	141.0921	0.0
	HMDB0062077	6-methylheptan-2,4-dione	C8H14O2	M-H	141.0921	0.0
	HMDB0062166	Vinyl hexanoate	C8H14O2	M-H	141.0921	0.0
	HMDB0013904	(3E)-2-Propylpent-3-enoic acid	C8H14O2	M-H	141.0921	0.0
	HMDB0013902	2-ene-Valproic acid	C8H14O2	M-H	141.0921	0.0
	HMDB0032164	Allyl valerate	C8H14O2	M-H	141.0921	0.0
	HMDB0032278	Ethyl trans-2-methyl-2-pentenoate	C8H14O2	M-H	141.0921	0.0
	HMDB0032207	cis-5-Octenoic acid	C8H14O2	M-H	141.0921	0.0
	HMDB0032267	Ethyl 5-hexenoate	C8H14O2	M-H	141.0921	0.0
	HMDB0059908	Ethyl-3-hexanoate	C8H14O2	M-H	141.0921	0.0
	HMDB0013897	4-ene-Valproic acid	C8H14O2	M-H	141.0921	0.0
	HMDB0013903	(3Z)-2-Propylpent-3-enoic acid	C8H14O2	M-H	141.0921	0.0
	HMDB0061342	(3Z)-2-Propylpent-3-enoic acid	C8H14O2	M-H	141.0921	0.0
141.1285	HMDB0031730	3,5,5-Trimethylhexanal	C9H18O	M-H	141.1285	0.1
	HMDB0041601	(E)-3-Nonen-1-ol	C9H18O	M-H	141.1285	0.1
	HMDB0163453	ZINC1986326	C9H18O	M-H	141.1285	0.1
	HMDB0167930	8-Nonen-2-ol	C9H18O	M-H	141.1285	0.1
	HMDB0031268	Amyl propyl ketone	C9H18O	M-H	141.1285	0.1
	HMDB0031417	2,6-Dimethyl-4-heptanone	C9H18O	M-H	141.1285	0.1
	HMDB0059835	Nonanal	C9H18O	M-H	141.1285	0.1
	HMDB0037304	2,6-Dimethyl-6-hepten-1-ol	C9H18O	M-H	141.1285	0.1
	HMDB0031684	2-Methyloctanal	C9H18O	M-H	141.1285	0.1
	HMDB0031266	2-Nonanone	C9H18O	M-H	141.1285	0.1
	HMDB0041498	2-Nonen-1-ol	C9H18O	M-H	141.1285	0.1
	HMDB0029557	Dihydroisophorol	C9H18O	M-H	141.1285	0.1
	HMDB0031267	3-Nonanone	C9H18O	M-H	141.1285	0.1
	HMDB0041499	(Z)-2-Nonen-1-ol	C9H18O	M-H	141.1285	0.1

	HMDB0034152	1-Nonen-3-ol	C9H18O	M-H	141.1285	0.1
	HMDB0030959	(Z)-3-Nonen-1-ol	C9H18O	M-H	141.1285	0.1
	HMDB0040581	(Z)-6-Nonen-1-ol	C9H18O	M-H	141.1285	0.1
	HMDB0059887	(E)-6-Nonenol	C9H18O	M-H	141.1285	0.1
	HMDB0167929	Nonen-2-ol	C9H18O	M-H	141.1285	0.1
142.0509	HMDB0032968	2,4-Dimethyloxazole	C5H7NO	M+FA-H	142.0510	-0.5
	HMDB0032970	4,5-Dimethyloxazole	C5H7NO	M+FA-H	142.0510	-0.5
	HMDB0167284	2-hydroxy-2-methylbut-3-enenitrile	C5H7NO	M+FA-H	142.0510	-0.5
	HMDB0032969	2,5-Dimethyloxazole	C5H7NO	M+FA-H	142.0510	-0.5
	HMDB0031339	1-Cyano-2-hydroxy-3-butene	C5H7NO	M+FA-H	142.0510	-0.5
	HMDB0177062	1-formyl-3,4-dihydro-2H-pyrrol-1-ium	C5H8NO	M+FA-H	142.0510	-0.5
	HMDB0000894	Vinylacetylglycine	C6H9NO3	M-H	142.0510	-0.5
	HMDB0014491	Trimethadione	C6H9NO3	M-H	142.0510	-0.5
	HMDB0032161	Acrylamide-acrylic acid resin	C6H9NO3	M-H	142.0510	-0.5
	HMDB0061705	6-Oxopiperidine-2-carboxylic acid	C6H9NO3	M-H	142.0510	-0.5
143.0352	HMDB0061082	5-ethyl-5-methyl-2,4-oxazolidinedione	C6H9NO3	M-H	142.0510	-0.5
	HMDB0034426	(-)-1-Methylpropyl 1-propenyl disulfide	C7H14S2	M-H2O-H	143.0353	-0.7
	HMDB0180627	2,4-Dioxohexanoic acid	C6H8O4	M-H	143.0350	1.5
	HMDB0240300	3-methylpent-2-enedioic acid	C6H8O4	M-H	143.0350	1.5
	HMDB0163711	(2Z)-5-hydroxy-3-methyl-4-oxopent-2-enoic acid	C6H8O4	M-H	143.0350	1.5
	HMDB0163710	3-acetyl-3-methyloxirane-2-carboxylic acid	C6H8O4	M-H	143.0350	1.5
	HMDB0163709	(2Z)-3-(hydroxymethyl)-4-oxopent-2-enoic acid	C6H8O4	M-H	143.0350	1.5
	HMDB0013311	trans-2-Hexenedioic acid	C6H8O4	M-H	143.0350	1.5
	HMDB0036232	Maleic acid homopolymer	C6H8O4	M-H	143.0350	1.5
	HMDB0040207	Ethyl hydrogen fumarate	C6H8O4	M-H	143.0350	1.5
	HMDB0031257	Dimethyl fumarate	C6H8O4	M-H	143.0350	1.5
	HMDB0002266	(E)-2-Methylglutaconic acid	C6H8O4	M-H	143.0350	1.5
	HMDB0000522	3-Methylglutaconic acid	C6H8O4	M-H	143.0350	1.5
	HMDB0000393	3-Hexenedioic acid	C6H8O4	M-H	143.0350	1.5
	HMDB0029171	3-Hydroxyadipic acid 3,6-lactone	C6H8O4	M-H	143.0350	1.5
	HMDB0062030	3-FURANMETHANOL	C5H6O2	M+FA-H	143.0350	1.5
	HMDB0040145	5-Hydroxy-4-pentenoic acid d-lactone	C5H6O2	M+FA-H	143.0350	1.5
	HMDB0029609	5-Methyl-2(3H)-furanone	C5H6O2	M+FA-H	143.0350	1.5
	HMDB0013742	2-Furanmethanol	C5H6O2	M+FA-H	143.0350	1.5
	HMDB0034245	2-Furanmethanol	C5H6O2	M+FA-H	143.0350	1.5
143.0464	HMDB0041946	N-Nitrosoproline	C5H8N2O3	M-H	143.0462	1.3
	HMDB0060768	4-Hydroxymethylpyrazole	C4H6N2O	M+FA-H	143.0462	1.3
143.0714	HMDB0180835	pentyl 2-oxoacetate	C7H12O3	M-H	143.0714	0.2
	HMDB0172013	4-methoxy-2,5-dimethyloxolan-3-one	C7H12O3	M-H	143.0714	0.2
	HMDB0180327	(2E)-3-[3-(2-hydroxyethyl)oxiran-2-yl]prop-2-en-1-ol	C7H12O3	M-H	143.0714	0.2
	HMDB0180326	(2E)-3-[3-(1-hydroxyethyl)oxiran-2-yl]prop-2-en-1-ol	C7H12O3	M-H	143.0714	0.2
	HMDB0166746	ACMC-mulz	C7H12O3	M-H	143.0714	0.2
	HMDB0166745	(2E)-6-hydroxyhept-2-enoic acid	C7H12O3	M-H	143.0714	0.2
	HMDB0166744	(2E)-4-hydroxyhept-2-enoic acid	C7H12O3	M-H	143.0714	0.2
	HMDB0166747	SCHEMBL088	C7H12O3	M-H	143.0714	0.2
	HMDB0166501	(4Z)-2-hydroxyhept-4-enoic acid	C7H12O3	M-H	143.0714	0.2
	HMDB0166500	SCHEMBL26282	C7H12O3	M-H	143.0714	0.2
	HMDB0166498	(4Z)-3-hydroxyhept-4-enoic acid	C7H12O3	M-H	143.0714	0.2
	HMDB0166499	SCHEMBL7994854	C7H12O3	M-H	143.0714	0.2
	HMDB0166497	(4Z)-6-hydroxyhept-4-enoic acid	C7H12O3	M-H	143.0714	0.2
	HMDB0165786	2(5)-ethyl-4-hydroxy-5(2)-methyl-3(2H)-furanone (ethylfuranol)	C7H12O3	M-H	143.0714	0.2
	HMDB0164728	4-hydroxy-4-(hydroxymethyl)cyclohexan-1-one	C7H12O3	M-H	143.0714	0.2
	HMDB0164729	2,4-dihydroxy-4-methylcyclohexan-1-one	C7H12O3	M-H	143.0714	0.2
	HMDB0163403	5-ethyl-3-hydroxy-4-methyloxolan-2-one	C7H12O3	M-H	143.0714	0.2
	HMDB0036594	Botryodiplodin	C7H12O3	M-H	143.0714	0.2
	HMDB0037114	Methyl (R)-3-methyl-2-oxopentanoate	C7H12O3	M-H	143.0714	0.2
	HMDB0061990	2-hydroxycyclohexanecarboxylic acid	C7H12O3	M-H	143.0714	0.2
	HMDB0040433	Ethyl levulinate	C7H12O3	M-H	143.0714	0.2
	HMDB0001988	4-Hydroxycyclohexylcarboxylic acid	C7H12O3	M-H	143.0714	0.2
	HMDB0031176	Tetrahydrofurfuryl acetate	C7H12O3	M-H	143.0714	0.2
	HMDB0165587	(2Z)-2-methylpenta-2,4-dien-1-ol	C6H10O	M+FA-H	143.0714	0.2
	HMDB0040264	(Z)-2-Hexenal	C6H10O	M+FA-H	143.0714	0.2
	HMDB0035239	4-Hexen-3-one	C6H10O	M+FA-H	143.0714	0.2
	HMDB0031196	4-Methyl-2-pentenal	C6H10O	M+FA-H	143.0714	0.2

	HMDB0033714	2-Methyl-2-pentenal	C6H10O	M+FA-H	143.0714	0.2
	HMDB0179336	cis,trans-2,4-hexadien-1-ol	C6H10O	M+FA-H	143.0714	0.2
	HMDB0031563	4-Methyl-3-penten-2-one, 9CI	C6H10O	M+FA-H	143.0714	0.2
	HMDB0030332	2-Methyl-4-pentenal	C6H10O	M+FA-H	143.0714	0.2
	HMDB0031564	4-Methyl-4-penten-2-one	C6H10O	M+FA-H	143.0714	0.2
	HMDB0033549	(E)-4-Hexenal	C6H10O	M+FA-H	143.0714	0.2
	HMDB0031498	(Z)-3-Hexenal	C6H10O	M+FA-H	143.0714	0.2
	HMDB0031497	3-Hexenal	C6H10O	M+FA-H	143.0714	0.2
	HMDB0040271	(Z)-4-Hexenal	C6H10O	M+FA-H	143.0714	0.2
	HMDB0062127	2-methylpent-1-en-3-one	C6H10O	M+FA-H	143.0714	0.2
	HMDB0062031	3e-hexene-2-one	C6H10O	M+FA-H	143.0714	0.2
	HMDB0003315	Cyclohexanone	C6H10O	M+FA-H	143.0714	0.2
	HMDB0031496	Hex-trans-2-en-1-al	C6H10O	M+FA-H	143.0714	0.2
	HMDB0176892	Hex-trans-2-en-1-al	C6H10O	M+FA-H	143.0714	0.2
	HMDB0033532	Dimethicone	C6H18OSi2	M-H20-H	143.0712	1.2
143.1078	HMDB0181105	8-hydroxyoctan-3-one	C8H16O2	M-H	143.1078	0.3
	HMDB0062151	Propyl 2-methylbutanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0061998	2-methylbutyl propanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0061931	Tetrahydro-2,5-dimethyl-2H-pyranmethanol	C8H16O2	M-H	143.1078	0.3
	HMDB0032272	Ethyl 4-methylpentanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0032225	1,1-Dimethoxy-trans-2-hexene	C8H16O2	M-H	143.1078	0.3
	HMDB0032335	3-Hydroxy-2-octanone	C8H16O2	M-H	143.1078	0.3
	HMDB0032203	cis- and trans-2-Isobutyl-4-methyl-1,3-dioxolane	C8H16O2	M-H	143.1078	0.3
	HMDB0032551	Valeraldehyde propyleneglycol acetal	C8H16O2	M-H	143.1078	0.3
	HMDB0181107	4-Hydroxyoctane-3-one	C8H16O2	M-H	143.1078	0.3
	HMDB0163321	8-Hydroxy-2-octanone	C8H16O2	M-H	143.1078	0.3
	HMDB0163323	1-hydroxy-2-octanone	C8H16O2	M-H	143.1078	0.3
	HMDB0163320	7-hydroxyoctan-2-one	C8H16O2	M-H	143.1078	0.3
	HMDB0181104	7-hydroxyoctan-3-one	C8H16O2	M-H	143.1078	0.3
	HMDB0181103	2-hydroxyoctan-3-one	C8H16O2	M-H	143.1078	0.3
	HMDB0031579	Ethyl 2-methylpentanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0034234	Ethyl 3-methylpentanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0001877	Valproic acid	C8H16O2	M-H	143.1078	0.3
	HMDB0031230	2-Ethylhexanoic acid	C8H16O2	M-H	143.1078	0.3
	HMDB0062546	2-Ethylhexanoic acid	C8H16O2	M-H	143.1078	0.3
	HMDB0031596	Methyl 5-methylhexanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0031587	2-Methylheptanoic acid	C8H16O2	M-H	143.1078	0.3
	HMDB0031703	2-Ethylbutyl acetate	C8H16O2	M-H	143.1078	0.3
	HMDB0034161	2-Methylpropyl butanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0031478	Methyl heptanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0034164	3-Methylbutyl propanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0034459	Heptyl formate	C8H16O2	M-H	143.1078	0.3
	HMDB0029980	Hexyl acetate	C8H16O2	M-H	143.1078	0.3
	HMDB0036165	3-(Hydroxymethyl)-2-heptanone	C8H16O2	M-H	143.1078	0.3
	HMDB0030368	(3R,5Z)-5-Octene-1,3-diol	C8H16O2	M-H	143.1078	0.3
	HMDB0031290	1-Hydroxy-3-octanone	C8H16O2	M-H	143.1078	0.3
	HMDB0000482	Caprylic acid	C8H16O2	M-H	143.1078	0.3
	HMDB0062511	Caprylic acid	C8H16O2	M-H	143.1078	0.3
	HMDB0040209	Ethyl hexanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0040298	Ethyl 2-ethylbutanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0040252	Isobutyl isobutyrate	C8H16O2	M-H	143.1078	0.3
	HMDB0040251	Butyl isobutyrate	C8H16O2	M-H	143.1078	0.3
	HMDB0032047	Propyl 3-methylbutanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0039620	Butyl butyrate	C8H16O2	M-H	143.1078	0.3
	HMDB0039217	Isopropyl 2-methylbutanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0031638	Pentyl propanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0031588	6-Methylheptanoic acid	C8H16O2	M-H	143.1078	0.3
	HMDB0032046	Isopropyl 3-methylbutanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0040296	Propyl pentanoate	C8H16O2	M-H	143.1078	0.3
	HMDB0035457	5-Hydroxy-4-octanone	C8H16O2	M-H	143.1078	0.3
	HMDB0062136	Methylcyclohexane	C7H14	M+FA-H	143.1078	0.3
	HMDB0061783	(E)-Hept-2-ene	C7H14	M+FA-H	143.1078	0.3
	HMDB0061892	2-Heptene	C7H14	M+FA-H	143.1078	0.3
	HMDB0061895	2,4-Dimethyl-2-pentene	C7H14	M+FA-H	143.1078	0.3
	HMDB0061894	(E)-4,4-Dimethyl-2-pentene	C7H14	M+FA-H	143.1078	0.3

	HMDB0061893	(E)-Hept-3-ene	C7H14	M+FA-H	143.1078	0.3
144.0455	HMDB0240308	2-Hydroxyquinoline	C9H7NO	M-H	144.0455	0.1
	HMDB0172134	isoquinolin-7-ol	C9H7NO	M-H	144.0455	0.1
	HMDB0172136	Isoquinolin-8-ol	C9H7NO	M-H	144.0455	0.1
	HMDB0165773	5-HYDROXYQUINOLINE	C9H7NO	M-H	144.0455	0.1
	HMDB0165771	6-Hydroxyquinoline	C9H7NO	M-H	144.0455	0.1
	HMDB0165770	7-HYDROXYQUINOLINE	C9H7NO	M-H	144.0455	0.1
	HMDB0029737	1H-Indole-3-carboxaldehyde	C9H7NO	M-H	144.0455	0.1
	HMDB0165772	Oxyquinoline	C9H7NO	M-H	144.0455	0.1
	HMDB0172135	Isoquinolin-6-ol	C9H7NO	M-H	144.0455	0.1
145.0506	HMDB0132474	2-methylbut-2-enoic acid	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0149276	SCHEMBL15659879	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0130837	2-methylbut-3-enoic acid	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0170858	Isopropenylacetic acid	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0163713	73255-29-5	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0180166	3-methyl-4-trans-hydroxy-2-butenal	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0163712	SCHEMBL69133	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0163714	1-(2-methyloxiran-2-yl)ethan-1-one	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0129418	3,3-dimethyloxirane-2-carbaldehyde	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0032351	Isopropenyl acetate	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0032459	2-Pentenoic acid	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0001470	Tiglic acid	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0032385	Methyl methacrylate	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0000509	Senecioic acid	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0001862	2-Ethylacrylic acid	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0035143	Dihydro-3-methyl-2(3H)-furanone	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0033978	Ethyl acrylate	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0031598	2,3-Pentanedione	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0031178	2-Methyltetrahydrofuran-3-one	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0031648	2,4-Pentanedione	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0033840	Dihydro-5-methyl-2(3H)-furanone	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0031602	4-Pentenoic acid	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0002167	3-Methylbutyrolactone	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0029608	Angelic acid	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0029599	Glutaral	C5H8O2	M+FA-H	145.0506	-0.2
	HMDB0240327	2,3-dimethylbutanedioate	C6H8O4	M-H	145.0506	-0.2
	HMDB0155922	Mevaldic acid	C6H10O4	M-H	145.0506	-0.2
	HMDB0000448	Adipic acid	C6H10O4	M-H	145.0506	-0.2
	HMDB0000752	Methylglutaric acid	C6H10O4	M-H	145.0506	-0.2
	HMDB0002074	2,2-Dimethylsuccinic acid	C6H10O4	M-H	145.0506	-0.2
	HMDB0002173	Solerol	C6H10O4	M-H	145.0506	-0.2
	HMDB0006900	(S)-2-Aceto-2-hydroxybutanoic acid	C6H10O4	M-H	145.0506	-0.2
	HMDB0000858	Monomethyl glutaric acid	C6H10O4	M-H	145.0506	-0.2
	HMDB0158745	SCHEMBL143458	C6H10O4	M-H	145.0506	-0.2
	HMDB0158746	SCHEMBL1268	C6H10O4	M-H	145.0506	-0.2
	HMDB0158747	2-(hydroxymethyl)-3-oxopentanoic acid	C6H10O4	M-H	145.0506	-0.2
	HMDB0000422	2-Methylglutaric acid	C6H10O4	M-H	145.0506	-0.2
	HMDB0161125	3-hydroxy-4-methyl-2-oxopentanoic acid	C6H10O4	M-H	145.0506	-0.2
	HMDB0161124	5-hydroxy-4-methyl-2-oxopentanoic acid	C6H10O4	M-H	145.0506	-0.2
	HMDB0161123	SCHEMBL193563	C6H10O4	M-H	145.0506	-0.2
	HMDB0159479	3-(hydroxymethyl)-2-oxopentanoic acid	C6H10O4	M-H	145.0506	-0.2
	HMDB0159478	SCHEMBL3185864	C6H10O4	M-H	145.0506	-0.2
	HMDB0159480	SCHEMBL85244	C6H10O4	M-H	145.0506	-0.2
	HMDB0159477	3-Hydroxy-3-methyl-2-oxopentanoate	C6H10O4	M-H	145.0506	-0.2
	HMDB0158748	SCHEMBL2592393	C6H10O4	M-H	145.0506	-0.2
	HMDB0033837	Dimethyl succinate	C6H10O4	M-H	145.0506	-0.2
	HMDB0061930	4-Ethoxy-4-oxobutanoic acid	C6H10O4	M-H	145.0506	-0.2
	HMDB0033050	Butyl isopropyl disulfide	C7H16S2	M-H20-H	145.0510	-2.4
	HMDB0033051	Butyl propyl disulfide	C7H16S2	M-H20-H	145.0510	-2.4
	HMDB0039783	1-(Methylthio)-1-hexanethiol	C7H16S2	M-H20-H	145.0510	-2.4
145.0619	HMDB0000641	L-Glutamine	C5H10N2O3	M-H	145.0619	0.2
	HMDB0006899	Alanylglycine	C5H10N2O3	M-H	145.0619	0.2
	HMDB0240333	4-[(C-hydroxycarbonimidoyl)amino]butanoate	C5H9N2O3	M-H	145.0619	0.2
	HMDB0002031	Ureidoisobutyric acid	C5H10N2O3	M-H	145.0619	0.2
	HMDB0003423	D-Glutamine	C5H10N2O3	M-H	145.0619	0.2

	HMDB0028687	Alanylglycine	C5H10N2O3	M-H	145.0619	0.2
	HMDB0031642	N-Nitroso-pyrrolidine	C4H8N2O	M+FA-H	145.0619	0.2
	HMDB0033952	Gyromitrin	C4H8N2O	M+FA-H	145.0619	0.2
145.0872	HMDB0059842	Ethyl 2-hydroxyisovalerate	C7H14O3	M-H	145.0870	1.3
	HMDB0061653	3-hydroxyheptanoic acid	C7H14O3	M-H	145.0870	1.3
	HMDB0161034	2-hydroxyheptanoic acid	C7H14O3	M-H	145.0870	1.3
	HMDB0032269	(+/-)-Ethyl 2-hydroxy-2-methylbutyrate	C7H14O3	M-H	145.0870	1.3
	HMDB0165835	Ethyl 2-(hydroxymethyl)butanoate	C7H14O3	M-H	145.0870	1.3
	HMDB0165836	SCHEMBL7861	C7H14O3	M-H	145.0870	1.3
	HMDB0165833	Ethyl 3-hydroxy-2-methylbutyrate	C7H14O3	M-H	145.0870	1.3
	HMDB0002207	3-Hydroxyisooheptanoic acid	C7H14O3	M-H	145.0870	1.3
	HMDB0165834	SCHEMBL934322	C7H14O3	M-H	145.0870	1.3
	HMDB0036231	Methyl DL-Leucate	C7H14O3	M-H	145.0870	1.3
	HMDB0039407	Methyl 3-hydroxyhexanoate	C7H14O3	M-H	145.0870	1.3
	HMDB0040254	Butyl lactate	C7H14O3	M-H	145.0870	1.3
	HMDB0161033	7-Hydroxyheptanoic acid	C7H14O3	M-H	145.0870	1.3
	HMDB0161032	6-hydroxyheptanoic acid	C7H14O3	M-H	145.0870	1.3
	HMDB0176555	3,3-Dimethylbutyraldehyde	C6H12O	M+FA-H	145.0870	1.3
	HMDB0062792	(2R,3S)-2-methyl-3-propyloxirane	C6H12O	M+FA-H	145.0870	1.3
	HMDB0165580	2-Penten-1-ol, 2-methyl-, (Z)-	C6H12O	M+FA-H	145.0870	1.3
	HMDB0179350	(E)-4-Hexen-1-ol	C6H12O	M+FA-H	145.0870	1.3
	HMDB0165149	3-methylidenepentane-1-ol	C6H12O	M+FA-H	145.0870	1.3
	HMDB0165150	3-Methyl-4-penten-1-ol	C6H12O	M+FA-H	145.0870	1.3
	HMDB0165144	3-METHYLPENTANAL	C6H12O	M+FA-H	145.0870	1.3
	HMDB0174748	Cyclohexanol	C6H12O	M+FA-H	145.0870	1.3
	HMDB0031220	2-Ethylbutanal	C6H12O	M+FA-H	145.0870	1.3
	HMDB0031503	1-Hexen-3-ol	C6H12O	M+FA-H	145.0870	1.3
	HMDB0031502	(E)-4-Hexen-1-ol	C6H12O	M+FA-H	145.0870	1.3
	HMDB0030003	(E)-3-Hexen-1-ol	C6H12O	M+FA-H	145.0870	1.3
	HMDB0030952	(E)-2-Hexen-1-ol	C6H12O	M+FA-H	145.0870	1.3
	HMDB0005994	Hexanal	C6H12O	M+FA-H	145.0870	1.3
	HMDB0005846	Ethyl isopropyl ketone	C6H12O	M+FA-H	145.0870	1.3
	HMDB0005842	2-Oxohexane	C6H12O	M+FA-H	145.0870	1.3
	HMDB0002939	Methyl isobutyl ketone	C6H12O	M+FA-H	145.0870	1.3
	HMDB0001318	4-Methylpentanal	C6H12O	M+FA-H	145.0870	1.3
	HMDB0164619	5-Hexenol	C6H12O	M+FA-H	145.0870	1.3
	HMDB0031578	2-Methylpentanal	C6H12O	M+FA-H	145.0870	1.3
	HMDB0062058	4-Methyl-3-penten-1-ol	C6H12O	M+FA-H	145.0870	1.3
	HMDB0062034	3-Methyl-2-pentanone	C6H12O	M+FA-H	145.0870	1.3
	HMDB0061882	3-Methyl-1-penten-3-ol	C6H12O	M+FA-H	145.0870	1.3
	HMDB0000753	3-Hexanone	C6H12O	M+FA-H	145.0870	1.3
145.0983	HMDB0000182	L-Lysine	C6H14N2O2	M-H	145.0983	0.3
	HMDB0142894	2,6-diaminohexanoic acid	C6H14N2O2	M-H	145.0983	0.3
	HMDB0012115	(3S,5S)-3,5-Diaminohexanoate	C6H14N2O2	M-H	145.0983	0.3
	HMDB0012114	(3S)-3,6-Diaminohexanoate	C6H14N2O2	M-H	145.0983	0.3
	HMDB0003405	D-Lysine	C6H14N2O2	M-H	145.0983	0.3
146.0247	HMDB0061933	1H-Indole-2,3-dione	C8H5NO2	M-H	146.0248	-0.4
	HMDB0006779	Indole-5,6-quinone	C8H5NO2	M-H	146.0248	-0.4
	HMDB0030481	Agrocybin	C8H5NO2	M-H	146.0248	-0.4
146.0460	HMDB0000148	L-Glutamic acid	C5H9NO4	M-H	146.0459	0.8
	HMDB0033550	3-(Carboxymethylamino)propanoic acid	C5H9NO4	M-H	146.0459	0.8
	HMDB0062183	N-lactoyl-glycine	C5H9NO4	M-H	146.0459	0.8
	HMDB0002931	N-Acetylserine	C5H9NO4	M-H	146.0459	0.8
	HMDB0002393	N-Methyl-D-aspartic acid	C5H9NO4	M-H	146.0459	0.8
	HMDB0003011	O-Acetylserine	C5H9NO4	M-H	146.0459	0.8
	HMDB0003339	D-Glutamic acid	C5H9NO4	M-H	146.0459	0.8
	HMDB0006556	L-4-Hydroxyglutamate semialdehyde	C5H9NO4	M-H	146.0459	0.8
	HMDB0060475	DL-Glutamate	C5H9NO4	M-H	146.0459	0.8
	HMDB0156263	glutamate(1-)	C5H8NO4	M-H	146.0459	0.8
	HMDB0165479	2,3-dihydroxy-2-methylpropanenitrile	C4H7NO2	M+FA-H	146.0459	0.8
	HMDB0029387	L-3-Aminodihydro-2(3H)-furanone	C4H7NO2	M+FA-H	146.0459	0.8
	HMDB0029615	(S)-2-Azetidinecarboxylic acid	C4H7NO2	M+FA-H	146.0459	0.8
	HMDB0036458	1-Aminocyclopropanecarboxylic acid	C4H7NO2	M+FA-H	146.0459	0.8
	HMDB0135275	3-phenyloxirane-2-carbaldehyde	C9H8O2	M-H	147.0452	-0.4
	HMDB0135648	3-(4-hydroxyphenyl)prop-2-enal	C9H8O2	M-H	147.0452	-0.4

147.0451	HMDB0128078	3-phenylprop-2-enoic acid	C9H8O2	M-H	147.0452	-0.4
	HMDB0135273	(2Z)-2-hydroxy-3-phenylprop-2-enal	C9H8O2	M-H	147.0452	-0.4
	HMDB0135274	(2E)-3-(3-hydroxyphenyl)prop-2-enal	C9H8O2	M-H	147.0452	-0.4
	HMDB0134039	3-(2-hydroxyphenyl)prop-2-enal	C9H8O2	M-H	147.0452	-0.4
	HMDB0000930	trans-Cinnamic acid	C9H8O2	M-H	147.0452	-0.4
	HMDB0040986	(E)-3-(4-Hydroxyphenyl)-2-propenal	C9H8O2	M-H	147.0452	-0.4
	HMDB0031725	(E)-3-(2-Hydroxyphenyl)-2-propenal	C9H8O2	M-H	147.0452	-0.4
	HMDB0035243	1-Phenyl-1,2-propanedione	C9H8O2	M-H	147.0452	-0.4
	HMDB0032947	Di-2-furanylmethane	C9H8O2	M-H	147.0452	-0.4
	HMDB0036626	3,4-Dihydro-2H-1-benzopyran-2-one	C9H8O2	M-H	147.0452	-0.4
	HMDB0000567	Cinnamic acid	C9H8O2	M-H	147.0452	-0.4
149.0096	HMDB0000289	Uric acid	C5H4N4O3	M-H2O-H	149.0100	-2.3
	HMDB0038889	2-Methyl-2-(methyldithio)propanal	C5H10OS2	M-H	149.0100	-2.9
	HMDB0029878	D-Tartaric acid	C4H6O6	M-H	149.0092	2.9
	HMDB0059916	Meso-Tartaric acid	C4H6O6	M-H	149.0092	2.9
	HMDB0062642	Meso-Tartaric acid	C4H6O6	M-H	149.0092	2.9
	HMDB0000956	Tartaric acid	C4H6O6	M-H	149.0092	2.9
	HMDB0006938	Tartronate semialdehyde	C3H4O4	M+FA-H	149.0092	3.0
	HMDB0001352	Hydroxypyruvic acid	C3H4O4	M+FA-H	149.0092	3.0
149.0609	HMDB0000691	Malonic acid	C3H4O4	M+FA-H	149.0092	3.0
	HMDB0135239	4-(prop-2-en-1-yl)benzene-1,2-diol	C9H10O2	M-H	149.0608	0.6
	HMDB0176418	2-Nonene-4,6-diyne-1,9-diol	C9H10O2	M-H	149.0608	0.6
	HMDB0170980	4-[(1Z)-prop-1-en-1-yl]benzene-1,2-diol	C9H10O2	M-H	149.0608	0.6
	HMDB0170763	4-(oxiran-2-ylmethyl)phenol	C9H10O2	M-H	149.0608	0.6
	HMDB0146657	2-hydroxycinnamyl alcohol	C9H10O2	M-H	149.0608	0.6
	HMDB0146635	4-vinyl-3-methoxyphenol	C9H10O2	M-H	149.0608	0.6
	HMDB0135280	3-[(1E)-3-hydroxyprop-1-en-1-yl]phenol	C9H10O2	M-H	149.0608	0.6
	HMDB0135279	3-(4-hydroxyphenyl)propanal	C9H10O2	M-H	149.0608	0.6
	HMDB0135281	(3-phenyloxiran-2-yl)methanol	C9H10O2	M-H	149.0608	0.6
	HMDB0135278	3-(3-hydroxyphenyl)propanal	C9H10O2	M-H	149.0608	0.6
	HMDB0135277	3-hydroxy-3-phenylpropanal	C9H10O2	M-H	149.0608	0.6
	HMDB0135276	2-hydroxy-3-phenylpropanal	C9H10O2	M-H	149.0608	0.6
	HMDB0134027	2-(3-hydroxyprop-1-en-1-yl)phenol	C9H10O2	M-H	149.0608	0.6
	HMDB0134026	3-(2-hydroxyphenyl)propanal	C9H10O2	M-H	149.0608	0.6
	HMDB0125532	3-ethenyl-5-methoxyphenol	C9H10O2	M-H	149.0608	0.6
	HMDB0062349	4-Chromanol	C9H10O2	M-H	149.0608	0.6
	HMDB0177508	4-(3-methyloxiran-2-yl)phenol	C9H10O2	M-H	149.0608	0.6
	HMDB0032592	2'-Hydroxy-5'-methylacetophenone	C9H10O2	M-H	149.0608	0.6
	HMDB0033967	Ethyl benzoate	C9H10O2	M-H	149.0608	0.6
	HMDB0032570	4'-Methoxyacetophenone	C9H10O2	M-H	149.0608	0.6
	HMDB0032075	p-Tolyl acetate	C9H10O2	M-H	149.0608	0.6
	HMDB0040428	2-Phenylethyl formate	C9H10O2	M-H	149.0608	0.6
	HMDB0032073	o-Tolyl acetate	C9H10O2	M-H	149.0608	0.6
	HMDB0032569	2'-Methoxyacetophenone	C9H10O2	M-H	149.0608	0.6
	HMDB0033970	4-Ethoxybenzaldehyde	C9H10O2	M-H	149.0608	0.6
	HMDB0031310	Benzyl acetate	C9H10O2	M-H	149.0608	0.6
	HMDB0011743	2-Phenylpropionate	C9H10O2	M-H	149.0608	0.6
	HMDB0003654	4-Coumaryl alcohol	C9H10O2	M-H	149.0608	0.6
	HMDB0002237	3,4-Dimethylbenzoic acid	C9H10O2	M-H	149.0608	0.6
	HMDB0002222	3-Methylphenylacetic acid	C9H10O2	M-H	149.0608	0.6
	HMDB0002097	4-Ethylbenzoic acid	C9H10O2	M-H	149.0608	0.6
	HMDB0013744	2-Methoxy-4-vinylphenol	C9H10O2	M-H	149.0608	0.6
	HMDB0032617	Methyl phenylacetate	C9H10O2	M-H	149.0608	0.6
	HMDB0040925	2-(2-Furanyl)-3-methyl-2-butenal	C9H10O2	M-H	149.0608	0.6
	HMDB0135644	4-(3-hydroxyprop-1-en-1-yl)phenol	C9H10O2	M-H	149.0608	0.6
	HMDB0176419	6-(3-methyloxiran-2-yl)hexa-3,5-diyne-1-ol	C9H10O2	M-H	149.0608	0.6
	HMDB0038355	2-Ethyl-4-(2-furanyl)-2-propenal	C9H10O2	M-H	149.0608	0.6
	HMDB0037715	1-Phenylethyl formate	C9H10O2	M-H	149.0608	0.6
	HMDB0059824	4-Hydroxy-3-methylacetophenone	C9H10O2	M-H	149.0608	0.6
	HMDB0000764	Hydrocinnamic acid	C9H10O2	M-H	149.0608	0.6
	HMDB0034240	Styrene	C8H8	M+FA-H	149.0608	0.7
	HMDB0061975	1,3,7-Octatrien-5-yne	C8H8	M+FA-H	149.0608	0.7
	HMDB0133616	2-methyl-3-phenylpropan-1-ol	C10H14O	M-H	149.0972	0.1
	HMDB0163107	(2E,4Z,7Z)-deca-2,4,7,9-tetraen-1-ol	C10H14O	M-H	149.0972	0.1
	HMDB0034846	2-(4-Methylphenyl)-1-propanol	C10H14O	M-H	149.0972	0.1

149.0972	HMDB0036061	Safranal	C10H14O	M-H	149.0972	0.1
	HMDB0035824	Carvone	C10H14O	M-H	149.0972	0.1
	HMDB0036070	1-Acetyl-4-isopropenylcyclopentene	C10H14O	M-H	149.0972	0.1
	HMDB0035591	3-Caren-5-one	C10H14O	M-H	149.0972	0.1
	HMDB0029652	2-(4-Methylphenyl)-2-propanol	C10H14O	M-H	149.0972	0.1
	HMDB0035770	5-Isopropyl-2-methylphenol	C10H14O	M-H	149.0972	0.1
	HMDB0033544	(2E,4Z,7Z)-2,4,7-Decatrienal	C10H14O	M-H	149.0972	0.1
	HMDB0036999	Piperitenone	C10H14O	M-H	149.0972	0.1
	HMDB0035172	2,6,6-Trimethyl-1,4-cyclohexadiene-1-carboxaldehyde	C10H14O	M-H	149.0972	0.1
	HMDB0031570	2-Methyl-1-phenyl-2-propanol	C10H14O	M-H	149.0972	0.1
	HMDB0031817	Cuminyl alcohol	C10H14O	M-H	149.0972	0.1
	HMDB0037561	Linden ether	C10H14O	M-H	149.0972	0.1
	HMDB0036089	(R)-Menthofuran	C10H14O	M-H	149.0972	0.1
	HMDB0001878	Thymol	C10H14O	M-H	149.0972	0.1
	HMDB0003647	Perillyl aldehyde	C10H14O	M-H	149.0972	0.1
	HMDB0004487	(S)-Carvone	C10H14O	M-H	149.0972	0.1
	HMDB0061788	(S)-Carvone	C10H14O	M-H	149.0972	0.1
	HMDB0038913	4,6-Decadiyn-1-ol	C10H14O	M-H	149.0972	0.1
	HMDB0031613	4-Phenyl-2-butanol	C10H14O	M-H	149.0972	0.1
	HMDB0034921	Teresantalal	C10H14O	M-H	149.0972	0.1
	HMDB0035089	(R)-Carvone	C10H14O	M-H	149.0972	0.1
	HMDB0035761	(-)-Pinocarvone	C10H14O	M-H	149.0972	0.1
	HMDB0035250	Myrtenal	C10H14O	M-H	149.0972	0.1
	HMDB0032626	1-Methoxy-4-propylbenzene	C10H14O	M-H	149.0972	0.1
	HMDB0032063	4-tert-Butylphenol	C10H14O	M-H	149.0972	0.1
	HMDB0062147	Perillene	C10H14O	M-H	149.0972	0.1
	HMDB0032213	2-trans-4-trans-7-cis-Decatrienal	C10H14O	M-H	149.0972	0.1
151.0403	HMDB0182861	SCHEMBL437438	C8H8O3	M-H	151.0401	1.5
	HMDB0171094	ortho-vanillin	C8H8O3	M-H	151.0401	1.5
	HMDB0166108	5-hydroxy-2-methoxybenzaldehyde	C8H8O3	M-H	151.0401	1.5
	HMDB0172092	3-Hydroxy-4-methoxybenzaldehyde	C8H8O3	M-H	151.0401	1.5
	HMDB0168664	Methyl 3-hydroxybenzoate	C8H8O3	M-H	151.0401	1.5
	HMDB0150437	6-methylsalicylic acid	C8H8O3	M-H	151.0401	1.5
	HMDB0166107	4-hydroxy-2-methoxybenzaldehyde	C8H8O3	M-H	151.0401	1.5
	HMDB0166109	3-hydroxy-2-methoxybenzaldehyde	C8H8O3	M-H	151.0401	1.5
	HMDB0166106	2-hydroxy-6-methoxybenzaldehyde	C8H8O3	M-H	151.0401	1.5
	HMDB0146889	SCHEMBL2128735	C8H8O3	M-H	151.0401	1.5
	HMDB0146870	SCHEMBL3679957	C8H8O3	M-H	151.0401	1.5
	HMDB0137457	4-[(E)-2-hydroxyethenyl]benzene-1,2-diol	C8H8O3	M-H	151.0401	1.5
	HMDB0125528	5-ethenylbenzene-1,2,3-triol	C8H8O3	M-H	151.0401	1.5
	HMDB0183904	mandelate	C8H7O3	M-H	151.0401	1.5
	HMDB0183905	4-hydroxyphenylacetate	C8H7O3	M-H	151.0401	1.5
	HMDB0124926	Mandelic acid	C8H8O3	M-H	151.0401	1.5
	HMDB0034172	Methyl 2-hydroxybenzoate	C8H8O3	M-H	151.0401	1.5
	HMDB0032606	3-Methoxybenzoic acid	C8H8O3	M-H	151.0401	1.5
	HMDB0029657	2,4'-Dihydroxyacetophenone	C8H8O3	M-H	151.0401	1.5
	HMDB0041283	1-(2-Furanyl)-1,3-butanedione	C8H8O3	M-H	151.0401	1.5
	HMDB0032919	Ethyl 2-furanyl diketone	C8H8O3	M-H	151.0401	1.5
	HMDB0036907	2-Propenyl 2-furancarboxylate	C8H8O3	M-H	151.0401	1.5
	HMDB0012308	Vanillin	C8H8O3	M-H	151.0401	1.5
	HMDB0032604	2-Methoxybenzoic acid	C8H8O3	M-H	151.0401	1.5
	HMDB0004815	4-Hydroxy-3-methylbenzoic acid	C8H8O3	M-H	151.0401	1.5
	HMDB0003791	3,4-Dihydroxyphenylacetaldehyde	C8H8O3	M-H	151.0401	1.5
	HMDB0002390	3-Cresotinic acid	C8H8O3	M-H	151.0401	1.5
	HMDB0000669	ortho-Hydroxyphenylacetic acid	C8H8O3	M-H	151.0401	1.5
	HMDB0000440	3-Hydroxyphenylacetic acid	C8H8O3	M-H	151.0401	1.5
	HMDB0000020	p-Hydroxyphenylacetic acid	C8H8O3	M-H	151.0401	1.5
	HMDB0001101	p-Anisic acid	C8H8O3	M-H	151.0401	1.5
	HMDB0029661	3',4'-Dihydroxyacetophenone	C8H8O3	M-H	151.0401	1.5
	HMDB0029662	3',5'-Dihydroxyacetophenone	C8H8O3	M-H	151.0401	1.5
	HMDB0062005	Dihydroxyacetophenone	C8H8O3	M-H	151.0401	1.5
	HMDB0060390	4-Hydroxyphenyl acetate	C8H8O3	M-H	151.0401	1.5
	HMDB0062635	(R)-mandelic Acid	C8H8O3	M-H	151.0401	1.5
	HMDB0032399	Methyl furfuracrylate	C8H8O3	M-H	151.0401	1.5
	HMDB0172091	2-Hydroxy-4-methoxybenzaldehyde	C8H8O3	M-H	151.0401	1.5

	HMDB0029660	2',6'-Dihydroxyacetophenone	C8H8O3	M-H	151.0401	1.5
	HMDB0029659	2',4'-Dihydroxyacetophenone	C8H8O3	M-H	151.0401	1.5
	HMDB0029658	2',3'-Dihydroxyacetophenone	C8H8O3	M-H	151.0401	1.5
	HMDB0031609	Phenoxyacetic acid	C8H8O3	M-H	151.0401	1.5
	HMDB0032594	2-(Hydroxymethyl)benzoic acid	C8H8O3	M-H	151.0401	1.5
	HMDB0033003	1-(5-Methyl-2-furanyl)-1,2-propanedione	C8H8O3	M-H	151.0401	1.5
	HMDB0032629	2',5'-Dihydroxyacetophenone	C8H8O3	M-H	151.0401	1.5
	HMDB0032572	Methylparaben	C8H8O3	M-H	151.0401	1.5
	HMDB0000703	Mandelic acid	C8H8O3	M-H	151.0401	1.5
	HMDB0006115	Benzaldehyde	C7H6O	M+FA-H	151.0401	1.5
151.0765	HMDB0150177	3-phenylpropane-1,2-diol	C9H12O2	M-H	151.0765	0.3
	HMDB0175243	SCHEMBL9169343	C9H12O2	M-H	151.0765	0.3
	HMDB0175244	4-(1-hydroxypropan-2-yl)phenol	C9H12O2	M-H	151.0765	0.3
	HMDB0175240	2-Phenyl-1,2-propanediol	C9H12O2	M-H	151.0765	0.3
	HMDB0175241	2-PHENYL-1,3-PROPANEDIOL	C9H12O2	M-H	151.0765	0.3
	HMDB0173825	1-[4-(Hydroxymethyl)phenyl]ethanol	C9H12O2	M-H	151.0765	0.3
	HMDB0173826	1-(4-methylphenyl)ethane-1,2-diol	C9H12O2	M-H	151.0765	0.3
	HMDB0150180	2-(3-hydroxypropyl)phenol	C9H12O2	M-H	151.0765	0.3
	HMDB0150178	1-Phenylpropane-1,3-diol	C9H12O2	M-H	151.0765	0.3
	HMDB0150179	3-(3-hydroxypropyl)phenol	C9H12O2	M-H	151.0765	0.3
	HMDB0146637	4-ETHYL-3-METHOXYPHENOL	C9H12O2	M-H	151.0765	0.3
	HMDB0125537	3-ethyl-5-methoxyphenol	C9H12O2	M-H	151.0765	0.3
	HMDB0032599	3-(4-Hydroxyphenyl)-1-propanol	C9H12O2	M-H	151.0765	0.3
	HMDB0040216	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	C9H12O2	M-H	151.0765	0.3
	HMDB0039801	1-(2-Furanyl)-1-pentanone	C9H12O2	M-H	151.0765	0.3
	HMDB0036227	2-Propenyl 2,4-hexadienoate	C9H12O2	M-H	151.0765	0.3
	HMDB0039956	4-(Ethoxymethyl)phenol	C9H12O2	M-H	151.0765	0.3
	HMDB0036169	3-(5-Methyl-2-furanyl)butanal	C9H12O2	M-H	151.0765	0.3
	HMDB0041326	(Dimethoxymethyl)benzene	C9H12O2	M-H	151.0765	0.3
	HMDB0040449	2-(Ethoxymethyl)phenol	C9H12O2	M-H	151.0765	0.3
	HMDB0032132	2-Isopropyl-1,4-benzenediol	C9H12O2	M-H	151.0765	0.3
	HMDB0040175	4-Ethyl-2-methoxyphenol	C9H12O2	M-H	151.0765	0.3
	HMDB0168680	(4-ethoxyphenyl)methanol	C9H12O2	M-H	151.0765	0.3
	HMDB0059853	3,5-Dimethoxytoluene	C9H12O2	M-H	151.0765	0.3
	HMDB0041804	2-Isopropoxyphenol	C9H12O2	M-H	151.0765	0.3
	HMDB0059810	m-Xylene	C8H10	M+FA-H	151.0765	0.3
	HMDB0059924	p-Xylene	C8H10	M+FA-H	151.0765	0.3
	HMDB0059851	o-Xylene	C8H10	M+FA-H	151.0765	0.3
	HMDB0059905	Ethylbenzene	C8H10	M+FA-H	151.0765	0.3
	HMDB0182523	p-Menth-1(7)-en-2-one	C10H16O	M-H	151.1128	2.4
	HMDB0187618	isopiperitenol	C10H16O	M-H	151.1128	2.4
	HMDB0187619	2-methyl-2-(4-methylcyclohex-3-en-1-yl)oxirane	C10H16O	M-H	151.1128	2.4
	HMDB0182597	SCHEMBL13931696	C10H16O	M-H	151.1128	2.4
	HMDB0182548	2-[(1R)-4-methylcyclohexa-2,4-dien-1-yl]propan-1-ol	C10H16O	M-H	151.1128	2.4
	HMDB0182545	(6S)-3-methyl-6-(propan-2-yl)cyclohexa-2,4-dien-1-ol	C10H16O	M-H	151.1128	2.4
	HMDB0182547	(5S)-2-methyl-5-(propan-2-yl)-7-oxabicyclo[4.1]hept-2-ene	C10H16O	M-H	151.1128	2.4
	HMDB0182544	SCHEMBL4374431	C10H16O	M-H	151.1128	2.4
	HMDB0182546	(4S)-1-methyl-4-(propan-2-yl)-7-oxabicyclo[4.1]hept-2-ene	C10H16O	M-H	151.1128	2.4
	HMDB0182543	(R)-p-Mentha-1,5-diene-8-ol	C10H16O	M-H	151.1128	2.4
	HMDB0182542	ZINC321828	C10H16O	M-H	151.1128	2.4
	HMDB0181809	2-[(1R)-4-methylidenebicyclo[3.1]hexan-1-yl]propan-1-ol	C10H16O	M-H	151.1128	2.4
	HMDB0181808	(1S)-4-methylidene-1-(propan-2-yl)bicyclo[3.1]hexan-6-ol	C10H16O	M-H	151.1128	2.4
	HMDB0181807	(5S)-2-methylidene-5-(propan-2-yl)bicyclo[3.1]hexan-1-ol	C10H16O	M-H	151.1128	2.4
	HMDB0181806	(1R)-4-methylidene-1-(propan-2-yl)bicyclo[3.1]hexan-2-ol	C10H16O	M-H	151.1128	2.4
	HMDB0181805	AC1O5B2Q	C10H16O	M-H	151.1128	2.4
	HMDB0181804	2-[(1R)-4-methylidenebicyclo[3.1]hexan-1-yl]propan-2-ol	C10H16O	M-H	151.1128	2.4
	HMDB0163091	(4Z,7Z)-deca-4,7-dienal	C10H16O	M-H	151.1128	2.4
	HMDB0163092	SCHEMBL5863926	C10H16O	M-H	151.1128	2.4

HMDB0030893	Isocitral	C10H16O	M-H	151.1128	2.4
HMDB0036115	(-)-3-Isothujone	C10H16O	M-H	151.1128	2.4
HMDB0036598	(E,E)-2,4-Decadienal	C10H16O	M-H	151.1128	2.4
HMDB0035656	3-Pinanone	C10H16O	M-H	151.1128	2.4
HMDB0035737	(R)-Piperitone	C10H16O	M-H	151.1128	2.4
HMDB0035738	(R)-Piperitone	C10H16O	M-H	151.1128	2.4
HMDB0038290	Photocitral A	C10H16O	M-H	151.1128	2.4
HMDB0035743	Pinocarveol	C10H16O	M-H	151.1128	2.4
HMDB0037025	Hop ether	C10H16O	M-H	151.1128	2.4
HMDB0032120	2,6-Dimethyl-1,7-octadien-3-one	C10H16O	M-H	151.1128	2.4
HMDB0036127	(-)-Pinocamphone	C10H16O	M-H	151.1128	2.4
HMDB0035744	(-)-Isopinocamphone	C10H16O	M-H	151.1128	2.4
HMDB0037009	Terpinolene oxide	C10H16O	M-H	151.1128	2.4
HMDB0037024	4-Acetyl-1,4-dimethyl-1-cyclohexene	C10H16O	M-H	151.1128	2.4
HMDB0034974	(R)-Carvotanacetone	C10H16O	M-H	151.1128	2.4
HMDB0040766	Anethofuran	C10H16O	M-H	151.1128	2.4
HMDB0035092	cis-Citral	C10H16O	M-H	151.1128	2.4
HMDB0037280	Junionone	C10H16O	M-H	151.1128	2.4
HMDB0036129	Verbenol	C10H16O	M-H	151.1128	2.4
HMDB0034973	(R)-Campholenic aldehyde	C10H16O	M-H	151.1128	2.4
HMDB0034985	(+)-Fenchone	C10H16O	M-H	151.1128	2.4
HMDB0034975	Piperitone	C10H16O	M-H	151.1128	2.4
HMDB0036128	(-)-trans-Pinocarveol	C10H16O	M-H	151.1128	2.4
HMDB0038557	xi-3,6-Dihydro-4-methyl-2-(2-methyl-1-propenyl)-2H-pyran	C10H16O	M-H	151.1128	2.4
HMDB0035622	(+)-cis-Carveol	C10H16O	M-H	151.1128	2.4
HMDB0036080	(1S,4S)-Dihydrocarvone	C10H16O	M-H	151.1128	2.4
HMDB0036114	(-)-3-Thujone	C10H16O	M-H	151.1128	2.4
HMDB0035054	(1S,4R)-p-Mentha-2,8-dien-1-ol	C10H16O	M-H	151.1128	2.4
HMDB0035077	(1R,4R)-p-Mentha-2,8-dien-1-ol	C10H16O	M-H	151.1128	2.4
HMDB0003667	Alpha-Pinene-oxide	C10H16O	M-H	151.1128	2.4
HMDB0003634	Perillyl alcohol	C10H16O	M-H	151.1128	2.4
HMDB0003450	(-)-trans-Carveol	C10H16O	M-H	151.1128	2.4
HMDB0035741	(-)-trans-Isopulegone	C10H16O	M-H	151.1128	2.4
HMDB0035600	(S)-Phellandral	C10H16O	M-H	151.1128	2.4
HMDB0034715	p-Mentha-1(6),8-dien-3-ol	C10H16O	M-H	151.1128	2.4
HMDB0037015	p-Mentha-1,8-dien-4-ol	C10H16O	M-H	151.1128	2.4
HMDB0037303	xi-p-Mentha-1(7),2-dien-4-ol	C10H16O	M-H	151.1128	2.4
HMDB0038251	xi-Pinol	C10H16O	M-H	151.1128	2.4
HMDB0035241	(Z)-2-Methyl-6-methylene-2,7-octadien-1-ol	C10H16O	M-H	151.1128	2.4
HMDB0037010	(2S,4R)-p-Mentha-1(7),8-dien-2-ol	C10H16O	M-H	151.1128	2.4
HMDB0035277	(2S,4R)-p-Mentha-1(7),5-dien-2-ol	C10H16O	M-H	151.1128	2.4
HMDB0036044	Marmelo oxide A	C10H16O	M-H	151.1128	2.4
HMDB0035203	(S)-9,-Cyclo-p-menth-1-en-4-ol	C10H16O	M-H	151.1128	2.4
HMDB0037302	xi-p-Mentha-3,8-dien-1-ol	C10H16O	M-H	151.1128	2.4
HMDB0035120	Dehydrolinalool	C10H16O	M-H	151.1128	2.4
HMDB0039008	3,4-Epoxy-p-menth-1(7)-ene	C10H16O	M-H	151.1128	2.4
HMDB0059838	Camphor	C10H16O	M-H	151.1128	2.4
HMDB0059827	3-Cyclohexene-1-carboxaldehyde, 1,3,4-trimethyl-	C10H16O	M-H	151.1128	2.4
HMDB0059761	4-(1-Methylethyl)-1-cyclohexene-4-carboxaldehyde	C10H16O	M-H	151.1128	2.4
HMDB0041631	3-Thujanone	C10H16O	M-H	151.1128	2.4
HMDB0059608	(+)-trans-Carveol	C10H16O	M-H	151.1128	2.4
HMDB0032242	(E)-3,7-Dimethyl-1,5,7-octatrien-3-ol	C10H16O	M-H	151.1128	2.4
HMDB0059875	Carvotanacetone	C10H16O	M-H	151.1128	2.4
HMDB0035604	Pulegone	C10H16O	M-H	151.1128	2.4
HMDB0061794	Pulegone	C10H16O	M-H	151.1128	2.4
HMDB0061292	SCHEMBL6943113	C10H16O	M-H	151.1128	2.4
HMDB0032536	2-(trans-2-Pentenyl)cyclopentanone	C10H16O	M-H	151.1128	2.4
HMDB0059885	p-Menth-1-en-9-al	C10H16O	M-H	151.1128	2.4
HMDB0031854	3-Methyl-5-propyl-2-cyclohexen-1-one	C10H16O	M-H	151.1128	2.4
HMDB0041013	Isocyclocitral	C10H16O	M-H	151.1128	2.4
HMDB0035100	2-Pinen--ol	C10H16O	M-H	151.1128	2.4
HMDB0035125	Darwinol	C10H16O	M-H	151.1128	2.4
HMDB0035280	Teresantalol	C10H16O	M-H	151.1128	2.4
HMDB0035078	Geranial	C10H16O	M-H	151.1128	2.4

	HMDB0036083	Carveol	C10H16O	M-H	151.1128	2.4
	HMDB0037008	6,8-Epoxy-p-menth-2-ene	C10H16O	M-H	151.1128	2.4
	HMDB0036082	(-)-cis-Carveol	C10H16O	M-H	151.1128	2.4
	HMDB0035158	1,2-Epoxy-p-menth-8-ene	C10H16O	M-H	151.1128	2.4
	HMDB0036085	Dehydro-1,8-cineole	C10H16O	M-H	151.1128	2.4
	HMDB0037017	(R)-p-Mentha-1,8-dien--ol	C10H16O	M-H	151.1128	2.4
	HMDB0036079	Dihydrocarvone	C10H16O	M-H	151.1128	2.4
	HMDB0035706	alpha-Cyclocitral	C10H16O	M-H	151.1128	2.4
	HMDB0036113	(+)-3-Thujone	C10H16O	M-H	151.1128	2.4
	HMDB0039816	2-Hexylfuran	C10H16O	M-H	151.1128	2.4
	HMDB0041011	beta-Cyclocitral	C10H16O	M-H	151.1128	2.4
	HMDB0034916	cis-2-Thujen-4-ol	C10H16O	M-H	151.1128	2.4
	HMDB0037172	Tetrahydro-5-isopropenyl-2-methyl-2-vinylfuran	C10H16O	M-H	151.1128	2.4
	HMDB0030892	p-Menth-3-en-9-al	C10H16O	M-H	151.1128	2.4
	HMDB0036087	(R)-p-Mentha-1,8-dien-7-ol	C10H16O	M-H	151.1128	2.4
	HMDB0036088	(R)-p-Mentha-1,8-dien-7-ol	C10H16O	M-H	151.1128	2.4
152.0353	HMDB0177404	4-(Hydroxyamino)benzoic acid	C7H7NO3	M-H	152.0353	-0.1
	HMDB0164041	2-(hydroxyamino)benzoic acid	C7H7NO3	M-H	152.0353	-0.1
	HMDB0059749	6-Methoxy-pyridine-3-carboxylic acid	C7H7NO3	M-H	152.0353	-0.1
	HMDB0001972	3-Aminosalicylic acid	C7H7NO3	M-H	152.0353	-0.1
	HMDB0059811	2-Nitro-p-cresol	C7H7NO3	M-H	152.0353	-0.1
	HMDB0001476	3-Hydroxyanthranilic acid	C7H7NO3	M-H	152.0353	-0.1
	HMDB0014389	Mesalazine	C7H7NO3	M-H	152.0353	-0.1
	HMDB0014378	Aminosalicylic Acid	C7H7NO3	M-H	152.0353	-0.1
152.9961	HMDB0172016	(1Z)-3-chloroprop-1-ene-1,2-diol	C3H5ClO2	M+FA-H	152.9960	0.6
	HMDB0172017	1-chloro-2,3-epoxypropanol	C3H5ClO2	M+FA-H	152.9960	0.6
	HMDB0030967	2,4,6-Octatriynoic acid	C8H4O2	M+Na-2H	152.9958	2.0
153.0557	HMDB0001858	p-Cresol	C7H8O	M+FA-H	153.0557	-0.1
	HMDB0033895	Anisole	C7H8O	M+FA-H	153.0557	-0.1
	HMDB0002048	m-Cresol	C7H8O	M+FA-H	153.0557	-0.1
	HMDB0003119	Benzyl alcohol	C7H8O	M+FA-H	153.0557	-0.1
	HMDB0002055	o-Cresol	C7H8O	M+FA-H	153.0557	-0.1
	HMDB0131231	5-methoxy-4-methylbenzene-1,3-diol	C8H10O3	M-H	153.0557	-0.1
	HMDB0131232	5-methoxy-2-methylbenzene-1,3-diol	C8H10O3	M-H	153.0557	-0.1
	HMDB0169080	2-Hydroxy-3-methoxybenzyl alcohol	C8H10O3	M-H	153.0557	-0.1
	HMDB0146894	4-Ethylpyrogallol	C8H10O3	M-H	153.0557	-0.1
	HMDB0146874	SCHEMBL093	C8H10O3	M-H	153.0557	-0.1
	HMDB0125534	5-ethylbenzene-1,2,3-triol	C8H10O3	M-H	153.0557	-0.1
	HMDB0131479	2,3-dimethoxyphenol	C8H10O3	M-H	153.0557	-0.1
	HMDB0059966	3,5-Dimethoxyphenol	C8H10O3	M-H	153.0557	-0.1
	HMDB0037724	Propyl 2-furoate	C8H10O3	M-H	153.0557	-0.1
	HMDB0034158	2,6-Dimethoxyphenol	C8H10O3	M-H	153.0557	-0.1
	HMDB0037728	2-Furanylmethyl propanoate	C8H10O3	M-H	153.0557	-0.1
	HMDB0032012	4-Hydroxy-3-methoxybenzenemethanol	C8H10O3	M-H	153.0557	-0.1
	HMDB0030570	Sylvopinol	C8H10O3	M-H	153.0557	-0.1
	HMDB0005784	Hydroxytyrosol	C8H10O3	M-H	153.0557	-0.1
	HMDB0126617	2,4-dimethylbenzene-1,3,5-triol	C8H10O3	M-H	153.0557	-0.1
	HMDB0135785	1-(4-hydroxyphenyl)ethane-1,2-diol	C8H10O3	M-H	153.0557	-0.1
153.0671	HMDB0035289	2,5-Dimethylpyrazine	C6H8N2	M+FA-H	153.0669	1.0
	HMDB0031849	2-Ethylpyrazine	C6H8N2	M+FA-H	153.0669	1.0
	HMDB0032971	2,3-Dimethylpyrazine	C6H8N2	M+FA-H	153.0669	1.0
	HMDB0035248	2,6-Dimethylpyrazine	C6H8N2	M+FA-H	153.0669	1.0
	HMDB0061897	(Z)-1,3-Octadiene	C8H12	M+FA-H	153.0921	0.0
	HMDB0167032	2E,6Z-nonadienoic acid	C9H14O2	M-H	153.0921	0.0
	HMDB0180434	(2E,4E)-9-hydroxynona-2,4-dienal	C9H14O2	M-H	153.0921	0.0
	HMDB0180433	trans-4,5-Epoxy-(E)-nonenal	C9H14O2	M-H	153.0921	0.0
	HMDB0180432	3-[(1E)-hex-1-en-1-yl]oxirane-2-carbaldehyde	C9H14O2	M-H	153.0921	0.0
	HMDB0180430	(2E,4E)-6-hydroxynona-2,4-dienal	C9H14O2	M-H	153.0921	0.0
	HMDB0180431	SCHEMBL179742	C9H14O2	M-H	153.0921	0.0
	HMDB0167038	(2E,6Z)-9-hydroxynona-2,6-dienal	C9H14O2	M-H	153.0921	0.0
	HMDB0167035	(2E,6Z)-5-hydroxynona-2,6-dienal	C9H14O2	M-H	153.0921	0.0
	HMDB0167034	(2E,6Z)-8-hydroxynona-2,6-dienal	C9H14O2	M-H	153.0921	0.0
	HMDB0167037	(2E)-5-(3-ethyloxiran-2-yl)pent-2-enal	C9H14O2	M-H	153.0921	0.0
	HMDB0167036	3-[(3Z)-hex-3-en-1-yl]oxirane-2-carbaldehyde	C9H14O2	M-H	153.0921	0.0
	HMDB0167033	(2E,6Z)-4-hydroxynona-2,6-dienal	C9H14O2	M-H	153.0921	0.0

HMDB0164921	1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O2	M-H	153.0921	0.0
HMDB0163467	(2Z)-2-methylocta-2,7-dienoic acid	C9H14O2	M-H	153.0921	0.0
HMDB0032442	2-Nonenoic acid gamma-lactone	C9H14O2	M-H	153.0921	0.0
HMDB0032314	2,4-Hexadienyl propionate	C9H14O2	M-H	153.0921	0.0
HMDB0040285	Anapear	C9H14O2	M-H	153.0921	0.0
HMDB0036177	3,5,5-Trimethyl-1,2-cyclohexanedione	C9H14O2	M-H	153.0921	0.0
HMDB0036239	3,5,5-Trimethyl-1,2-cyclohexanedione	C9H14O2	M-H	153.0921	0.0
HMDB0037276	Octahydro-2H-1-benzopyran-2-one	C9H14O2	M-H	153.0921	0.0
HMDB0031302	Methyl 2-octynoate	C9H14O2	M-H	153.0921	0.0
HMDB0038268	Allyl hexenoate	C9H14O2	M-H	153.0921	0.0
HMDB0038697	xi-2,2,6-Trimethyl-1,4-cyclohexanedione	C9H14O2	M-H	153.0921	0.0
HMDB0060285	4-Oxo-2-nonenal	C9H14O2	M-H	153.0921	0.0
HMDB0035135	(E)-2,6-Dimethyl-2,5-heptadienoic acid	C9H14O2	M-H	153.0921	0.0
HMDB0061802	5-Methyl-2-(1-methylethyl)-cyclohexanone	C10H18O	M-H	153.1285	0.1
HMDB0187564	CTK8I1689	C10H18O	M-H	153.1285	0.1
HMDB0163116	(4Z,7Z)-deca-4,7-dien-1-ol	C10H18O	M-H	153.1285	0.1
HMDB0032530	(+)-thujan-3-ol	C10H18O	M-H	153.1285	0.1
HMDB0035815	(+)-Isoborneol	C10H18O	M-H	153.1285	0.1
HMDB0036100	3,7-Dimethyl-1,6-octadien-3-ol	C10H18O	M-H	153.1285	0.1
HMDB0035825	(-)-Dihydrocarveol	C10H18O	M-H	153.1285	0.1
HMDB0035783	(+)-Menthone	C10H18O	M-H	153.1285	0.1
HMDB0037016	p-Menth-1-en-5-ol	C10H18O	M-H	153.1285	0.1
HMDB0035954	(1R*,3R*,6S*)-3-Caranol	C10H18O	M-H	153.1285	0.1
HMDB0035820	(R)-Citronellal	C10H18O	M-H	153.1285	0.1
HMDB0035842	(R)-Citronellal	C10H18O	M-H	153.1285	0.1
HMDB0034848	9-Decenal	C10H18O	M-H	153.1285	0.1
HMDB0037019	6,8-Epoxy-p-menthane	C10H18O	M-H	153.1285	0.1
HMDB0036077	p-Menth-8-en-3-ol	C10H18O	M-H	153.1285	0.1
HMDB0034976	(-)-Borneol	C10H18O	M-H	153.1285	0.1
HMDB0035818	(-)-Borneol	C10H18O	M-H	153.1285	0.1
HMDB0037048	m-Menth-1-en-8-ol	C10H18O	M-H	153.1285	0.1
HMDB0032118	2,6-Dimethyl-7-octen-3-one	C10H18O	M-H	153.1285	0.1
HMDB0035841	Citronellal	C10H18O	M-H	153.1285	0.1
HMDB0037007	p-Menth-1-en-9-ol	C10H18O	M-H	153.1285	0.1
HMDB0036991	delta-Terpineol	C10H18O	M-H	153.1285	0.1
HMDB0036993	gamma-Terpineol	C10H18O	M-H	153.1285	0.1
HMDB0036097	Rose oxide	C10H18O	M-H	153.1285	0.1
HMDB0037133	Linaloyl oxide	C10H18O	M-H	153.1285	0.1
HMDB0036096	1,4-Cineole	C10H18O	M-H	153.1285	0.1
HMDB0035819	(-)-Isoborneol	C10H18O	M-H	153.1285	0.1
HMDB0041034	(4Z,7Z)-4,7-Decadien-1-ol	C10H18O	M-H	153.1285	0.1
HMDB0031410	3-Decen-2-one	C10H18O	M-H	153.1285	0.1
HMDB0037049	(R)-m-Menth-1(6)-en-8-ol	C10H18O	M-H	153.1285	0.1
HMDB0038025	xi-p-Menth-3-en-1-ol	C10H18O	M-H	153.1285	0.1
HMDB0035861	trans-(-)-p-Menth-1-en-3-ol	C10H18O	M-H	153.1285	0.1
HMDB0005812	Geraniol	C10H18O	M-H	153.1285	0.1
HMDB0004043	alpha-Terpineol	C10H18O	M-H	153.1285	0.1
HMDB0036126	(-)-Pinocampheol	C10H18O	M-H	153.1285	0.1
HMDB0036112	(1R,4S,5R)-4-Thujanol	C10H18O	M-H	153.1285	0.1
HMDB0036068	Campholenic alcohol	C10H18O	M-H	153.1285	0.1
HMDB0035955	(1R*,2S*,3S*,6S*)-2-Caranol	C10H18O	M-H	153.1285	0.1
HMDB0036196	(2E,4E)-2,4-Decadien-1-ol	C10H18O	M-H	153.1285	0.1
HMDB0037047	(-)-trans-m-Menth-8-en-1-ol	C10H18O	M-H	153.1285	0.1
HMDB0004472	Eucalyptol	C10H18O	M-H	153.1285	0.1
HMDB0059869	p-tert-Butylcyclohexanone	C10H18O	M-H	153.1285	0.1
HMDB0059881	Ocimenol	C10H18O	M-H	153.1285	0.1
HMDB0036086	(S)-alpha-Terpineol	C10H18O	M-H	153.1285	0.1
HMDB0035833	p-Menth-1-en-4-ol	C10H18O	M-H	153.1285	0.1
HMDB0035272	p-Menthan-2-one	C10H18O	M-H	153.1285	0.1
HMDB0036107	Myrcenol	C10H18O	M-H	153.1285	0.1
HMDB0036101	(R)-3,7-Dimethyl-1,6-octadien-3-ol	C10H18O	M-H	153.1285	0.1
HMDB0036102	(R)-3,7-Dimethyl-1,6-octadien-3-ol	C10H18O	M-H	153.1285	0.1
HMDB0030999	2-Decenal	C10H18O	M-H	153.1285	0.1
HMDB0035155	beta-Geraniol	C10H18O	M-H	153.1285	0.1
HMDB0041014	4-Decenal	C10H18O	M-H	153.1285	0.1

	HMDB0037215	trans-beta-Terpineol	C10H18O	M-H	153.1285	0.1
	HMDB0037161	2-Isopropyl-5-methyl-2-hexenal	C10H18O	M-H	153.1285	0.1
	HMDB0035823	(S)-p-Menth-1-en-4-ol	C10H18O	M-H	153.1285	0.1
	HMDB0036041	(R)-Lavandulol	C10H18O	M-H	153.1285	0.1
	HMDB0034972	Isomenthone	C10H18O	M-H	153.1285	0.1
	HMDB0034932	Fenchol	C10H18O	M-H	153.1285	0.1
	HMDB0035162	(-)-Menthone	C10H18O	M-H	153.1285	0.1
	HMDB0059864	(-)-Menthone	C10H18O	M-H	153.1285	0.1
	HMDB0035838	Piperitol	C10H18O	M-H	153.1285	0.1
	HMDB0038185	Ocimen quintoxide	C10H18O	M-H	153.1285	0.1
	HMDB0036078	(-)-Isopulegol	C10H18O	M-H	153.1285	0.1
	HMDB0034969	(-)-Carvomenthone	C10H18O	M-H	153.1285	0.1
	HMDB0036996	cis-beta-Terpineol	C10H18O	M-H	153.1285	0.1
	HMDB0037214	cis-beta-Terpineol	C10H18O	M-H	153.1285	0.1
	HMDB0040448	2-(1-Methylpropyl)cyclohexanone	C10H18O	M-H	153.1285	0.1
	HMDB0037006	cis-Isopulegone	C10H18O	M-H	153.1285	0.1
155.0352	HMDB0172619	SCHEMBL17148379	C7H8O4	M-H	155.0350	1.4
	HMDB0172142	(furan-2-yl)methyl 2-hydroxyacetate	C7H8O4	M-H	155.0350	1.4
	HMDB0140891	5-methoxybenzene-1,2,3-triol	C7H8O4	M-H	155.0350	1.4
	HMDB0140890	6-methoxybenzene-1,2,4-triol	C7H8O4	M-H	155.0350	1.4
	HMDB0125077	2-methoxybenzene-1,3,5-triol	C7H8O4	M-H	155.0350	1.4
	HMDB0059731	2,3-Methyleneglutaric acid	C7H8O4	M-H	155.0350	1.4
	HMDB0029610	Ascladiol	C7H8O4	M-H	155.0350	1.4
	HMDB0125064	4-methoxybenzene-1,2,3-triol	C7H8O4	M-H	155.0350	1.4
	HMDB0002434	Hydroquinone	C6H6O2	M+FA-H	155.0350	1.4
	HMDB0031180	(E,E)-2,4-Hexadienedial	C6H6O2	M+FA-H	155.0350	1.4
	HMDB0033127	2-Acetylfuran	C6H6O2	M+FA-H	155.0350	1.4
	HMDB0033002	5-Methyl-2-furancarboxaldehyde	C6H6O2	M+FA-H	155.0350	1.4
	HMDB0032037	1,3-Benzenediol	C6H6O2	M+FA-H	155.0350	1.4
	HMDB0000957	Pyrocatechol	C6H6O2	M+FA-H	155.0350	1.4
	HMDB0187589	2-Cyclohexene-1,4-dione	C6H6O2	M+FA-H	155.0350	1.4
155.0463	HMDB0000544	5-Hydroxymethyl-4-methyluracil	C6H8N2O3	M-H	155.0462	0.5
	HMDB0185113	AKO22715792	C6H8N2O3	M-H	155.0462	0.5
	HMDB0062719	3-(5-hydroxy-1H-imidazol-4-yl)propanoic acid	C6H8N2O3	M-H	155.0462	0.5
	HMDB0001014	4-Imidazolone-5-propionic acid	C6H8N2O3	M-H	155.0462	0.5
	HMDB0002320	Imidazolelactic acid	C6H8N2O3	M-H	155.0462	0.5
	HMDB0003905	Imidazole-4-acetaldehyde	C5H6N2O	M+FA-H	155.0462	0.6
	HMDB0033156	Methoxypyrazine	C5H6N2O	M+FA-H	155.0462	0.6
	HMDB0060741	3-Hydroxy-4-aminopyridine	C5H6N2O	M+FA-H	155.0462	0.6
155.0713	HMDB0029728	2-Ethyl-5-methylfuran	C7H10O	M+FA-H	155.0714	-0.4
	HMDB0061891	(E,Z)-2,4-Heptadienal	C7H10O	M+FA-H	155.0714	-0.4
	HMDB0040278	2-Isopropylfuran	C7H10O	M+FA-H	155.0714	-0.4
	HMDB0031541	3-Methyl-2-cyclohexen-1-one	C7H10O	M+FA-H	155.0714	-0.4
	HMDB0029721	2,3,5-Trimethylfuran	C7H10O	M+FA-H	155.0714	-0.4
	HMDB0040277	2-Propylfuran	C7H10O	M+FA-H	155.0714	-0.4
	HMDB0159132	2-(4-oxocyclohexyl)acetic Acid	C8H12O3	M-H	155.0714	-0.4
	HMDB0031101	8-Hydroxy-5,6-octadienoic acid	C8H12O3	M-H	155.0714	-0.4
	HMDB0032232	2,5-Dimethyl-4-ethoxy-3(2H)-furanone	C8H12O3	M-H	155.0714	-0.4
	HMDB0061900	2,4-Octadiene	C8H14	M+FA-H	155.1078	-0.3
	HMDB0061902	2,5-Dimethyl-2,4-hexadiene	C8H14	M+FA-H	155.1078	-0.3
	HMDB0061899	2-(Methylenebutyl)-cyclopropane	C8H14	M+FA-H	155.1078	-0.3
	HMDB0061901	Dimethylhexa-1,4-diene	C8H14	M+FA-H	155.1078	-0.3
	HMDB0040966	1,3-Octadiene	C8H14	M+FA-H	155.1078	-0.3
	HMDB0166519	6-(hydroxymethyl)-2,2-dimethylcyclohexan-1-one	C9H16O2	M-H	155.1078	-0.3
	HMDB0167040	(6Z)-5-hydroxynon-6-enal	C9H16O2	M-H	155.1078	-0.3
	HMDB0167039	(6Z)-8-hydroxynon-6-enal	C9H16O2	M-H	155.1078	-0.3
	HMDB0167041	5-(3-ethyloxiran-2-yl)pentanal	C9H16O2	M-H	155.1078	-0.3
	HMDB0167042	(6Z)-9-hydroxynon-6-enal	C9H16O2	M-H	155.1078	-0.3
	HMDB0167045	(2E,6Z)-nona-2,6-diene-1,9-diol	C9H16O2	M-H	155.1078	-0.3
	HMDB0167043	(6Z)-2-hydroxynon-6-enal	C9H16O2	M-H	155.1078	-0.3
	HMDB0166518	2-(hydroxymethyl)-2,6-dimethylcyclohexan-1-one	C9H16O2	M-H	155.1078	-0.3
	HMDB0163459	(2Z)-8-hydroxy-2-methyloct-2-enal	C9H16O2	M-H	155.1078	-0.3
	HMDB0163454	SCHEMBL11263	C9H16O2	M-H	155.1078	-0.3
	HMDB0163455	(2Z)-2-(hydroxymethyl)oct-2-enal	C9H16O2	M-H	155.1078	-0.3
	HMDB0163458	2-methyl-3-pentyloxirane-2-carbaldehyde	C9H16O2	M-H	155.1078	-0.3

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HMDB0163457	(2Z)-7-hydroxy-2-methyloct-2-enal	C9H16O2	M-H	155.1078	-0.3
HMDB0163456	(2Z)-4-hydroxy-2-methyloct-2-enal	C9H16O2	M-H	155.1078	-0.3
HMDB0179750	7-hydroxynon-8-en-3-one	C9H16O2	M-H	155.1078	-0.3
HMDB0179788	(5E)-3-hydroxynon-5-en-2-one	C9H16O2	M-H	155.1078	-0.3
HMDB0179787	(5E)-1-hydroxynon-5-en-2-one	C9H16O2	M-H	155.1078	-0.3
HMDB0179806	(3Z)-9-hydroxynon-3-en-2-one	C9H16O2	M-H	155.1078	-0.3
HMDB0179805	Ethanone, 1-(3-pentyloxiranyl)-	C9H16O2	M-H	155.1078	-0.3
HMDB0179804	(3Z)-8-hydroxynon-3-en-2-one	C9H16O2	M-H	155.1078	-0.3
HMDB0179803	(3Z)-5-hydroxynon-3-en-2-one	C9H16O2	M-H	155.1078	-0.3
HMDB0179807	(3Z)-1-hydroxynon-3-en-2-one	C9H16O2	M-H	155.1078	-0.3
HMDB0180000	7-METHYL-7-OCTENOIC ACID	C9H16O2	M-H	155.1078	-0.3
HMDB0180426	(2E,4E)-nona-2,4-diene-1,8-diol	C9H16O2	M-H	155.1078	-0.3
HMDB0180428	(2E)-3-(3-butyloxiran-2-yl)prop-2-en-1-ol	C9H16O2	M-H	155.1078	-0.3
HMDB0180427	{3-[(1E)-hex-1-en-1-yl]oxiran-2-yl}methanol	C9H16O2	M-H	155.1078	-0.3
HMDB0180425	(2E,4E)-nona-2,4-diene-1,6-diol	C9H16O2	M-H	155.1078	-0.3
HMDB0180429	(2E,4E)-nona-2,4-diene-1,9-diol	C9H16O2	M-H	155.1078	-0.3
HMDB0179786	(5E)-9-hydroxynon-5-en-2-one	C9H16O2	M-H	155.1078	-0.3
HMDB0179784	(5E)-8-hydroxynon-5-en-2-one	C9H16O2	M-H	155.1078	-0.3
HMDB0167044	(2E,6Z)-nona-2,6-diene-1,8-diol	C9H16O2	M-H	155.1078	-0.3
HMDB0167048	(2E,6Z)-nona-2,6-diene-1,5-diol	C9H16O2	M-H	155.1078	-0.3
HMDB0167047	(2E,6Z)-nona-2,6-diene-1,4-diol	C9H16O2	M-H	155.1078	-0.3
HMDB0167049	{3-[(3Z)-hex-3-en-1-yl]oxiran-2-yl}methanol	C9H16O2	M-H	155.1078	-0.3
HMDB0167050	(2E)-5-(3-ethyloxiran-2-yl)pent-2-en-1-ol	C9H16O2	M-H	155.1078	-0.3
HMDB0167057	6Z-Nonenoic acid	C9H16O2	M-H	155.1078	-0.3
HMDB0179752	7-(oxiran-2-yl)heptan-3-one	C9H16O2	M-H	155.1078	-0.3
HMDB0179754	4-hydroxynon-8-en-3-one	C9H16O2	M-H	155.1078	-0.3
HMDB0179751	2-hydroxynon-8-en-3-one	C9H16O2	M-H	155.1078	-0.3
HMDB0179753	SCHEMBL18838844	C9H16O2	M-H	155.1078	-0.3
HMDB0179782	(5E)-7-hydroxynon-5-en-2-one	C9H16O2	M-H	155.1078	-0.3
HMDB0179783	4-Hydroxynon-5-en-2-one	C9H16O2	M-H	155.1078	-0.3
HMDB0179785	4-(3-propyloxiran-2-yl)butan-2-one	C9H16O2	M-H	155.1078	-0.3
HMDB0039794	Methyl 4Z-octenoate	C9H16O2	M-H	155.1078	-0.3
HMDB0038275	cis-3-Hexenyl propanoate	C9H16O2	M-H	155.1078	-0.3
HMDB0031271	2-Nonenoic acid	C9H16O2	M-H	155.1078	-0.3
HMDB0038272	trans-2-Hexenyl propanoate	C9H16O2	M-H	155.1078	-0.3
HMDB0036208	2-Propenyl 2-ethylbutanoate	C9H16O2	M-H	155.1078	-0.3
HMDB0032413	Methyl 2-octenoate	C9H16O2	M-H	155.1078	-0.3
HMDB0032491	Prenyl isobutyrate	C9H16O2	M-H	155.1078	-0.3
HMDB0032265	cis-Ethyl 4-heptenoate	C9H16O2	M-H	155.1078	-0.3
HMDB0032307	Hept-trans-2-en-1-yl acetate	C9H16O2	M-H	155.1078	-0.3
HMDB0059728	Methyl 3-Octenoate	C9H16O2	M-H	155.1078	-0.3
HMDB0059817	(Z)-Oak lactone	C9H16O2	M-H	155.1078	-0.3
HMDB0059894	(Z)-Oak lactone	C9H16O2	M-H	155.1078	-0.3
HMDB0037629	Isobutyl angelate	C9H16O2	M-H	155.1078	-0.3
HMDB0031514	6-Butyltetrahydro-2H-pyran-2-one	C9H16O2	M-H	155.1078	-0.3
HMDB0004362	4-Hydroxynonanal	C9H16O2	M-H	155.1078	-0.3
HMDB0035307	Quercuslactone a	C9H16O2	M-H	155.1078	-0.3
HMDB0037618	(E)-3-Heptenyl acetate	C9H16O2	M-H	155.1078	-0.3
HMDB0037023	2-Hydroxy-2,6,6-trimethylcyclohexanone	C9H16O2	M-H	155.1078	-0.3
HMDB0031531	Dihydro-5-pentyl-2(3H)-furanone	C9H16O2	M-H	155.1078	-0.3
HMDB0036222	Cyclohexyl propionate	C9H16O2	M-H	155.1078	-0.3
HMDB0039736	6-Hydroxy-4,6-dimethyl-3-hepten-2-one	C9H16O2	M-H	155.1078	-0.3
HMDB0031263	2,4-Nonanedione	C9H16O2	M-H	155.1078	-0.3
HMDB0034716	4-Oxononanal	C9H16O2	M-H	155.1078	-0.3
HMDB0033167	Ethyl cyclohexanecarboxylate	C9H16O2	M-H	155.1078	-0.3
HMDB0040210	2-Propenyl hexanoate	C9H16O2	M-H	155.1078	-0.3
HMDB0037496	Methyl (E)-2-octenoate	C9H16O2	M-H	155.1078	-0.3
HMDB0059840	(E)-2-Ethyl heptenoate	C9H16O2	M-H	155.1078	-0.3
HMDB0060286	3,4-Epoxyonanal	C9H16O2	M-H	155.1078	-0.3
HMDB0170941	8-nonylenic acid	C9H16O2	M-H	155.1078	-0.3
HMDB0035094	L-Citronellol	C10H20O	M-H	155.1441	-0.3
HMDB0062106	dihydromyrcenol	C10H20O	M-H	155.1441	-0.3
HMDB0037171	alpha-Citronellol	C10H20O	M-H	155.1441	-0.3
HMDB0171174	Citronellol	C10H20O	M-H	155.1441	-0.3
HMDB0035763	(+)-Neomenthol	C10H20O	M-H	155.1441	-0.3

155.1441	HMDB0034717	Menthanol	C10H20O	M-H	155.1441	-0.3
	HMDB0035765	p-Menthan-3-ol	C10H20O	M-H	155.1441	-0.3
	HMDB0035093	D-Citronellol	C10H20O	M-H	155.1441	-0.3
	HMDB0031409	2-Decanone	C10H20O	M-H	155.1441	-0.3
	HMDB0035764	(-)-Neoisomenthol	C10H20O	M-H	155.1441	-0.3
	HMDB0039854	1-Decen-3-ol	C10H20O	M-H	155.1441	-0.3
	HMDB0011623	Decanal	C10H20O	M-H	155.1441	-0.3
	HMDB0037020	p-Menthan-1-ol	C10H20O	M-H	155.1441	-0.3
	HMDB0035726	p-Menthan-4-ol	C10H20O	M-H	155.1441	-0.3
	HMDB0037806	Dihydrocitronellal	C10H20O	M-H	155.1441	-0.3
	HMDB0059861	9-Decenol	C10H20O	M-H	155.1441	-0.3
	HMDB0013810	(E)-3-decen-1-ol	C10H20O	M-H	155.1441	-0.3
	HMDB0041628	(+)-Neoisomenthol	C10H20O	M-H	155.1441	-0.3
	HMDB0032206	cis-4-Decenol	C10H20O	M-H	155.1441	-0.3
	HMDB0032532	2-DECENOL	C10H20O	M-H	155.1441	-0.3
	HMDB0032241	3,7-Dimethyloctanal	C10H20O	M-H	155.1441	-0.3
	HMDB0032274	(+/-)-4-Ethylactanal	C10H20O	M-H	155.1441	-0.3
	HMDB0032212	3-Decanone	C10H20O	M-H	155.1441	-0.3
	HMDB0037223	Carvomenthol	C10H20O	M-H	155.1441	-0.3
	HMDB0003352	Menthol	C10H20O	M-H	155.1441	-0.3
156.0303	HMDB0001241	2-Aminomuconic acid	C6H7NO4	M-H	156.0302	0.4
	HMDB0004230	Pyrrole-2-carboxylic acid	C5H5NO2	M+FA-H	156.0302	0.5
	HMDB0038175	2-Acetyloxazole	C5H5NO2	M+FA-H	156.0302	0.5
	HMDB0031577	Berteroin	C7H13NS2	M-H2O-H	156.0306	-1.6
	HMDB0166085	(4-isothiocyanatobutyl)dimethylsulfonium	C7H14NS2	M-H2O-H	156.0306	-1.6
157.0251	HMDB0029402	L-2-Amino-3-(oxalylamino)propanoic acid	C5H8N2O5	M-H2O-H	157.0249	1.1
	HMDB0038668	L-3-Amino-2-(oxalylamino)propanoic acid	C5H8N2O5	M-H2O-H	157.0249	1.1
	HMDB0159928	N-carbamoylaspartic acid	C5H8N2O5	M-H2O-H	157.0249	1.1
	HMDB0000828	Ureidosuccinic acid	C5H8N2O5	M-H2O-H	157.0249	1.1
	HMDB0000300	Uracil	C4H4N2O2	M+FA-H	157.0255	-2.4
	HMDB0060760	4-Carboxypyrazole	C4H4N2O2	M+FA-H	157.0255	-2.4
	HMDB0000528	4,5-Dihydroorotic acid	C5H6N2O4	M-H	157.0255	-2.4
	HMDB0003349	L-Dihydroorotic acid	C5H6N2O4	M-H	157.0255	-2.4
157.0508	HMDB0163408	5-(1-hydroxyethyl)-4-methyloxolane-2,3-dione	C7H10O4	M-H	157.0506	1.1
	HMDB0163409	5-(2-hydroxyethyl)-4-methyloxolane-2,3-dione	C7H10O4	M-H	157.0506	1.1
	HMDB0163405	5-ethyl-3-hydroxy-4-(hydroxymethyl)-2,5-dihydrofuran-2-one	C7H10O4	M-H	157.0506	1.1
	HMDB0163406	3-hydroxy-5-(1-hydroxyethyl)-4-methyl-2,5-dihydrofuran-2-one	C7H10O4	M-H	157.0506	1.1
	HMDB0163407	3-hydroxy-5-(2-hydroxyethyl)-4-methyl-2,5-dihydrofuran-2-one	C7H10O4	M-H	157.0506	1.1
	HMDB0000635	Succinylacetone	C7H10O4	M-H	157.0506	1.1
	HMDB0059815	Ethyl 5-oxotetrahydro-2-furancarboxylate	C7H10O4	M-H	157.0506	1.1
	HMDB0012241	Isopropylmaleate	C7H10O4	M-H	157.0506	1.1
	HMDB0036380	xi-2,3-Dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one	C7H10O4	M-H	157.0506	1.1
	HMDB0040260	5,5-Dimethyl-2(5H)-furanone	C6H8O2	M+FA-H	157.0506	1.1
	HMDB0034247	2-(Methoxymethyl)furan	C6H8O2	M+FA-H	157.0506	1.1
	HMDB0033569	Syoyualdehyde	C6H8O2	M+FA-H	157.0506	1.1
	HMDB0039778	xi-3,5-Dimethyl-2(5H)-furanone	C6H8O2	M+FA-H	157.0506	1.1
	HMDB0031344	1,2-Cyclohexanedione	C6H8O2	M+FA-H	157.0506	1.1
	HMDB0001164	trans-1,2-Dihydrobenzene-1,2-diol	C6H8O2	M+FA-H	157.0506	1.1
	HMDB0031759	(E)-4-Oxo-2-hexen-1-al	C6H8O2	M+FA-H	157.0506	1.1
	HMDB0031543	3-Methyl-1,2-cyclopentanedione	C6H8O2	M+FA-H	157.0506	1.1
	HMDB0029581	(2E,4E)-2,4-Hexadienoic acid	C6H8O2	M+FA-H	157.0506	1.1
	HMDB0032233	2,5-Dimethyl-3(2H)-furanone	C6H8O2	M+FA-H	157.0506	1.1
	HMDB0187593	1,4-Cyclohexanedione	C6H8O2	M+FA-H	157.0506	1.1
	HMDB0179338	(2Z,4E)-6-hydroxyhexa-2,4-dienal	C6H8O2	M+FA-H	157.0506	1.1
	HMDB0179339	3-[(1E)-prop-1-en-1-yl]oxirane-2-carbaldehyde	C6H8O2	M+FA-H	157.0506	1.1
	HMDB0179340	(2Z)-3-(3-methyloxiran-2-yl)prop-2-enal	C6H8O2	M+FA-H	157.0506	1.1
	HMDB0179337	(2Z,4E)-hexa-2,4-dienoic acid	C6H8O2	M+FA-H	157.0506	1.1
	HMDB0062028	3-Ethylcyclopentanone	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0061994	2-methyl-2-hexenal	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0061985	2-ethylcyclopentan-1-one	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0032301	trans-2-trans-4-Heptadien-1-ol	C7H12O	M+FA-H	157.0870	-0.7

157.0869	HMDB0031540	4-Methylcyclohexanone	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0031483	(Z)-4-Heptenal	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0040339	2,5-Heptadien-1-ol	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0034372	xi-3-Methyl-3-cyclohexen-1-ol	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0031487	(E)-4-Hepten-2-one	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0031550	5-Methyl-3-hexen-2-one	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0031539	2-Methylcyclohexanone	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0061957	(Z)-2-Heptenal	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0031486	3-Hepten-2-one	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0033827	(2E)-2-Heptenal	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0033667	(R)-3-Methylcyclohexanone	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0031488	2-Hepten-4-one	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0031551	5-Methyl-5-hexen-2-one	C7H12O	M+FA-H	157.0870	-0.7
	HMDB0158406	(2Z)-7-hydroxyoct-2-enoic acid	C8H14O3	M-H	157.0870	-0.8
	HMDB0158405	(2Z)-4-hydroxyoct-2-enoic acid	C8H14O3	M-H	157.0870	-0.8
	HMDB0158407	SCHEMBL63	C8H14O3	M-H	157.0870	-0.8
	HMDB0158408	(2Z)-8-hydroxyoct-2-enoic acid	C8H14O3	M-H	157.0870	-0.8
	HMDB0062788	isobutyric acid anhydride	C8H14O3	M-H	157.0870	-0.8
	HMDB0041616	Propyl levulinate	C8H14O3	M-H	157.0870	-0.8
	HMDB0000451	cis-4-Hydroxycyclohexylacetic acid	C8H14O3	M-H	157.0870	-0.8
	HMDB0010721	3-Oxoctanoic acid	C8H14O3	M-H	157.0870	-0.8
	HMDB0000909	trans-4-Hydroxycyclohexylacetic acid	C8H14O3	M-H	157.0870	-0.8
	HMDB0036230	1-Methyl-2-oxopropyl butyrate	C8H14O3	M-H	157.0870	-0.8
	HMDB0036395	2-Methylpropyl 3-oxobutanoate	C8H14O3	M-H	157.0870	-0.8
	HMDB0031307	Ethyl 3-oxohexanoate	C8H14O3	M-H	157.0870	-0.8
	HMDB0030303	6-Ethyl-1-methyl-2,7,8-trioxabicyclo[3.2.1]octane	C8H14O3	M-H	157.0870	-0.8
	HMDB0059939	6-Butyl-1,4-dioxan-2-one	C8H14O3	M-H	157.0870	-0.8
	HMDB0040447	Butyl acetoacetate	C8H14O3	M-H	157.0870	-0.8
	HMDB0060685	3-Oxovalproic acid	C8H14O3	M-H	157.0870	-0.8
	HMDB0059938	5-Butyl-1,4-dioxan-2-one	C8H14O3	M-H	157.0870	-0.8
	HMDB0060683	2-n-Propyl-4-oxopentanoic acid	C8H14O3	M-H	157.0870	-0.8
	HMDB0013211	Alpha-Ketooctanoic acid	C8H14O3	M-H	157.0870	-0.8
	HMDB0031177	Tetrahydrofurfuryl propionate	C8H14O3	M-H	157.0870	-0.8
	HMDB0038305	3-Methylbutyl 2-oxopropanoate	C8H14O3	M-H	157.0870	-0.8
	HMDB0164642	2,3,7-trihydroxyoctanal	C8H16O4	M-H2O-H	157.0865	2.7
	HMDB0164641	3,7,8-trihydroxyoctanal	C8H16O4	M-H2O-H	157.0865	2.7
	HMDB0161158	2,8-dihydroxy-octanoic acid	C8H16O4	M-H2O-H	157.0865	2.7
	HMDB0159450	2,7-dihydroxyoctanoic acid	C8H16O4	M-H2O-H	157.0865	2.7
	HMDB0159449	7,8-dihydroxyoctanoic acid	C8H16O4	M-H2O-H	157.0865	2.7
157.1233	HMDB0061911	4-Methyl-3-heptene	C8H16	M+FA-H	157.1234	-0.6
	HMDB0061908	3-Methyl-1-heptene	C8H16	M+FA-H	157.1234	-0.6
	HMDB0061910	(E)-4-Methyl-2-heptene	C8H16	M+FA-H	157.1234	-0.6
	HMDB0061909	3-Methyl-3-heptene	C8H16	M+FA-H	157.1234	-0.6
	HMDB0061907	3-Methyleneheptane	C8H16	M+FA-H	157.1234	-0.6
	HMDB0061906	(E)-3-Octene	C8H16	M+FA-H	157.1234	-0.6
	HMDB0061905	(Z)-3-Octene	C8H16	M+FA-H	157.1234	-0.6
	HMDB0094705	6-methylhept-1-ene	C8H16	M+FA-H	157.1234	-0.6
	HMDB0061903	(Z)-2-Octene	C8H16	M+FA-H	157.1234	-0.6
	HMDB0032449	1-Octene	C8H16	M+FA-H	157.1234	-0.6
	HMDB0061904	(E)-2-Octene	C8H16	M+FA-H	157.1234	-0.6
	HMDB0163461	(2Z)-2-methyloct-2-ene-1,4-diol	C9H18O2	M-H	157.1234	-0.7
	HMDB0163472	2-methyl-octanoic acid	C9H18O2	M-H	157.1234	-0.7
	HMDB0031557	4-Methyloctanoic acid	C9H18O2	M-H	157.1234	-0.7
	HMDB0030331	xi-2-Ethylheptanoic acid	C9H18O2	M-H	157.1234	-0.7
	HMDB0039219	1-Methylbutyl butanoate	C9H18O2	M-H	157.1234	-0.7
	HMDB0031480	Heptyl acetate	C9H18O2	M-H	157.1234	-0.7
	HMDB0034162	Pentyl butanoate	C9H18O2	M-H	157.1234	-0.7
	HMDB0000847	Pelargonic acid	C9H18O2	M-H	157.1234	-0.7
	HMDB0179988	Isononanoic acid	C9H18O2	M-H	157.1234	-0.7
	HMDB0179811	2-nonanon-3-ol	C9H18O2	M-H	157.1234	-0.7
	HMDB0179808	8-hydroxynonan-2-one	C9H18O2	M-H	157.1234	-0.7
	HMDB0179810	1-hydroxy-2-nonanone	C9H18O2	M-H	157.1234	-0.7
	HMDB0179167	1-hydroxynonan-4-one	C9H18O2	M-H	157.1234	-0.7
	HMDB0171040	non-8-ene-2,7-diol	C9H18O2	M-H	157.1234	-0.7
	HMDB0171041	SCHEMBL926	C9H18O2	M-H	157.1234	-0.7

HMDB0171042	SCHEMBL7123711	C9H18O2	M-H	157.1234	-0.7
HMDB0163464	(2Z)-2-methyloct-2-ene-1,8-diol	C9H18O2	M-H	157.1234	-0.7
HMDB0163460	2-Hexylidene-1,3-propanediol	C9H18O2	M-H	157.1234	-0.7
HMDB0036234	3-Methylbutyl 2-methylpropanoate	C9H18O2	M-H	157.1234	-0.7
HMDB0163462	(2Z)-2-methyloct-2-ene-1,7-diol	C9H18O2	M-H	157.1234	-0.7
HMDB0163463	(2-methyl-3-pentylloxiran-2-yl)methanol	C9H18O2	M-H	157.1234	-0.7
HMDB0039216	Butyl 2-methylbutanoate	C9H18O2	M-H	157.1234	-0.7
HMDB0034165	Propyl hexanoate	C9H18O2	M-H	157.1234	-0.7
HMDB0179809	9-hydroxynonan-2-one	C9H18O2	M-H	157.1234	-0.7
HMDB0032042	Butyl 3-methylbutanoate	C9H18O2	M-H	157.1234	-0.7
HMDB0062123	2-methylpropyl pentanoate	C9H18O2	M-H	157.1234	-0.7
HMDB0040221	Isoamyl butyrate	C9H18O2	M-H	157.1234	-0.7
HMDB0038040	2-Methylpropyl 3-methylbutanoate	C9H18O2	M-H	157.1234	-0.7
HMDB0000798	Oenanthic ether	C9H18O2	M-H	157.1234	-0.7
HMDB0032406	5-Methylhexyl acetate	C9H18O2	M-H	157.1234	-0.7
HMDB0032309	3-Heptyl acetate	C9H18O2	M-H	157.1234	-0.7
HMDB0032454	3-Octyl formate	C9H18O2	M-H	157.1234	-0.7
HMDB0059822	Ethyl 5-methylhexanoate	C9H18O2	M-H	157.1234	-0.7
HMDB0031291	Methyl caprylate	C9H18O2	M-H	157.1234	-0.7
HMDB0034606	Hexyl propionate	C9H18O2	M-H	157.1234	-0.7
HMDB0040295	Butyl pentanoate	C9H18O2	M-H	157.1234	-0.7
HMDB0038603	Octyl formate	C9H18O2	M-H	157.1234	-0.7
HMDB0037288	4-Methyl-2-pentyl-1,3-dioxolane	C9H18O2	M-H	157.1234	-0.7
HMDB0037164	3-(Hydroxymethyl)-2-octanone	C9H18O2	M-H	157.1234	-0.7
HMDB0037143	1-Hydroxy-3-nonanone	C9H18O2	M-H	157.1234	-0.7
HMDB0040430	Isopropyl hexanoate	C9H18O2	M-H	157.1234	-0.7
HMDB0061676	2,2-Dimethylglutaric acid	C7H12O4	M-H	159.0663	0.7
HMDB0059738	2-Ethylglutaric acid	C7H12O4	M-H	159.0663	0.7
HMDB0059722	Mono-methyl-adipate	C7H12O4	M-H	159.0663	0.7
HMDB0059893	Ethyl methyl succinate	C7H12O4	M-H	159.0663	0.7
HMDB0041605	Propyleneglycol diacetate	C7H12O4	M-H	159.0663	0.7
HMDB0029167	2-Methyladipic acid	C7H12O4	M-H	159.0663	0.7
HMDB0165010	2-(acetyloxy)-3-methylButanoic acid	C7H12O4	M-H	159.0663	0.7
HMDB0000857	Pimelic acid	C7H12O4	M-H	159.0663	0.7
HMDB0061239	2-Propylsuccinic acid	C7H12O4	M-H	159.0663	0.7
HMDB0000555	3-Methyladipic acid	C7H12O4	M-H	159.0663	0.7
HMDB0002441	3,3-Dimethylglutaric acid	C7H12O4	M-H	159.0663	0.7
HMDB0175388	ss-Acetoxyisovaleriansaure	C7H12O4	M-H	159.0663	0.7
HMDB0029573	Diethyl malonate	C7H12O4	M-H	159.0663	0.7
HMDB0179341	(4E)-6-hydroxyhex-4-enal	C6H10O2	M+FA-H	159.0663	0.7
HMDB0179344	cis-2,4-hexadien-1,6-diol	C6H10O2	M+FA-H	159.0663	0.7
HMDB0179346	(2Z)-3-(3-methyloxiran-2-yl)prop-2-en-1-ol	C6H10O2	M+FA-H	159.0663	0.7
HMDB0179351	4-Hexenoic acid	C6H10O2	M+FA-H	159.0663	0.7
HMDB0179342	(4E)-3-hydroxyhex-4-enal	C6H10O2	M+FA-H	159.0663	0.7
HMDB0165584	(2Z)-5-hydroxy-2-methylpent-2-enal	C6H10O2	M+FA-H	159.0663	0.7
HMDB0165581	(2Z)-2-(hydroxymethyl)pent-2-enal	C6H10O2	M+FA-H	159.0663	0.7
HMDB0165583	2-Methyl-3-ethyloxirane-2-carbaldehyde	C6H10O2	M+FA-H	159.0663	0.7
HMDB0165582	(2Z)-4-hydroxy-2-methylpent-2-enal	C6H10O2	M+FA-H	159.0663	0.7
HMDB0163702	Pentanal, 3-methyl-4-oxo-	C6H10O2	M+FA-H	159.0663	0.7
HMDB0163354	(4Z)-2-hydroxyhex-4-enal	C6H10O2	M+FA-H	159.0663	0.7
HMDB0169664	(E)-3-Methyl-2-pentenoic acid	C6H10O2	M+FA-H	159.0663	0.7
HMDB0179345	{3-[(1E)-prop-1-en-1-yl]oxiran-2-yl}methanol	C6H10O2	M+FA-H	159.0663	0.7
HMDB0163352	(4Z)-3-hydroxyhex-4-enal	C6H10O2	M+FA-H	159.0663	0.7
HMDB0169695	(Z)-3-methyl-2-pentenoic acid	C6H10O2	M+FA-H	159.0663	0.7
HMDB0163353	3-(3-methyloxiran-2-yl)propanal	C6H10O2	M+FA-H	159.0663	0.7
HMDB0163351	(4Z)-6-hydroxyhex-4-enal	C6H10O2	M+FA-H	159.0663	0.7
HMDB0163350	(Z)-hex-4-enoic acid	C6H10O2	M+FA-H	159.0663	0.7
HMDB0179343	(4E)-2-hydroxyhex-4-enal	C6H10O2	M+FA-H	159.0663	0.7
HMDB0163703	(3Z)-5-hydroxy-3-methylpent-3-en-2-one	C6H10O2	M+FA-H	159.0663	0.7
HMDB0003843	Gamma-Caprolactone	C6H10O2	M+FA-H	159.0663	0.7
HMDB0039581	Ethyl crotonate	C6H10O2	M+FA-H	159.0663	0.7
HMDB0032490	Prenyl formate	C6H10O2	M+FA-H	159.0663	0.7
HMDB0060476	epsilon-Caprolactone	C6H10O2	M+FA-H	159.0663	0.7
HMDB0031559	4-Methyl-2,3-pentanedione	C6H10O2	M+FA-H	159.0663	0.7
HMDB0240384	4-Hydroxyhexanal	C6H10O2	M+FA-H	159.0663	0.7

	HMDB0031562	2-Methyl-3-pentenoic acid	C6H10O2	M+FA-H	159.0663	0.7
	HMDB0031491	2,3-Hexanedione	C6H10O2	M+FA-H	159.0663	0.7
	HMDB0031560	2-Methyl-2-pentenoic acid	C6H10O2	M+FA-H	159.0663	0.7
	HMDB0000453	delta-Hexanolactone	C6H10O2	M+FA-H	159.0663	0.7
	HMDB0010719	Isohydrosorbic acid	C6H10O2	M+FA-H	159.0663	0.7
	HMDB0031561	4-Methyl-2-pentenoic acid	C6H10O2	M+FA-H	159.0663	0.7
	HMDB0031492	3,4-Hexanedione	C6H10O2	M+FA-H	159.0663	0.7
	HMDB0040328	Methyl 4-pentenoate	C6H10O2	M+FA-H	159.0663	0.7
	HMDB0033568	5-Oxohexanal	C6H10O2	M+FA-H	159.0663	0.7
	HMDB0029487	Allyl propionate	C6H10O2	M+FA-H	159.0663	0.7
	HMDB0031501	3-Hexenoic acid	C6H10O2	M+FA-H	159.0663	0.7
	HMDB0061929	Dihydro-4,4-dimethyl-2(3H)-furanone	C6H10O2	M+FA-H	159.0663	0.7
	HMDB0031158	2-Methyl-4-pentenoic acid	C6H10O2	M+FA-H	159.0663	0.7
	HMDB0061965	1-methyl-2,3-dioxabicyclo[2.2.1]heptane	C6H10O2	M+FA-H	159.0663	0.7
	HMDB0062135	methyl (2E)-2-methylbut-2-enoate	C6H10O2	M+FA-H	159.0663	0.7
	HMDB0029569	Dibutyl disulfide	C8H18S2	M-H2O-H	159.0666	-1.3
	HMDB0040348	1,8-Octanedithiol	C8H18S2	M-H2O-H	159.0666	-1.3
159.1026	HMDB0175178	6-Hepten-1-ol	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0062059	4-methylhexan-3-one	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0061896	2-Methyl-3-hexanone	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0059693	1-Methylcyclohexanol	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0166735	trans-2-Hepten-1-ol	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0032405	3-Methylhexanal	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0031538	3-Methylcyclohexanol	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0005841	Ethyl isobutyl ketone	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0040191	2-Methylhexanal	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0003671	2-Heptanone	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0041320	(2R,4Z)-4-Hepten-2-ol	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0031475	Heptanal	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0031482	3-Heptanone	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0031429	2,4-Dimethyl-3-pentanone	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0004814	4-Heptanone	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0038052	1-Ethoxy-3-methyl-2-butene	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0031549	5-Methyl-2-hexanone	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0031405	(Z)-4-Hepten-1-ol	C7H14O	M+FA-H	159.1027	-0.4
	HMDB0002264	(R)-2-Hydroxycaprylic acid	C8H16O3	M-H	159.1027	-0.4
	HMDB0172044	SCHEMBL8569867	C8H16O3	M-H	159.1027	-0.4
	HMDB0172042	NSC616278	C8H16O3	M-H	159.1027	-0.4
	HMDB0172043	ethyl 3-(hydroxymethyl)pentanoate	C8H16O3	M-H	159.1027	-0.4
	HMDB0172041	SCHEMBL9153763	C8H16O3	M-H	159.1027	-0.4
	HMDB0062596	(7R)-7-hydroxyoctanoic acid	C8H16O3	M-H	159.1027	-0.4
	HMDB0164640	3,7-dihydroxyoctanal	C8H16O3	M-H	159.1027	-0.4
	HMDB0000711	Hydroxyoctanoic acid	C8H16O3	M-H	159.1027	-0.4
	HMDB0061914	8-Hydroxyoctanoate	C8H16O3	M-H	159.1027	-0.4
	HMDB0032270	(+/-)-Ethyl 2-hydroxy-3-methylvalerate	C8H16O3	M-H	159.1027	-0.4
	HMDB0013898	5-Hydroxyvalproic acid	C8H16O3	M-H	159.1027	-0.4
	HMDB0013900	4-Hydroxyvalproic acid	C8H16O3	M-H	159.1027	-0.4
	HMDB0000486	7-Hydroxyoctanoic acid	C8H16O3	M-H	159.1027	-0.4
	HMDB0059825	Isoamyl lactate	C8H16O3	M-H	159.1027	-0.4
	HMDB0059867	Ethyl 2-hydroxy-4-methylpentanoate	C8H16O3	M-H	159.1027	-0.4
	HMDB0001954	(S)-3-hydroxyoctanoic acid	C8H16O3	M-H	159.1027	-0.4
	HMDB0032827	Peroxyoctanoic acid	C8H16O3	M-H	159.1027	-0.4
	HMDB0031509	Ethyl 3-hydroxyhexanoate	C8H16O3	M-H	159.1027	-0.4
	HMDB0010722	(R)-3-Hydroxyoctanoic acid	C8H16O3	M-H	159.1027	-0.4
	HMDB0013899	3-Hydroxyvalproic acid	C8H16O3	M-H	159.1027	-0.4
	HMDB0172040	CTK811333	C8H16O3	M-H	159.1027	-0.4
160.0072	HMDB0162809	[(2,3-dihydro-1H-pyrrol-3-yl)methoxy]sulfonic acid	C5H9NO4S	M-H2O-H	160.0068	2.3
	HMDB0029415	S-Carboxymethyl-L-cysteine	C5H9NO4S	M-H2O-H	160.0068	2.3
	HMDB0166857	1,4-dimethyl 2-hydroxybutanedioate	C6H10O5	M-H	161.0455	1.0
	HMDB0158873	2-Hydroxy-2-methylglutaric acid	C6H10O5	M-H	161.0455	1.0
	HMDB0158875	2-hydroxy-4-methylpentanedioic acid	C6H10O5	M-H	161.0455	1.0
	HMDB0158874	2-(hydroxymethyl)pentanedioic acid	C6H10O5	M-H	161.0455	1.0
	HMDB0166862	21583-38	C6H10O5	M-H	161.0455	1.0
	HMDB0041561	D-1,5-Anhydrofructose	C6H10O5	M-H	161.0455	1.0
	HMDB0032873	Diethyl dicarbonate	C6H10O5	M-H	161.0455	1.0

161.0457	HMDB0029934	D-1-Deoxy-erythro-hexo-2,3-diulose	C6H10O5	M-H	161.0455	1.0
	HMDB0000640	Levogluconan	C6H10O5	M-H	161.0455	1.0
	HMDB0000368	2(R)-Hydroxyadipic acid	C6H10O5	M-H	161.0455	1.0
	HMDB0000345	3-Hydroxyadipic acid	C6H10O5	M-H	161.0455	1.0
	HMDB0000321	2-Hydroxyadipic acid	C6H10O5	M-H	161.0455	1.0
	HMDB0000355	3-Hydroxymethylglutaric acid	C6H10O5	M-H	161.0455	1.0
	HMDB0059737	3-Hydroxymethylglutaric acid	C6H10O5	M-H	161.0455	1.0
	HMDB0029169	(2S,3R)-3-hydroxy-2-methylpentanedioic acid	C6H10O5	M-H	161.0455	1.0
	HMDB0166863	4-ethoxy-2-hydroxy-4-oxobutanoic acid	C6H10O5	M-H	161.0455	1.0
	HMDB0061362	(2R)-1-(formyloxy)-3-hydroxypropan-2-yl acetate	C6H10O5	M-H	161.0455	1.0
	HMDB0166864	Butanedioic acid, 2-hydroxy-, 1-ethyl ester	C6H10O5	M-H	161.0455	1.0
	HMDB0059758	2-Hydroxy-2-ethylsuccinic acid	C6H10O5	M-H	161.0455	1.0
	HMDB0169666	SCHEMBL4558754	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0128916	4-hydroxy-3-methylbut-2-enoic acid	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0129096	(2Z)-2-(hydroxymethyl)but-2-enoic acid	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0128943	(2E)-4-hydroxy-3-methylbut-2-enoic acid	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0003771	2-Methylacetoacetic acid	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0177210	4-hydroxytiglic acid	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0128917	dimethyloxirane-2-carboxylic acid	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0168838	Ethyl 2,3-epoxypropanoate	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0177209	2-Hydroxymethyl-trans-crotonsaure	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0129098	2,3-dimethyloxirane-2-carboxylic acid	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0168839	2-HYDROXYETHYL ACRYLATE	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0029172	2-Methylacetoacetic acid	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0034466	Acetoxyacetone	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0012233	Glutarate semialdehyde	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0001865	2-Oxovaleric acid	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0000310	Methylacetoacetic acid	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0031643	Ethyl pyruvate	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0000019	alpha-Ketoisovaleric acid	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0000720	Levulinic acid	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0132477	2-(hydroxymethyl)but-2-enoic acid	C5H8O3	M+FA-H	161.0455	1.0
	HMDB0129097	4-hydroxy-2-methylbut-2-enoic acid	C5H8O3	M+FA-H	161.0455	1.0
163.0764	HMDB0059899	alpha-Methylstyrene	C9H10	M+FA-H	163.0765	-0.3
	HMDB0062099	cyclopropylbenzene	C9H10	M+FA-H	163.0765	-0.3
	HMDB0059837	Indane	C9H10	M+FA-H	163.0765	-0.3
	HMDB0041612	Phenyl butyrate	C10H12O2	M-H	163.0765	-0.3
	HMDB0133507	4-(3-hydroxyphenyl)butan-2-one	C10H12O2	M-H	163.0765	-0.3
	HMDB0133617	2-methyl-3-phenylpropanoic acid	C10H12O2	M-H	163.0765	-0.3
	HMDB0133727	3-[(1E)-3-hydroxybut-1-en-1-yl]phenol	C10H12O2	M-H	163.0765	-0.3
	HMDB0133725	(3E)-4-phenylbut-3-ene-1,2-diol	C10H12O2	M-H	163.0765	-0.3
	HMDB0133728	4-(4-Hydroxyphenyl)-3-buten-2-ol	C10H12O2	M-H	163.0765	-0.3
	HMDB0133729	1-(3-phenyloxiran-2-yl)ethan-1-ol	C10H12O2	M-H	163.0765	-0.3
	HMDB0133753	1-hydroxy-4-phenylbutan-2-one	C10H12O2	M-H	163.0765	-0.3
	HMDB0133754	4-hydroxy-4-phenylbutan-2-one	C10H12O2	M-H	163.0765	-0.3
	HMDB0135737	3-(4-methoxyphenyl)propanal	C10H12O2	M-H	163.0765	-0.3
	HMDB0146616	2-Propen-1-ol, 3-(2-methoxyphenyl)-	C10H12O2	M-H	163.0765	-0.3
	HMDB0151234	AKO1788443	C10H12O2	M-H	163.0765	-0.3
	HMDB0170842	Estragole oxide	C10H12O2	M-H	163.0765	-0.3
	HMDB0179484	2-methyl-5-(prop-1-en-2-yl)benzene-1,4-diol	C10H12O2	M-H	163.0765	-0.3
	HMDB0179725	SCHEMBL1438714	C10H12O2	M-H	163.0765	-0.3
	HMDB0133608	4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]phenol	C10H12O2	M-H	163.0765	-0.3
	HMDB0133609	(2-methyl-3-phenyloxiran-2-yl)methanol	C10H12O2	M-H	163.0765	-0.3
	HMDB0133610	2-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]phenol	C10H12O2	M-H	163.0765	-0.3
	HMDB0146615	3-(2-methoxyphenyl)propanal	C10H12O2	M-H	163.0765	-0.3
	HMDB0127494	1-ethenyl-3,5-dimethoxybenzene	C10H12O2	M-H	163.0765	-0.3
	HMDB0133603	3-hydroxy-2-methyl-3-phenylpropanal	C10H12O2	M-H	163.0765	-0.3
	HMDB0133601	2-benzyl-3-hydroxypropanal	C10H12O2	M-H	163.0765	-0.3
	HMDB0133600	2-hydroxy-2-methyl-3-phenylpropanal	C10H12O2	M-H	163.0765	-0.3
	HMDB0133607	3-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]phenol	C10H12O2	M-H	163.0765	-0.3
	HMDB0133604	3-(3-hydroxyphenyl)-2-methylpropanal	C10H12O2	M-H	163.0765	-0.3
	HMDB0133605	3-(4-hydroxyphenyl)-2-methylpropanal	C10H12O2	M-H	163.0765	-0.3
	HMDB0133606	2-(phenylmethylidene)propane-1,3-diol	C10H12O2	M-H	163.0765	-0.3
	HMDB0000543	Benzenebutanoic acid	C10H12O2	M-H	163.0765	-0.3
	HMDB0035268	4-Isopropylbenzoic acid	C10H12O2	M-H	163.0765	-0.3

	HMDB0030060	Methyl 3-phenylpropanoate	C10H12O2	M-H	163.0765	-0.3
	HMDB0035414	Lepalone	C10H12O2	M-H	163.0765	-0.3
	HMDB0031761	Propyl benzoate	C10H12O2	M-H	163.0765	-0.3
	HMDB0037160	4-Methyl-2-phenyl-1,3-dioxolane	C10H12O2	M-H	163.0765	-0.3
	HMDB0038184	Egomaketone	C10H12O2	M-H	163.0765	-0.3
	HMDB0032618	Ethyl phenylacetate	C10H12O2	M-H	163.0765	-0.3
	HMDB0034471	3-Phenylpropyl formate	C10H12O2	M-H	163.0765	-0.3
	HMDB0032620	1-Phenylethyl acetate	C10H12O2	M-H	163.0765	-0.3
	HMDB0036098	Isoegomaketone	C10H12O2	M-H	163.0765	-0.3
	HMDB0032891	1-(4-Methoxyphenyl)-2-propanone	C10H12O2	M-H	163.0765	-0.3
	HMDB0040460	4-Methylbenzyl alcohol acetate	C10H12O2	M-H	163.0765	-0.3
	HMDB0170973	(Z)-Isoeugenol	C10H12O2	M-H	163.0765	-0.3
	HMDB0033945	2-Phenylethyl acetate	C10H12O2	M-H	163.0765	-0.3
	HMDB0041473	(3-Methylphenyl)methyl acetate	C10H12O2	M-H	163.0765	-0.3
	HMDB0034615	Epoxyanethole	C10H12O2	M-H	163.0765	-0.3
	HMDB0000329	2-Phenylbutyric acid	C10H12O2	M-H	163.0765	-0.3
	HMDB0001955	3-Phenylbutyric acid	C10H12O2	M-H	163.0765	-0.3
	HMDB0005802	Isoeugenol	C10H12O2	M-H	163.0765	-0.3
	HMDB0005809	Eugenol	C10H12O2	M-H	163.0765	-0.3
	HMDB0037174	p-Mentha-2,4(8)-dien-9,3-olide	C10H12O2	M-H	163.0765	-0.3
	HMDB0030063	Benzyl propionate	C10H12O2	M-H	163.0765	-0.3
	HMDB0032038	Isopropyl benzoate	C10H12O2	M-H	163.0765	-0.3
	HMDB0035213	beta-Thujaplicin	C10H12O2	M-H	163.0765	-0.3
	HMDB0033723	4-(4-Hydroxyphenyl)-2-butanone	C10H12O2	M-H	163.0765	-0.3
	HMDB0041472	2-Methylbenzyl alcohol acetate	C10H12O2	M-H	163.0765	-0.3
	HMDB0032586	3-(4-Methoxyphenyl)-2-propen-1-ol	C10H12O2	M-H	163.0765	-0.3
	HMDB0040359	1,2-Dimethoxy-4-vinylbenzene	C10H12O2	M-H	163.0765	-0.3
	HMDB0034732	Thymoquinone	C10H12O2	M-H	163.0765	-0.3
	HMDB0032336	3-Hydroxy-4-phenylbutan-2-one	C10H12O2	M-H	163.0765	-0.3
	HMDB0135738	3-(4-methoxyphenyl)prop-2-en-1-ol	C10H12O2	M-H	163.0765	-0.3
164.0717	HMDB0062407	5-(3-Pyridyl)-2-hydroxytetrahydrofuran	C9H11NO2	M-H	164.0717	0.0
	HMDB0034169	Methyl N-methylanthranilate	C9H11NO2	M-H	164.0717	0.0
	HMDB0006044	Norsalsolinol	C9H11NO2	M-H	164.0717	0.0
	HMDB0001007	3-Pyridinebutanoic acid	C9H11NO2	M-H	164.0717	0.0
	HMDB0004992	Benzocaine	C9H11NO2	M-H	164.0717	0.0
	HMDB0033485	Gentiatibetine	C9H11NO2	M-H	164.0717	0.0
	HMDB0033589	Ethyl 2-aminobenzoate	C9H11NO2	M-H	164.0717	0.0
	HMDB0062402	4-Hydroxy-1-(3-pyridinyl)-1-butanone	C9H11NO2	M-H	164.0717	0.0
	HMDB0059934	Benzyl glycinate	C9H11NO2	M-H	164.0717	0.0
	HMDB0000159	L-Phenylalanine	C9H11NO2	M-H	164.0717	0.0
165.0408	HMDB0159744	L-Phenylalanine	C9H11NO2	M-H	164.0717	0.0
	HMDB0060256	欽婁-Xylonic acid	C5H10O6	M-H	165.0405	2.0
	HMDB0000867	Ribonic acid	C5H10O6	M-H	165.0405	2.0
	HMDB0059750	欽婦-欽婦ylonic acid	C5H10O6	M-H	165.0405	2.0
	HMDB0060255	欽婁-欽婁yxonic acid	C5H10O6	M-H	165.0405	2.0
	HMDB0000539	Arabinonic acid	C5H10O6	M-H	165.0405	2.0
	HMDB0154797	68516-39-2	C4H8O4	M+FA-H	165.0405	2.1
	HMDB0000360	2,4-Dihydroxybutanoic acid	C4H8O4	M+FA-H	165.0405	2.1
	HMDB0000498	4-Deoxyerythronic acid	C4H8O4	M+FA-H	165.0405	2.1
	HMDB0002453	4-Deoxythreonic acid	C4H8O4	M+FA-H	165.0405	2.1
	HMDB0002601	A,b-Dihydroxyisobutyric acid	C4H8O4	M+FA-H	165.0405	2.1
	HMDB0002649	Erythrose	C4H8O4	M+FA-H	165.0405	2.1
	HMDB0006293	L-Erythrulose	C4H8O4	M+FA-H	165.0405	2.1
	HMDB0000337	(S)-3,4-Dihydroxybutyric acid	C4H8O4	M+FA-H	165.0405	2.1
	HMDB0062348	3,5-Dimethoxybenzaldehyde	C9H10O3	M-H	165.0557	0.5
	HMDB0041611	Ethyl 2-furanacrylate	C9H10O3	M-H	165.0557	0.5
	HMDB0168681	4-ethoxybenzoic acid	C9H10O3	M-H	165.0557	0.5
	HMDB0166065	4-hydroxybenzyl acetate	C9H10O3	M-H	165.0557	0.5
	HMDB0166615	4-[(1Z)-3-hydroxyprop-1-en-1-yl]benzene-1,2-diol	C9H10O3	M-H	165.0557	0.5
	HMDB0167324	AKO23569996	C9H10O3	M-H	165.0557	0.5
	HMDB0168656	2-hydroxyethyl benzoate	C9H10O3	M-H	165.0557	0.5
	HMDB0168684	4-Ethoxy-3-hydroxybenzaldehyde	C9H10O3	M-H	165.0557	0.5
	HMDB0168682	4-ethoxy-2-hydroxybenzaldehyde	C9H10O3	M-H	165.0557	0.5
	HMDB0168683	4-(2-hydroxyethoxy)benzaldehyde	C9H10O3	M-H	165.0557	0.5
	HMDB0171689	(4-Methylphenoxy)acetic acid	C9H10O3	M-H	165.0557	0.5

165.0558	HMDB0177510	1-(4-hydroxyphenyl)prop-1-ene-1,2-diol	C9H10O3	M-H	165.0557	0.5
	HMDB0180874	SCHEMBL7737611	C9H10O3	M-H	165.0557	0.5
	HMDB0180875	620-15-1	C9H10O3	M-H	165.0557	0.5
	HMDB0180872	5-Allylbenzene-1,2,3-triol	C9H10O3	M-H	165.0557	0.5
	HMDB0180873	SCHEMBL978929	C9H10O3	M-H	165.0557	0.5
	HMDB0240325	2-(4-Hydroxyphenyl)propionate	C9H9O3	M-H	165.0557	0.5
	HMDB0142136	2-(2-hydroxyphenyl)propanoic acid	C9H10O3	M-H	165.0557	0.5
	HMDB0141766	4-[3-(hydroxymethyl)oxiran-2-yl]phenol	C9H10O3	M-H	165.0557	0.5
	HMDB0125519	4-ethenyl-6-methoxybenzene-1,3-diol	C9H10O3	M-H	165.0557	0.5
	HMDB0125525	5-ethenyl-3-methoxybenzene-1,2-diol	C9H10O3	M-H	165.0557	0.5
	HMDB0125539	4-ethenyl-2-methoxybenzene-1,3-diol	C9H10O3	M-H	165.0557	0.5
	HMDB0134035	3-hydroxy-3-(2-hydroxyphenyl)propanal	C9H10O3	M-H	165.0557	0.5
	HMDB0134033	3-(2,5-dihydroxyphenyl)propanal	C9H10O3	M-H	165.0557	0.5
	HMDB0134034	2-hydroxy-3-(2-hydroxyphenyl)propanal	C9H10O3	M-H	165.0557	0.5
	HMDB0134032	3-(2,3-dihydroxyphenyl)propanal	C9H10O3	M-H	165.0557	0.5
	HMDB0134037	2-[3-(hydroxymethyl)oxiran-2-yl]phenol	C9H10O3	M-H	165.0557	0.5
	HMDB0134038	2-(3-hydroxyprop-1-en-1-yl)benzene-1,4-diol	C9H10O3	M-H	165.0557	0.5
	HMDB0134036	3-(3-hydroxyprop-1-en-1-yl)benzene-1,2-diol	C9H10O3	M-H	165.0557	0.5
	HMDB0137472	4-[(E)-2-hydroxyethenyl]-2-methoxyphenol	C9H10O3	M-H	165.0557	0.5
	HMDB0141765	4-[(1E)-3-hydroxyprop-1-en-1-yl]benzene-1,2-diol	C9H10O3	M-H	165.0557	0.5
	HMDB0124925	(R)-3-hydroxy-3-phenylpropionic acid	C9H10O3	M-H	165.0557	0.5
	HMDB0032030	Guaicyl acetate	C9H10O3	M-H	165.0557	0.5
	HMDB0040645	3-Hydroxy-1-(4-hydroxyphenyl)-1-propanone	C9H10O3	M-H	165.0557	0.5
	HMDB0034243	Ipomeanine	C9H10O3	M-H	165.0557	0.5
	HMDB0032605	Methyl 2-methoxybenzoate	C9H10O3	M-H	165.0557	0.5
	HMDB0032573	Ethylparaben	C9H10O3	M-H	165.0557	0.5
	HMDB0032639	Methyl 4-methoxybenzoate	C9H10O3	M-H	165.0557	0.5
	HMDB0031132	3,4-Dihydroxyphenylacetone	C9H10O3	M-H	165.0557	0.5
	HMDB0032138	3,4-Dimethoxybenzaldehyde	C9H10O3	M-H	165.0557	0.5
	HMDB0033752	3-(2-Hydroxyphenyl)propanoic acid	C9H10O3	M-H	165.0557	0.5
	HMDB0142137	2-hydroxy-2-phenylpropanoic acid	C9H10O3	M-H	165.0557	0.5
	HMDB0041683	4-Hydroxyphenyl-2-propionic acid	C9H10O3	M-H	165.0557	0.5
	HMDB0029665	Ethyl vanillin	C9H10O3	M-H	165.0557	0.5
	HMDB0034993	4-Methoxybenzyl formate	C9H10O3	M-H	165.0557	0.5
	HMDB0000563	D-Phenyllactic acid	C9H10O3	M-H	165.0557	0.5
	HMDB0002199	Desaminotyrosine	C9H10O3	M-H	165.0557	0.5
	HMDB0000375	3-(3-Hydroxyphenyl)propanoic acid	C9H10O3	M-H	165.0557	0.5
	HMDB0000748	L-3-Phenyllactic acid	C9H10O3	M-H	165.0557	0.5
	HMDB0000779	Phenyllactic acid	C9H10O3	M-H	165.0557	0.5
	HMDB0002072	4-Methoxyphenylacetic acid	C9H10O3	M-H	165.0557	0.5
	HMDB0002229	3-Phenoxypropionic acid	C9H10O3	M-H	165.0557	0.5
	HMDB0005175	Homovanillin	C9H10O3	M-H	165.0557	0.5
	HMDB0029817	Ethyl salicylate	C9H10O3	M-H	165.0557	0.5
	HMDB0166610	3-(3,4-dihydroxyphenyl)propanal	C9H10O3	M-H	165.0557	0.5
	HMDB0062590	Tropate	C9H10O3	M-H	165.0557	0.5
	HMDB0168657	Ethyl 3-hydroxybenzoate	C9H10O3	M-H	165.0557	0.5
	HMDB0062026	3-23-1	C9H10O3	M-H	165.0557	0.5
	HMDB0059969	3-Methoxyphenylacetic acid	C9H10O3	M-H	165.0557	0.5
	HMDB0013815	2,3-Dihydrobenzofuran	C8H8O	M+FA-H	165.0557	0.5
	HMDB0033910	Acetophenone	C8H8O	M+FA-H	165.0557	0.5
	HMDB0006236	Phenylacetaldehyde	C8H8O	M+FA-H	165.0557	0.5
	HMDB0124943	3-ethenylphenol	C8H8O	M+FA-H	165.0557	0.5
	HMDB0062765	styrene oxide	C8H8O	M+FA-H	165.0557	0.5
	HMDB0029638	4-Methylbenzaldehyde	C8H8O	M+FA-H	165.0557	0.5
	HMDB0029636	2-Methylbenzaldehyde	C8H8O	M+FA-H	165.0557	0.5
	HMDB0172088	2-Vinylphenol	C8H8O	M+FA-H	165.0557	0.5
	HMDB0038997	Lentialexin	C8H8O	M+FA-H	165.0557	0.5
	HMDB0029637	3-Methylbenzaldehyde	C8H8O	M+FA-H	165.0557	0.5
	HMDB0004072	4-Hydroxystyrene	C8H8O	M+FA-H	165.0557	0.5
	HMDB0040458	1,2,4-Tris(methylene)cyclohexane	C9H12	M+FA-H	165.0921	-0.6
	HMDB0059877	Propylbenzene	C9H12	M+FA-H	165.0921	-0.6
	HMDB0059819	o-Ethyltoluene	C9H12	M+FA-H	165.0921	-0.6
	HMDB0013733	1,2,4-Trimethylbenzene	C9H12	M+FA-H	165.0921	-0.6
	HMDB0059848	m-Ethyl toluene	C9H12	M+FA-H	165.0921	-0.6
	HMDB0041924	Mesitylene	C9H12	M+FA-H	165.0921	-0.6

HMDB0059901	Hemimellitene	C9H12	M+FA-H	165.0921	-0.6
HMDB0061962	1-ethyl-4-methylbenzene	C9H12	M+FA-H	165.0921	-0.6
HMDB0034029	Isopropylbenzene	C9H12	M+FA-H	165.0921	-0.6
HMDB0179460	NSC143559	C10H14O2	M-H	165.0921	-0.6
HMDB0163096	4,5-epoxy-(e,z)-2,7-decadienal	C10H14O2	M-H	165.0921	-0.6
HMDB0163098	(4Z,7Z)--hydroxydeca-2,4,7-trienal	C10H14O2	M-H	165.0921	-0.6
HMDB0163095	3-[(1Z,4Z)-hepta-1,4-dien-1-yl]oxirane-2-carbaldehyde	C10H14O2	M-H	165.0921	-0.6
HMDB0163097	(2E,4Z)-6-(3-ethyloxiran-2-yl)hexa-2,4-dienal	C10H14O2	M-H	165.0921	-0.6
HMDB0163094	(2E,7Z)-9-hydroxydeca-2,4,7-trienal	C10H14O2	M-H	165.0921	-0.6
HMDB0163093	SCHEMBL36924	C10H14O2	M-H	165.0921	-0.6
HMDB0146631	3-(2-methoxyphenyl)propan-1-ol	C10H14O2	M-H	165.0921	-0.6
HMDB0179459	5-methyl-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O2	M-H	165.0921	-0.6
HMDB0180472	2-(4-methylphenyl)propane-1,2-diol	C10H14O2	M-H	165.0921	-0.6
HMDB0180474	p-Cymene-9,-diol	C10H14O2	M-H	165.0921	-0.6
HMDB0181689	4-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M-H	165.0921	-0.6
HMDB0181688	1-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M-H	165.0921	-0.6
HMDB0181686	2-(hydroxymethyl)-3-methyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M-H	165.0921	-0.6
HMDB0181687	5-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M-H	165.0921	-0.6
HMDB0181685	3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M-H	165.0921	-0.6
HMDB0180473	2-[4-(hydroxymethyl)phenyl]propan-1-ol	C10H14O2	M-H	165.0921	-0.6
HMDB0041584	3-Hydroxy-p-mentha-1,8-dien-7-al	C10H14O2	M-H	165.0921	-0.6
HMDB0135742	3-(4-methoxyphenyl)propan-1-ol	C10H14O2	M-H	165.0921	-0.6
HMDB0127496	1-ethyl-3,5-dimethoxybenzene	C10H14O2	M-H	165.0921	-0.6
HMDB0062603	2-(4-methoxyphenyl)propan-2-ol	C10H14O2	M-H	165.0921	-0.6
HMDB0032462	Pentyl 2-furyl ketone	C10H14O2	M-H	165.0921	-0.6
HMDB0029691	Wine lactone	C10H14O2	M-H	165.0921	-0.6
HMDB0031085	6-Pentyl-2H-pyran-2-one	C10H14O2	M-H	165.0921	-0.6
HMDB0037011	5-Hydroxy-p-mentha-6,8-dien-2-one	C10H14O2	M-H	165.0921	-0.6
HMDB0032062	2-tert-Butyl-1,4-benzenediol	C10H14O2	M-H	165.0921	-0.6
HMDB0036878	1,4-Epidioxy-p-mentha-2,8-diene	C10H14O2	M-H	165.0921	-0.6
HMDB0037012	2-Hydroxy-p-mentha-1,8-dien-6-one	C10H14O2	M-H	165.0921	-0.6
HMDB0037044	Rotundifolone	C10H14O2	M-H	165.0921	-0.6
HMDB0032615	1,1-Dimethoxy-2-phenylethane	C10H14O2	M-H	165.0921	-0.6
HMDB0035328	Perilla ketone	C10H14O2	M-H	165.0921	-0.6
HMDB0035063	Epinepetalactone	C10H14O2	M-H	165.0921	-0.6
HMDB0036879	1,2,3,4-Diepoxy-p-menth-8-ene	C10H14O2	M-H	165.0921	-0.6
HMDB0035235	2,4,7-Decatrienoic acid	C10H14O2	M-H	165.0921	-0.6
HMDB0036084	Isomintlactone	C10H14O2	M-H	165.0921	-0.6
HMDB0179461	2-methyl-5-(propan-2-yl)benzene-1,4-diol	C10H14O2	M-H	165.0921	-0.6
HMDB0032135	2-Methoxy-4-propylphenol	C10H14O2	M-H	165.0921	-0.6
HMDB0039382	(1xi,4xi,6xi)-Carvone oxide	C10H14O2	M-H	165.0921	-0.6
HMDB0034922	alpha-Teresantalic acid	C10H14O2	M-H	165.0921	-0.6
HMDB0036042	Marmelolactone A	C10H14O2	M-H	165.0921	-0.6
HMDB0004586	Perillic acid	C10H14O2	M-H	165.0921	-0.6
HMDB0041000	Karahana lactone	C10H14O2	M-H	165.0921	-0.6
HMDB0040176	4-Ethyl-1,2-dimethoxybenzene	C10H14O2	M-H	165.0921	-0.6
HMDB0182628	2-[3-(hydroxymethyl)-2,2-dimethylcyclopent-3-en-1-yl]acetic acid	C10H16O3	M-H2O-H	165.0916	2.7
HMDB0182627	2-[2-(hydroxymethyl)-2,3-dimethylcyclopent-3-en-1-yl]acetic acid	C10H16O3	M-H2O-H	165.0916	2.7
HMDB0178772	(4Z,8Z)-6-hydroxydeca-4,8-dienoic acid	C10H16O3	M-H2O-H	165.0916	2.7
HMDB0039710	1-Acetylcyclohexyl acetate	C10H16O3	M-H2O-H	165.0916	2.7
HMDB0039052	(4S,8R)-8,9-Dihydroxy-p-menth-1(6)-en-2-one	C10H16O3	M-H2O-H	165.0916	2.7
HMDB0182630	2-{1,2,2-trimethyl-6-oxabicyclo[3.1]hexan-3-yl}acetic acid	C10H16O3	M-H2O-H	165.0916	2.7
HMDB0131084	(5E)-2,2,5-trimethyl-7-oxohept-5-enoic acid	C10H16O3	M-H2O-H	165.0916	2.7
HMDB0182631	SCHEMBL59867	C10H16O3	M-H2O-H	165.0916	2.7
HMDB0182629	SCHEMBL5986763	C10H16O3	M-H2O-H	165.0916	2.7
HMDB0178770	(4Z,8Z)--hydroxydeca-4,8-dienoic acid	C10H16O3	M-H2O-H	165.0916	2.7
HMDB0179403	SCHEMBL12833	C10H16O3	M-H2O-H	165.0916	2.7

	HMDB0178771	(4Z,8Z)-3-hydroxydeca-4,8-dienoic acid	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0179404	(2E,4Z)--hydroxydeca-2,4-dienoic acid	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0178774	3-{3-[(3Z)-pent-3-en-1-yl]oxiran-2-yl}propanoic acid	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0178773	(4Z)-7-(3-methyloxiran-2-yl)hept-4-enoic acid	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0178775	(4Z,8Z)-2-hydroxydeca-4,8-dienoic acid	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0179400	(4Z)-6-hydroxydeca-2,4-dienoic acid	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0176286	3,6-dihydroxy-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0176284	6,6-dihydroxy-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0040883	(E)--Oxo-8-decenoic acid	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0179402	3-[(1Z)-hept-1-en-1-yl]oxirane-2-carboxylic acid	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0178769	(4Z,8Z)-7-hydroxydeca-4,8-dienoic acid	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0036998	(S)-Oleuropeic acid	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0036117	(1'R)-Nepetalic acid	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0176282	6-hydroxy-1-(hydroxymethyl)-7,7-dimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0176283	1-Methyl-6-hydroxy-7-methyl-7-(hydroxymethyl)norbornane-2-one	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0176285	5,6-dihydroxy-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M-H2O-H	165.0916	2.7
	HMDB0179401	(2E,4Z)-9-hydroxydeca-2,4-dienoic acid	C10H16O3	M-H2O-H	165.0916	2.7
166.0508	HMDB0035281	2-Acetylpyridine	C7H7NO	M+FA-H	166.0510	-1.0
	HMDB0004461	Benzamide	C7H7NO	M+FA-H	166.0510	-1.0
	HMDB0033131	3-Acetylpyridine	C7H7NO	M+FA-H	166.0510	-1.0
	HMDB0181253	Tetrahydro-1H-isoindole-1,3,5(2H,6H)-trione	C8H9NO3	M-H	166.0510	-1.0
	HMDB0167787	3,7a-dihydroxy-3a,4,7,7a-tetrahydro-1H-isoindol-1-one	C8H9NO3	M-H	166.0510	-1.0
	HMDB0167786	Tetrahydrophthalimide epoxide	C8H9NO3	M-H	166.0510	-1.0
	HMDB0240370	2-hydroxy-n-(2-hydroxyphenyl)acetamide	C8H9NO3	M-H	166.0510	-1.0
	HMDB0181280	octahydroisoindoletrione	C8H9NO3	M-H	166.0510	-1.0
	HMDB0060374	3-Methoxyanthranilate	C8H9NO3	M-H	166.0510	-1.0
	HMDB0001545	Pyridoxal	C8H9NO3	M-H	166.0510	-1.0
	HMDB0034887	3alpha,4,5,7alpha-Tetrahydro-5-hydroxy-1H-isoindole-1,3(2H)-dione	C8H9NO3	M-H	166.0510	-1.0
	HMDB0034889	3alpha,4,7,7alpha-Tetrahydro-4-hydroxy-1H-isoindole-1,3(2H)-dione	C8H9NO3	M-H	166.0510	-1.0
	HMDB0004290	Isopyridoxal	C8H9NO3	M-H	166.0510	-1.0
	HMDB0155837	5-(2-amino-1-hydroxyethyl)benzene-1,2,3-triol	C8H11NO4	M-H2O-H	166.0504	2.3
	HMDB0155838	4-(2-amino-1-hydroxyethyl)benzene-1,2,3-triol	C8H11NO4	M-H2O-H	166.0504	2.3
	HMDB0155839	2623-77	C8H11NO4	M-H2O-H	166.0504	2.3
167.0350	HMDB0184098	2,4-dihydroxy-m-toluic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0171313	Methyl 2,5-dihydroxybenzoate	C8H8O4	M-H	167.0350	0.1
	HMDB0240257	Quinolacetic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0150427	o-orsellinic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0125536	3-hydroxy-5-methoxybenzoic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0171312	methyl 2,3-dihydroxybenzoate	C8H8O4	M-H	167.0350	0.1
	HMDB0146634	2-Hydroxy-6-methoxybenzoic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0146638	4-hydroxy-2-methoxybenzoic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0140902	3-hydroxy-2-methoxybenzoic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0184097	2-hydroxy-3-(hydroxymethyl)benzoic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0184096	3-Methylgentisic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0183283	2-(2,5-dioxocyclohex-3-en-1-yl)acetic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0150438	SCHEMBL11571511	C8H8O4	M-H	167.0350	0.1
	HMDB0137458	5-[(E)-2-hydroxyethenyl]benzene-1,2,3-triol	C8H8O4	M-H	167.0350	0.1
	HMDB0137459	4-[(E)-2-hydroxyethenyl]benzene-1,2,3-triol	C8H8O4	M-H	167.0350	0.1
	HMDB0094709	3,5-dihydroxyphenylacetic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0184099	2,4-dihydroxy-3-methylbenzoic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0137460	5-[(E)-2-hydroxyethenyl]benzene-1,2,4-triol	C8H8O4	M-H	167.0350	0.1
	HMDB0166110	5-hydroxy-2-methoxybenzoic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0001336	3,4-Dihydroxybenzeneacetic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0059713	3-Methoxysalicylic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0029644	2',4',6'-Trihydroxyacetophenone	C8H8O4	M-H	167.0350	0.1
	HMDB0131176	2-hydroxy-4-methoxybenzoic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0029673	2,6-Dimethoxy-1,4-benzoquinone	C8H8O4	M-H	167.0350	0.1
	HMDB0033129	3-Acetyl-4-hydroxy-6-methyl-2H-pyran-2-one	C8H8O4	M-H	167.0350	0.1

	HMDB0034335	Thermophilin	C8H8O4	M-H	167.0350	0.1
	HMDB0006242	3,4-Dihydroxymandelaldehyde	C8H8O4	M-H	167.0350	0.1
	HMDB0001868	5-Methoxysalicylic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0000822	p-Hydroxymandelic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0000750	3-Hydroxymandelic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0000484	Vanillic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0000130	Homogentisic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0060003	Isovanillic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0062008	2-(2,3-dihydroxyphenyl)acetic acid	C8H8O4	M-H	167.0350	0.1
	HMDB0001870	Benzoic acid	C7H6O2	M+FA-H	167.0350	0.1
	HMDB0011718	4-Hydroxybenzaldehyde	C7H6O2	M+FA-H	167.0350	0.1
	HMDB0186744	3-hydroxybenzaldehyde	C7H6O2	M+FA-H	167.0350	0.1
	HMDB0032918	3-(2-Furanyl)-2-propenal	C7H6O2	M+FA-H	167.0350	0.1
	HMDB0034170	2-Hydroxybenzaldehyde	C7H6O2	M+FA-H	167.0350	0.1
167.0465	HMDB0013159	2,3-Diaminosalicylic acid	C7H8N2O3	M-H	167.0462	1.7
	HMDB0059778	2-Pyrroloylglycine	C7H8N2O3	M-H	167.0462	1.7
	HMDB0001406	Niacinamide	C6H6N2O	M+FA-H	167.0462	1.7
	HMDB0031861	2-Acetylpyrazine	C6H6N2O	M+FA-H	167.0462	1.7
167.0713	HMDB0030540	2,5-Dimethylphenol	C8H10O	M+FA-H	167.0714	-0.4
	HMDB0062024	2,7-Dimethyloxyepine	C8H10O	M+FA-H	167.0714	-0.4
	HMDB0041609	4-Methylbenzyl alcohol	C8H10O	M+FA-H	167.0714	-0.4
	HMDB0032150	2,6-Dimethylphenol	C8H10O	M+FA-H	167.0714	-0.4
	HMDB0032074	1-Methoxy-2-methylbenzene	C8H10O	M+FA-H	167.0714	-0.4
	HMDB0032151	3,4-Dimethylphenol	C8H10O	M+FA-H	167.0714	-0.4
	HMDB0059873	3-Ethylphenol	C8H10O	M+FA-H	167.0714	-0.4
	HMDB0029306	4-Ethylphenol	C8H10O	M+FA-H	167.0714	-0.4
	HMDB0033944	2-Phenylethanol	C8H10O	M+FA-H	167.0714	-0.4
	HMDB0032076	1-Methoxy-4-methylbenzene	C8H10O	M+FA-H	167.0714	-0.4
	HMDB0032148	2,3-Dimethylphenol	C8H10O	M+FA-H	167.0714	-0.4
	HMDB0032619	1-Phenylethanol	C8H10O	M+FA-H	167.0714	-0.4
	HMDB0131223	3,5-dimethoxy-2-methylphenol	C9H12O3	M-H	167.0714	-0.4
	HMDB0151518	SCHEMBL1954	C9H12O3	M-H	167.0714	-0.4
	HMDB0125521	4-ethyl-6-methoxybenzene-1,3-diol	C9H12O3	M-H	167.0714	-0.4
	HMDB0125531	5-ethyl-3-methoxybenzene-1,2-diol	C9H12O3	M-H	167.0714	-0.4
	HMDB0125541	4-ethyl-2-methoxybenzene-1,3-diol	C9H12O3	M-H	167.0714	-0.4
	HMDB0126600	5-methoxy-2,4-dimethylbenzene-1,3-diol	C9H12O3	M-H	167.0714	-0.4
	HMDB0168685	2-(4-(Hydroxymethyl)phenoxy)ethanol	C9H12O3	M-H	167.0714	-0.4
	HMDB0032921	Ethyl 2-furanpropionate	C9H12O3	M-H	167.0714	-0.4
	HMDB0030472	4-Ipomeanol	C9H12O3	M-H	167.0714	-0.4
	HMDB0059963	1,3,5-Trimethoxybenzene	C9H12O3	M-H	167.0714	-0.4
	HMDB0032252	Epoxyoxophorone	C9H12O3	M-H	167.0714	-0.4
	HMDB0030473	1-Ipomeanol	C9H12O3	M-H	167.0714	-0.4
	HMDB0038925	(4-Hydroxy-3-methoxyphenyl)ethanol	C9H12O3	M-H	167.0714	-0.4
	HMDB0029680	2,6-Dimethoxy-4-methylphenol	C9H12O3	M-H	167.0714	-0.4
	HMDB0037729	2-Furanylmethyl butanoate	C9H12O3	M-H	167.0714	-0.4
	HMDB0030992	5-Butyltetrahydro-2-oxo-3-furancarboxylic acid	C9H14O4	M-H2O-H	167.0708	2.9
	HMDB0030988	5-(2-Methylpropyl)tetrahydro-2-oxo-3-furancarboxylic acid	C9H14O4	M-H2O-H	167.0708	2.9
	HMDB0061784	3-Allyl-1-cyclohexene	C9H14	M+FA-H	167.1078	-0.3
	HMDB0038140	Santene	C9H14	M+FA-H	167.1078	-0.3
	HMDB0176281	6-hydroxycamphor	C10H16O2	M-H	167.1078	-0.3
	HMDB0169534	geranic acid	C10H16O2	M-H	167.1078	-0.3
	HMDB0182617	25435-53-4	C10H16O2	M-H	167.1078	-0.3
	HMDB0181693	3-(hydroxymethyl)-2,3-dimethyltricyclo[2.2.1,heptan-1-ol	C10H16O2	M-H	167.1078	-0.3
	HMDB0181692	7-(hydroxymethyl)-1,7-dimethyltricyclo[2.2.1,heptan-3-ol	C10H16O2	M-H	167.1078	-0.3
	HMDB0181691	[7-(hydroxymethyl)-7-methyltricyclo[2.2.1,heptan-1-yl]methanol	C10H16O2	M-H	167.1078	-0.3
	HMDB0181690	[3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptan-3-yl]methanol	C10H16O2	M-H	167.1078	-0.3
	HMDB0181638	2-methyl-5-(propan-2-yl)bicyclo[3.1]hex-3-ene-2,6-	C10H16O2	M-H	167.1078	-0.3
	HMDB0181639	5-(1-hydroxypropan-2-yl)-2-methylbicyclo[3.1]hex-3-en-2-ol	C10H16O2	M-H	167.1078	-0.3

HMDB0181635	5-(2-hydroxypropan-2-yl)-2-methylbicyclo[3.1]hex-3-en-2-ol	C10H16O2	M-H	167.1078	-0.3
HMDB0181634	2-(hydroxymethyl)-5-(propan-2-yl)bicyclo[3.1]hex-3-en-2-ol	C10H16O2	M-H	167.1078	-0.3
HMDB0181636	5-methyl-1-(propan-2-yl)-3-oxatricyclo[4.1,heptan-5-ol	C10H16O2	M-H	167.1078	-0.3
HMDB0181637	2-methyl-5-(propan-2-yl)bicyclo[3.1]hex-3-ene-1,2-	C10H16O2	M-H	167.1078	-0.3
HMDB0179485	14-64-6	C10H16O2	M-H	167.1078	-0.3
HMDB0182618	2-hydroxy-2-(2,2,3-trimethylcyclopent-3-en-1-yl)acetaldehyde	C10H16O2	M-H	167.1078	-0.3
HMDB0182619	2-[2-(hydroxymethyl)-2,3-dimethylcyclopent-3-en-1-yl]acetaldehyde	C10H16O2	M-H	167.1078	-0.3
HMDB0240639	(1S,4R,6R)-1,3,3-Trimethyl-6-hydroxybicyclo[2.2.1]heptane-2-one	C10H16O2	M-H	167.1078	-0.3
HMDB0182798	(1S,4R,6S)-1,3,3-Trimethyl-6-hydroxybicyclo[2.2.1]heptane-2-one	C10H16O2	M-H	167.1078	-0.3
HMDB0182796	3-(hydroxymethyl)-1,3-dimethylbicyclo[2.2.1]heptan-2-one	C10H16O2	M-H	167.1078	-0.3
HMDB0182797	7-hydroxy-1,3,3-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O2	M-H	167.1078	-0.3
HMDB0182799	5-hydroxy-1,3,3-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O2	M-H	167.1078	-0.3
HMDB0182685	6-Hydroxycarvotanacetone	C10H16O2	M-H	167.1078	-0.3
HMDB0182684	SCHEMBL6689811	C10H16O2	M-H	167.1078	-0.3
HMDB0182683	1-methyl-4-(propan-2-yl)-7-oxabicyclo[4.1]heptan-2-one	C10H16O2	M-H	167.1078	-0.3
HMDB0182680	2-(hydroxymethyl)-5-(propan-2-yl)cyclohex-2-en-1-	C10H16O2	M-H	167.1078	-0.3
HMDB0182620	2-[3-(hydroxymethyl)-2,2-dimethylcyclopent-3-en-1-yl]acetaldehyde	C10H16O2	M-H	167.1078	-0.3
HMDB0182621	SCHEMBL14359771	C10H16O2	M-H	167.1078	-0.3
HMDB0179394	2E,4Z-decadienoic acid	C10H16O2	M-H	167.1078	-0.3
HMDB0178761	SCHEMBL7756279	C10H16O2	M-H	167.1078	-0.3
HMDB0163117	(z,z)-4,7-decadienoic acid	C10H16O2	M-H	167.1078	-0.3
HMDB0136694	6-hydroxy-3,7-dimethylocta-2,7-dienal	C10H16O2	M-H	167.1078	-0.3
HMDB0163110	(2E,4Z)-6-(3-ethyloxiran-2-yl)hexa-2,4-dien-1-ol	C10H16O2	M-H	167.1078	-0.3
HMDB0163108	{3-[(1Z,4Z)-hepta-1,4-dien-1-yl]oxiran-2-yl}methanol	C10H16O2	M-H	167.1078	-0.3
HMDB0163109	(2E)-3-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}prop-2-en-1-ol	C10H16O2	M-H	167.1078	-0.3
HMDB0163104	(4Z,7Z)-2-hydroxydeca-4,7-dienal	C10H16O2	M-H	167.1078	-0.3
HMDB0163106	(4Z,7Z)-deca-2,4,7-triene-1,-diol	C10H16O2	M-H	167.1078	-0.3
HMDB0163103	(4Z,7Z)--hydroxydeca-4,7-dienal	C10H16O2	M-H	167.1078	-0.3
HMDB0163105	(2E,7Z)-deca-2,4,7-triene-1,9-diol	C10H16O2	M-H	167.1078	-0.3
HMDB0163101	3-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}propanal	C10H16O2	M-H	167.1078	-0.3
HMDB0163099	(4Z,7Z)-3-hydroxydeca-4,7-dienal	C10H16O2	M-H	167.1078	-0.3
HMDB0163102	(4Z)-6-(3-ethyloxiran-2-yl)hex-4-enal	C10H16O2	M-H	167.1078	-0.3
HMDB0163100	(7Z)-9-hydroxydeca-4,7-dienal	C10H16O2	M-H	167.1078	-0.3
HMDB0182795	ACMC-mnp1	C10H16O2	M-H	167.1078	-0.3
HMDB0013105	trans-4,5-epoxy-2(E)-decenal	C10H16O2	M-H	167.1078	-0.3
HMDB0182682	4-hydroxy-2-methyl-5-(propan-2-yl)cyclohex-2-en-1-one	C10H16O2	M-H	167.1078	-0.3
HMDB0032434	(+/-)-2-(5-Methyl-5-vinyltetrahydrofuran-2-yl)propionaldehyde	C10H16O2	M-H	167.1078	-0.3
HMDB0032319	cis-3-Hexenyl crotonate	C10H16O2	M-H	167.1078	-0.3
HMDB0032313	2,4-Hexadienyl isobutyrate	C10H16O2	M-H	167.1078	-0.3
HMDB0032312	2,4-Hexadienyl butyrate	C10H16O2	M-H	167.1078	-0.3
HMDB0182681	8-Hydroxycarvotanacetone	C10H16O2	M-H	167.1078	-0.3
HMDB0037014	gamma-Diosphenol	C10H16O2	M-H	167.1078	-0.3
HMDB0034670	6-Hydroxy-2,6-dimethyl-2,7-octadien-4-one	C10H16O2	M-H	167.1078	-0.3
HMDB0035829	Dihydronepetalactone	C10H16O2	M-H	167.1078	-0.3
HMDB0032219	(+/-)-Dihydromintlactone	C10H16O2	M-H	167.1078	-0.3
HMDB0035766	Ascaridole	C10H16O2	M-H	167.1078	-0.3
HMDB0035714	Epoxysteremisia ketone	C10H16O2	M-H	167.1078	-0.3
HMDB0040639	(xi)-(Z)-5-(3-Hexenyl)dihydro-2(3H)-furanone	C10H16O2	M-H	167.1078	-0.3
HMDB0037175	4-Isopropyl-3-cyclohexene-1-carboxylic acid	C10H16O2	M-H	167.1078	-0.3
HMDB0036103	Geranic acid	C10H16O2	M-H	167.1078	-0.3
HMDB0034452	5,6-Dihydro-6-pentyl-2H-pyran-2-one	C10H16O2	M-H	167.1078	-0.3
HMDB0033700	(-)-(Z)-Tetrahydro-6-(2-pentenyl)-2H-pyran-2-one	C10H16O2	M-H	167.1078	-0.3
HMDB0037821	xi-1,8,8-Trimethyl-2-oxabicyclo[3.2.1]octan-3-one	C10H16O2	M-H	167.1078	-0.3

	HMDB0031156	Ethyl (4Z)-4,7-octadienoate	C10H16O2	M-H	167.1078	-0.3
	HMDB0031273	Methyl octynecarboxylate	C10H16O2	M-H	167.1078	-0.3
	HMDB0036067	Epoxycampholenic aldehyde	C10H16O2	M-H	167.1078	-0.3
	HMDB0164896	6,7-dihydroxy-7-methyl-3-methylideneoctanal	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0180511	Oxiraneoctanoic acid	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0039533	(E)--Hydroxy-8-decenoic acid	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0039587	5-Hexyl-1,4-dioxan-2-one	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0010724	3-Oxodecanoic acid	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0164962	1-(2-hydroxypropan-2-yl)-4-methylbicyclo[3.1]hexane-2,4-diol	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0033010	(1S,2S,4S,5R)-1,8-Epoxy-p-menthane-2,5-diol	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0039582	6-Hexyl-1,4-dioxan-2-one	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0038692	6-Methyl-2-methylene-6-octene-1,3,8-triol	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0180051	(6E)-8-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0041376	exo,exo-1,8-Epoxy-p-menthane-2,6-diol	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0180512	2-hydroxydec-9-enoic acid	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0180510	8-hydroxy-9-decenoic acid	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0180052	(6E)-5-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0180507	5-hydroxydec-9-enoic acid	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0180506	4-hydroxydec-9-enoic acid	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0180508	6-hydroxydec-9-enoic acid	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0180505	3-hydroxy-9-decenoic acid	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0180148	1-(hydroxymethyl)-3,3-dimethyl-2-oxabicyclo[2.2.2]octan-6-ol	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0180055	(6E)-2-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0038978	(1beta,2beta,5beta)-p-Menth-3-ene-1,2,5-triol	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0180054	(6E)-9-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0030367	Ethyl (3R,5Z)-3-hydroxy-5-octenoate	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0180053	5-[3-(propan-2-yl)oxiran-2-yl]pentanoic acid	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0040205	3-Methylbutyl 3-hydroxy-2-methylidenebutanoate	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0041545	(1R,2R,4R)-1,8-Epoxy-p-menthane-2,4-diol	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0040204	2-Methylbutyl 3-hydroxy-2-methylidenebutanoate	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0030369	3-Hydroxy-5Z-octenyl acetate	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0180509	7-hydroxydec-9-enoic acid	C10H18O3	M-H2O-H	167.1072	3.0
	HMDB0163825	5-(1,2-dihydroxypropan-2-yl)-2-methylcyclohexan-1-one	C10H18O3	M-H2O-H	167.1072	3.0
168.0433	HMDB0060244	Phosphodimethylethanolamine	C4H12NO4P	M-H	168.0431	1.1
	HMDB0005785	Indole-3-carbinol	C9H9NO	M+Na-2H	168.0431	1.3
	HMDB0172056	3-(2-hydroxyphenyl)propanenitrile	C9H9NO	M+Na-2H	168.0431	1.3
	HMDB0159222	3-methyl-1H-indol-6-ol	C9H9NO	M+Na-2H	168.0431	1.3
	HMDB0159224	1125-35-5	C9H9NO	M+Na-2H	168.0431	1.3
	HMDB0159223	5-Hydroxy-3-methylindole	C9H9NO	M+Na-2H	168.0431	1.3
	HMDB0159225	3-Methyl-1H-indol-4-ol	C9H9NO	M+Na-2H	168.0431	1.3
	HMDB0172057	3-Hydroxy-3-phenylpropanenitrile	C9H9NO	M+Na-2H	168.0431	1.3
	HMDB0172058	3-(3-hydroxyphenyl)propanenitrile	C9H9NO	M+Na-2H	168.0431	1.3
	HMDB0172059	3-(4-Hydroxyphenyl)propionitrile	C9H9NO	M+Na-2H	168.0431	1.3
	HMDB0030204	1-(2-Furanylmethyl)-1H-pyrrole	C9H9NO	M+Na-2H	168.0431	1.3
	HMDB0040009	4-(2-Furanylmethylene)-3,4-dihydro-2H-pyrrole	C9H9NO	M+Na-2H	168.0431	1.3
	HMDB0040011	3-(2-Furanylmethyl)-1H-pyrrole	C9H9NO	M+Na-2H	168.0431	1.3
169.0506	HMDB0135619	3-methoxyphenol	C7H8O2	M+FA-H	169.0506	-0.2
	HMDB0001398	Guaiacol	C7H8O2	M+FA-H	169.0506	-0.2
	HMDB0040280	1-(2-Furanyl)-1-propanone	C7H8O2	M+FA-H	169.0506	-0.2
	HMDB0059709	2-Hydroxybenzyl alcohol	C7H8O2	M+FA-H	169.0506	-0.2
	HMDB0059712	3-Hydroxybenzyl alcohol	C7H8O2	M+FA-H	169.0506	-0.2
	HMDB0032917	1-(2-Furanyl)-2-propanone	C7H8O2	M+FA-H	169.0506	-0.2
	HMDB0038963	4,6-Heptadiyne-1,3-diol	C7H8O2	M+FA-H	169.0506	-0.2
	HMDB0000873	4-Methylcatechol	C7H8O2	M+FA-H	169.0506	-0.2
	HMDB0035226	2-Acetyl-5-methylfuran	C7H8O2	M+FA-H	169.0506	-0.2
	HMDB0011724	4-Hydroxybenzyl alcohol	C7H8O2	M+FA-H	169.0506	-0.2
	HMDB0029696	Mequinol	C7H8O2	M+FA-H	169.0506	-0.2
	HMDB0034877	2-Acetyl-3-methylfuran	C7H8O2	M+FA-H	169.0506	-0.2
	HMDB0179996	SCHEMBL285344	C8H10O4	M-H	169.0506	-0.2
	HMDB0173106	2,5-dimethoxycyclohex-2-ene-1,4-dione	C8H10O4	M-H	169.0506	-0.2
	HMDB0132906	3,5-dimethoxybenzene-1,2-diol	C8H10O4	M-H	169.0506	-0.2

	HMDB0153684	2-(hydroxymethyl)-5-methoxybenzene-1,3-diol	C8H10O4	M-H	169.0506	-0.2
	HMDB0133971	3,4-dimethoxybenzene-1,2-diol	C8H10O4	M-H	169.0506	-0.2
	HMDB0133982	4,5-dimethoxybenzene-1,3-diol	C8H10O4	M-H	169.0506	-0.2
	HMDB0133972	2,3-dimethoxybenzene-1,4-diol	C8H10O4	M-H	169.0506	-0.2
	HMDB0032966	Furaneol acetate	C8H10O4	M-H	169.0506	-0.2
	HMDB0038761	Herierin IV	C8H10O4	M-H	169.0506	-0.2
	HMDB0038760	Herierin III	C8H10O4	M-H	169.0506	-0.2
	HMDB0000318	3,4-Dihydroxyphenylglycol	C8H10O4	M-H	169.0506	-0.2
	HMDB0059756	3,4-Methyleneadipic acid	C8H10O4	M-H	169.0506	-0.2
	HMDB0132907	2,6-dimethoxybenzene-1,4-diol	C8H10O4	M-H	169.0506	-0.2
	HMDB0153685	6-methoxy-3-methylbenzene-1,2,4-triol	C8H10O4	M-H	169.0506	-0.2
	HMDB0040141	2-Methoxy-5-methylpyrazine	C6H8N2O	M+FA-H	169.0619	2.6
169.0623	HMDB0004181	Methylimidazole acetaldehyde	C6H8N2O	M+FA-H	169.0619	2.6
	HMDB0031852	2-Methoxy-3-methylpyrazine	C6H8N2O	M+FA-H	169.0619	2.6
	HMDB0040143	2-Methoxy-6-methylpyrazine	C6H8N2O	M+FA-H	169.0619	2.6
	HMDB0033238	2-Isopropyl-5-methylfuran	C8H12O	M+FA-H	169.0870	-0.1
169.0870	HMDB0061898	Methyl-1-cyclopenten-1-yl)-ethanone	C8H12O	M+FA-H	169.0870	-0.1
	HMDB0032447	1,5-Octadien-3-one	C8H12O	M+FA-H	169.0870	-0.1
	HMDB0032446	trans, trans-3,5-Octadien-2-one	C8H12O	M+FA-H	169.0870	-0.1
	HMDB0040246	3,5,5-Trimethyl-2-cyclopenten-1-one	C8H12O	M+FA-H	169.0870	-0.1
	HMDB0039844	(E,E)-2,6-Octadienal	C8H12O	M+FA-H	169.0870	-0.1
	HMDB0031582	6-Methyl-3,5-heptadien-2-one	C8H12O	M+FA-H	169.0870	-0.1
	HMDB0040272	2-Butylfuran	C8H12O	M+FA-H	169.0870	-0.1
	HMDB0031414	2,3-Dimethyl-2-cyclohexen-1-one	C8H12O	M+FA-H	169.0870	-0.1
	HMDB0062073	5-Octen-2-yn-4-ol	C8H12O	M+FA-H	169.0870	-0.1
	HMDB0031686	(E,E)-2,4-Octadienal	C8H12O	M+FA-H	169.0870	-0.1
	HMDB0164923	3-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M-H	169.0870	-0.1
	HMDB0030471	1,4-Ipomeadiol	C9H14O3	M-H	169.0870	-0.1
	HMDB0038276	cis-3-Hexenyl pyruvate	C9H14O3	M-H	169.0870	-0.1
	HMDB0167056	(2E,6Z)-9-hydroxynona-2,6-dienoic acid	C9H14O3	M-H	169.0870	-0.1
	HMDB0167055	(2E)-5-(3-ethyloxiran-2-yl)pent-2-enoic acid	C9H14O3	M-H	169.0870	-0.1
	HMDB0167053	(2E,6Z)-5-hydroxynona-2,6-dienoic acid	C9H14O3	M-H	169.0870	-0.1
	HMDB0164924	7-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M-H	169.0870	-0.1
	HMDB0164926	5-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M-H	169.0870	-0.1
	HMDB0164922	1,3-bis(hydroxymethyl)bicyclo[2.2.1]heptan-2-one	C9H14O3	M-H	169.0870	-0.1
	HMDB0167051	(2E,6Z)-4-hydroxynona-2,6-dienoic acid	C9H14O3	M-H	169.0870	-0.1
	HMDB0164925	6-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M-H	169.0870	-0.1
	HMDB0167052	(2E,6Z)-8-hydroxynona-2,6-dienoic acid	C9H14O3	M-H	169.0870	-0.1
	HMDB0167054	3-[(3Z)-hex-3-en-1-yl]oxirane-2-carboxylic acid	C9H14O3	M-H	169.0870	-0.1
	HMDB0031415	2,6-Dimethyl-2,4-heptadiene	C9H16	M+FA-H	169.1234	-0.6
	HMDB0061920	Prop-2-enylcyclohexane	C9H16	M+FA-H	169.1234	-0.6
	HMDB0037777	2-Isopropyl-1,4-hexadiene	C9H16	M+FA-H	169.1234	-0.6
	HMDB0032344	Isobutylene-isoprene copolymer	C9H16	M+FA-H	169.1234	-0.6
	HMDB0182601	4-Hydroxypiperitone	C10H18O2	M-H	169.1234	-0.6
	HMDB0182595	8-hydroxy-p-menthan-3-one	C10H18O2	M-H	169.1234	-0.6
	HMDB0182598	2-hydroxy-p-menthanone-(3)	C10H18O2	M-H	169.1234	-0.6
	HMDB0182596	2-(2-Hydroxy-1-methylethyl)-5-methylcyclohexanone	C10H18O2	M-H	169.1234	-0.6
	HMDB0182594	5-Hydroxy-2-isopropyl-5-methylcyclohexanone	C10H18O2	M-H	169.1234	-0.6
	HMDB0182528	SCHEMBL12683693	C10H18O2	M-H	169.1234	-0.6
	HMDB0182525	2-(hydroxymethyl)-5-(propan-2-yl)cyclohexan-1-one	C10H18O2	M-H	169.1234	-0.6
	HMDB0182524	2-hydroxy-6-methyl-3-(propan-2-yl)cyclohexan-1-one	C10H18O2	M-H	169.1234	-0.6
	HMDB0182526	Oxytetrahydrocarvon	C10H18O2	M-H	169.1234	-0.6
	HMDB0182527	4-hydroxy-2-methyl-5-(propan-2-yl)cyclohexan-1-one	C10H18O2	M-H	169.1234	-0.6
	HMDB0182520	SCHEMBL12683689	C10H18O2	M-H	169.1234	-0.6
	HMDB0182521	5-(2-hydroxypropan-2-yl)-2-methylcyclohexan-1-one	C10H18O2	M-H	169.1234	-0.6
	HMDB0182522	AC1LCBYF	C10H18O2	M-H	169.1234	-0.6
	HMDB0181920	AC1MS2IY	C10H18O2	M-H	169.1234	-0.6
	HMDB0181921	1,3,3-trimethylbicyclo[2.2.1]heptane-2,5-diol	C10H18O2	M-H	169.1234	-0.6
	HMDB0181919	1,3,3-trimethylbicyclo[2.2.1]heptane-2,7-diol	C10H18O2	M-H	169.1234	-0.6
	HMDB0182600	5-(hydroxymethyl)-2-(propan-2-yl)cyclohexan-1-one	C10H18O2	M-H	169.1234	-0.6
	HMDB0182599	(+)-4-hydroxy-p-menth-3-one	C10H18O2	M-H	169.1234	-0.6

HMDB0182701	(1S)-1,7,7-trimethylbicyclo[2.2.1]heptane-2,5-diol	C10H18O2	M-H	169.1234	-0.6
HMDB0182700	1,7,7-trimethylbicyclo[2.2.1]heptane-2,6-diol	C10H18O2	M-H	169.1234	-0.6
HMDB0182698	(1S)-1,7,7-trimethylbicyclo[2.2.1]heptane-2,3-diol	C10H18O2	M-H	169.1234	-0.6
HMDB0182699	(1S)-1,7,7-trimethylbicyclo[2.2.1]heptane-2,2-diol	C10H18O2	M-H	169.1234	-0.6
HMDB0182696	SCHEMBL15462834	C10H18O2	M-H	169.1234	-0.6
HMDB0182697	(1S)-7-(hydroxymethyl)-1,7-dimethylbicyclo[2.2.1]heptan-2-ol	C10H18O2	M-H	169.1234	-0.6
HMDB0182626	2-{1,2,2-trimethyl-6-oxabicyclo[3.1]hexan-3-yl}ethan-1-ol	C10H18O2	M-H	169.1234	-0.6
HMDB0182624	SCHEMBL5398	C10H18O2	M-H	169.1234	-0.6
HMDB0182622	2-[2-(hydroxymethyl)-2,3-dimethylcyclopent-3-en-1-yl]ethan-1-ol	C10H18O2	M-H	169.1234	-0.6
HMDB0182623	2-[3-(hydroxymethyl)-2,2-dimethylcyclopent-3-en-1-yl]ethan-1-ol	C10H18O2	M-H	169.1234	-0.6
HMDB0182625	5-(2-hydroxyethyl)-3,4,4-trimethylcyclopent-2-en-1-ol	C10H18O2	M-H	169.1234	-0.6
HMDB0182602	SCHEMBL16581455	C10H18O2	M-H	169.1234	-0.6
HMDB0181916	62853-86-5	C10H18O2	M-H	169.1234	-0.6
HMDB0181918	1,3,3-trimethylbicyclo[2.2.1]heptane-2,2-diol	C10H18O2	M-H	169.1234	-0.6
HMDB0181917	3-(hydroxymethyl)-1,3-dimethylbicyclo[2.2.1]heptan-2-ol	C10H18O2	M-H	169.1234	-0.6
HMDB0161932	SCHEMBL9863268	C10H18O2	M-H	169.1234	-0.6
HMDB0161931	(2Z)-3,7-dimethylocta-2,6-diene-1,4-diol	C10H18O2	M-H	169.1234	-0.6
HMDB0179965	3-exo-hydroxy-1,8-cineole	C10H18O2	M-H	169.1234	-0.6
HMDB0131081	(2E)-7-hydroxy-3,6,6-trimethylhept-2-enal	C10H18O2	M-H	169.1234	-0.6
HMDB0161933	SCHEMBL15361567	C10H18O2	M-H	169.1234	-0.6
HMDB0161934	8-hydroxyneryl	C10H18O2	M-H	169.1234	-0.6
HMDB0180591	4-methylnon-8-enoic acid	C10H18O2	M-H	169.1234	-0.6
HMDB0180590	4-methylidenenonanoic acid	C10H18O2	M-H	169.1234	-0.6
HMDB0180496	2-hydroxydec-9-enal	C10H18O2	M-H	169.1234	-0.6
HMDB0180494	SCHEMBL186654	C10H18O2	M-H	169.1234	-0.6
HMDB0180495	SCHEMBL58664	C10H18O2	M-H	169.1234	-0.6
HMDB0180493	7-hydroxydec-9-enal	C10H18O2	M-H	169.1234	-0.6
HMDB0180491	5-hydroxydec-9-enal	C10H18O2	M-H	169.1234	-0.6
HMDB0180489	3-hydroxydec-9-enal	C10H18O2	M-H	169.1234	-0.6
HMDB0180490	4-hydroxydec-9-enal	C10H18O2	M-H	169.1234	-0.6
HMDB0180492	6-hydroxydec-9-enal	C10H18O2	M-H	169.1234	-0.6
HMDB0180107	8-METHYL-8-NONENOIC ACID	C10H18O2	M-H	169.1234	-0.6
HMDB0161936	2,3-Epoxy-3,7-dimethyloct-6-enol	C10H18O2	M-H	169.1234	-0.6
HMDB0161935	(2Z)-3,7-dimethylocta-2,6-diene-1,5-diol	C10H18O2	M-H	169.1234	-0.6
HMDB0161937	(2Z)-3,7-Dimethyl-6,7-epoxy-2-octene-1-ol	C10H18O2	M-H	169.1234	-0.6
HMDB0059852	2-Hydroxycineol	C10H18O2	M-H	169.1234	-0.6
HMDB0035837	Citronelllic acid	C10H18O2	M-H	169.1234	-0.6
HMDB0035907	Linalyl oxide	C10H18O2	M-H	169.1234	-0.6
HMDB0039768	5-Decenoic acid	C10H18O2	M-H	169.1234	-0.6
HMDB0030031	6-Methyl-5-hepten-2-yl acetate	C10H18O2	M-H	169.1234	-0.6
HMDB0040213	cis-3-Hexenyl isobutyrate	C10H18O2	M-H	169.1234	-0.6
HMDB0036990	2,6-Dimethyl-3,7-octadiene-2,6-diol	C10H18O2	M-H	169.1234	-0.6
HMDB0031362	Cyclohexylethyl acetate	C10H18O2	M-H	169.1234	-0.6
HMDB0036211	Hexyl crotonate	C10H18O2	M-H	169.1234	-0.6
HMDB0035365	Cnidial C	C10H18O2	M-H	169.1234	-0.6
HMDB0040330	Menthone lactone	C10H18O2	M-H	169.1234	-0.6
HMDB0040530	Isopentyl 3-methyl-2-butenate	C10H18O2	M-H	169.1234	-0.6
HMDB0031003	9-Decenoic acid	C10H18O2	M-H	169.1234	-0.6
HMDB0040194	Methyl 2-nonenate	C10H18O2	M-H	169.1234	-0.6
HMDB0034880	3-Methyl-2,4-nonanediene	C10H18O2	M-H	169.1234	-0.6
HMDB0029859	Methyl (xi)-3-nonenate	C10H18O2	M-H	169.1234	-0.6
HMDB0059610	2-Exo-hydroxy-1,8-cineole	C10H18O2	M-H	169.1234	-0.6
HMDB0031441	Linalool oxide III	C10H18O2	M-H	169.1234	-0.6
HMDB0041630	Linalool oxide III	C10H18O2	M-H	169.1234	-0.6
HMDB0031440	Linalool oxide (trans-pyranoid)	C10H18O2	M-H	169.1234	-0.6
HMDB0032393	2-Methylbutyl 3-methyl-2-butenate	C10H18O2	M-H	169.1234	-0.6
HMDB0061293	1-p-Menthene-8,9-diol	C10H18O2	M-H	169.1234	-0.6
HMDB0032452	1-Octen-3-yl acetate	C10H18O2	M-H	169.1234	-0.6
HMDB0032275	Ethyl 3-octenoate	C10H18O2	M-H	169.1234	-0.6
HMDB0033377	cis-3-Hexenyl butyrate	C10H18O2	M-H	169.1234	-0.6

HMDB0031297	2-Octenyl acetate	C10H18O2	M-H	169.1234	-0.6
HMDB0036992	1-Cyclopropyl-4-methyl-1,3-cyclohexanediol	C10H18O2	M-H	169.1234	-0.6
HMDB0035122	(S,E)-2,6-Dimethyl-5,7-octadiene-2,3-diol	C10H18O2	M-H	169.1234	-0.6
HMDB0037632	xi-Tetrahydro-3-pentyl-2H-pyran-2-one	C10H18O2	M-H	169.1234	-0.6
HMDB0037217	xi-5-Hexyldihydro-2(3H)-furanone	C10H18O2	M-H	169.1234	-0.6
HMDB0035839	(E)-3-(Tetrahydro-5,5-dimethyl-2-furanyl)-2-buten-1-ol	C10H18O2	M-H	169.1234	-0.6
HMDB0038744	9-Hydroxygeraniol	C10H18O2	M-H	169.1234	-0.6
HMDB0039149	(+)-6-Hydroxy-2,6-dimethyl-7-octen-4-one	C10H18O2	M-H	169.1234	-0.6
HMDB0012183	8-Methylnonenoate	C10H18O2	M-H	169.1234	-0.6
HMDB0010726	trans-Dec-2-enoic acid	C10H18O2	M-H	169.1234	-0.6
HMDB0004980	cis-4-Decenoic acid	C10H18O2	M-H	169.1234	-0.6
HMDB0037116	delta-Decalactone	C10H18O2	M-H	169.1234	-0.6
HMDB0037497	Ethyl (E)-2-octenoate	C10H18O2	M-H	169.1234	-0.6
HMDB0040208	2-Propenyl heptanoate	C10H18O2	M-H	169.1234	-0.6
HMDB0039795	Ethyl 4Z-octenoate	C10H18O2	M-H	169.1234	-0.6
HMDB0034581	2-Hexenyl butanoate	C10H18O2	M-H	169.1234	-0.6
HMDB0034427	Cyclohexyl butanoate	C10H18O2	M-H	169.1234	-0.6
HMDB0037021	trans-p-Menth-2-ene-1,4-diol	C10H18O2	M-H	169.1234	-0.6
HMDB0032119	4-Hydroxy-2,6-dimethyl-7-octen-3-one	C10H18O2	M-H	169.1234	-0.6
HMDB0029358	5Z-Octenyl acetate	C10H18O2	M-H	169.1234	-0.6
HMDB0041012	6-Decenoic acid	C10H18O2	M-H	169.1234	-0.6
HMDB0036099	Lilac alcohol	C10H18O2	M-H	169.1234	-0.6
HMDB0040726	cis-Linalyl oxide	C10H18O2	M-H	169.1234	-0.6
HMDB0031002	3-Decenoic acid	C10H18O2	M-H	169.1234	-0.6
HMDB0033203	6-Decanolide	C10H18O2	M-H	169.1234	-0.6
HMDB0040727	trans-Linalyl oxide	C10H18O2	M-H	169.1234	-0.6
HMDB0164952	4-methyl-1-(propan-2-yl)bicyclo[3.1]hexane-2,4-diol	C10H18O2	M-H	169.1234	-0.6
HMDB0062152	Propyl cyclohexanecarboxylate	C10H18O2	M-H	169.1234	-0.6
HMDB0033574	(1R,2R,4R,8R)-p-Menthane-2,8,9-triol	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0010725	(R)-3-Hydroxydecanoic acid	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0002203	3-Hydroxycapric acid	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0094656	2s-hydroxy-decanoic acid	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0179932	(5E)-3-(hydroxymethyl)-7-methyloct-5-ene-1,7-diol	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0039893	(1R,2R,4S)-p-Menthane-1,2,8-triol	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0040329	xi-5-Hydroxydecanoic acid	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0034783	cis-p-Menthane-1,7,8-triol	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0039470	(1S,2S,4R,8R)-p-Menthane-1,2,9-triol	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0041600	Ethyl 3-hydroxyoctanoate	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0033640	7-Methyl-3-methylene-1,6,7-octanetriol	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0039669	2-Hexyl-1,3-dioxolane-4-methanol	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0180106	SCHEMBL4626344	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0180105	9-hydroxy-8-methylnonanoic acid	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0180104	8-Hydroxy-8-methylnonanoic acid	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0179930	4-[3-(2-hydroxypropan-2-yl)oxiran-2-yl]-3-methylbutan-1-ol	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0179931	(3E)-2,6-dimethyloct-3-ene-1,2,8-triol	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0179929	(5E)-3,7-dimethyloct-5-ene-1,4,7-triol	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0179928	(5E)-3,7-dimethyloct-5-ene-1,3,7-triol	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0038186	2,6-Dimethyl-7-octene-2,3,6-triol	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0180588	9-hydroxy-4-methylnonanoic acid	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0039668	2-Hexyl-1,3-dioxan-5-ol	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0180589	SCHEMBL45681	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0033201	9-Hydroxydecanoic acid	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0180585	AKO19123491	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0180586	8-hydroxy-4-methylnonanoic acid	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0180587	4-(hydroxymethyl)nonanoic acid	C10H20O3	M-H2O-H	169.1229	2.6
HMDB0163244	(Z)-5-Undecen-1-ol	C11H22O	M-H	169.1598	-0.5
HMDB0033713	2-Undecanone	C11H22O	M-H	169.1598	-0.5
HMDB0031016	-Undecen-1-ol	C11H22O	M-H	169.1598	-0.5
HMDB0030943	6-Undecanone	C11H22O	M-H	169.1598	-0.5
HMDB0031064	(Z)-3-Methyl-3-decen-1-ol	C11H22O	M-H	169.1598	-0.5
HMDB0032379	trans- and cis-1-Methoxy-1-decene	C11H22O	M-H	169.1598	-0.5
HMDB0032371	1-Menthyl methyl ether	C11H22O	M-H	169.1598	-0.5
HMDB0031065	(E)-3-Methyl-4-decen-1-ol	C11H22O	M-H	169.1598	-0.5
HMDB0030941	Undecanal	C11H22O	M-H	169.1598	-0.5

	HMDB0034856	2-Undecen-1-ol	C11H22O	M-H	169.1598	-0.5
	HMDB0034151	1,1-Dimethoxynonane	C11H24O2	M-H2O-H	169.1592	2.7
171.0065	HMDB0002520	beta-Glycerophosphoric acid	C3H9O6P	M-H	171.0064	0.6
	HMDB0000126	Glycerol 3-phosphate	C3H9O6P	M-H	171.0064	0.6
	HMDB0061734	Dimethyl hydrogen phosphate	C2H7O4P	M+FA-H	171.0064	0.6
	HMDB0012228	Ethylphosphate	C2H7O4P	M+FA-H	171.0064	0.6
	HMDB0040528	1,4-Benzodioxin-2(3H)-one	C8H6O3	M+Na-2H	171.0064	0.8
	HMDB0032612	3,4-Methylenedioxybenzaldehyde	C8H6O3	M+Na-2H	171.0064	0.8
	HMDB0032598	4-Hydroxyphthalide	C8H6O3	M+Na-2H	171.0064	0.8
	HMDB0031515	(E)-8-Hydroxy-2-octene-4,6-diynoic acid	C8H6O3	M+Na-2H	171.0064	0.8
	HMDB0001587	Phenylglyoxylic acid	C8H6O3	M+Na-2H	171.0064	0.8
171.0412	HMDB0034322	L-alpha-Amino-5-oxo-2(5H)-isoxazolepropanoic acid	C6H8N2O4	M-H	171.0411	0.4
	HMDB0001212	Hydantoin-5-propionic acid	C6H8N2O4	M-H	171.0411	0.4
	HMDB0160104	bis(hydroxymethyl)pyrimidine-2,4-diol	C6H8N2O4	M-H	171.0411	0.4
	HMDB0029736	1H-Imidazole-1-acetic acid	C5H6N2O2	M+FA-H	171.0411	0.4
	HMDB0002024	Imidazoleacetic acid	C5H6N2O2	M+FA-H	171.0411	0.4
	HMDB0060261	Imidazoleacetic acid	C5H6N2O2	M+FA-H	171.0411	0.4
171.0664	HMDB0000262	Thymine	C5H6N2O2	M+FA-H	171.0411	0.4
	HMDB0173107	2,5-dimethoxycyclohexane-1,4-dione	C8H12O4	M-H	171.0663	0.7
	HMDB0159134	2-(3-hydroxy-4-oxocyclohexyl)acetic acid	C8H12O4	M-H	171.0663	0.7
	HMDB0159135	2-hydroxy-2-(4-oxocyclohexyl)acetic acid	C8H12O4	M-H	171.0663	0.7
	HMDB0013312	trans-3-Octenedioic acid	C8H12O4	M-H	171.0663	0.7
	HMDB0032352	3-Isopropenylpentanedioic acid	C8H12O4	M-H	171.0663	0.7
	HMDB0000341	2-Octenedioic acid	C8H12O4	M-H	171.0663	0.7
	HMDB0034851	Ethyl 2,4-dioxohexanoate	C8H12O4	M-H	171.0663	0.7
	HMDB0038601	Diethyl fumarate	C8H12O4	M-H	171.0663	0.7
	HMDB0004982	cis-4-Octenedioic acid	C8H12O4	M-H	171.0663	0.7
	HMDB0037026	3,4-Dimethyl-1,2-cyclopentanedione	C7H10O2	M+FA-H	171.0663	0.7
	HMDB0040445	2-(Ethoxymethyl)furan	C7H10O2	M+FA-H	171.0663	0.7
	HMDB0031223	Enol-3-Ethyl-1,2-cyclopentanedione	C7H10O2	M+FA-H	171.0663	0.7
	HMDB0034835	3-(3-Ethylloxiranyl)-2-propenal	C7H10O2	M+FA-H	171.0663	0.7
	HMDB0041474	xi-5-Isopropyl-2(5H)-furanone	C7H10O2	M+FA-H	171.0663	0.7
	HMDB0031222	3-Ethyl-1,2-cyclopentanedione	C7H10O2	M+FA-H	171.0663	0.7
	HMDB0033629	xi-4-Hydroxy-4-methyl-2-cyclohexen-1-one	C7H10O2	M+FA-H	171.0663	0.7
	HMDB0037027	3,5-Dimethyl-1,2-cyclopentanedione	C7H10O2	M+FA-H	171.0663	0.7
	HMDB0032333	4-Hydroxy-4-methyl-5-hexenoic acid gamma lactone	C7H10O2	M+FA-H	171.0663	0.7
	HMDB0034080	3-Methyl-1,2-cyclohexanedione	C7H10O2	M+FA-H	171.0663	0.7
	HMDB0029582	Methyl sorbate	C7H10O2	M+FA-H	171.0663	0.7
	HMDB0032067	Allyl crotonate	C7H10O2	M+FA-H	171.0663	0.7
171.0778	HMDB0011178	Prolylglycine	C7H12N2O3	M-H	171.0775	1.7
	HMDB0000721	Glycylproline	C7H12N2O3	M-H	171.0775	1.7
171.1026	HMDB0181106	7-Octen-3-one	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0062529	3,5-Dimethyl-1-hexyn-3-ol	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0163322	7-octen-2-one	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0039770	(Z)-5-Octenal	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0040146	2,5-Octadien-1-ol	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0031590	3-Methyl-3-hepten-2-one	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0037152	2-Ethylidenhexanal	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0030961	2-Octenal	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0031309	1-Octen-3-one	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0033547	3-Octen-2-one	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0035915	Sulcatone	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0040151	(2E,4E)-2,4-Octadien-1-ol	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0031197	2,4,4-Trimethylcyclopentanone	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0030966	(3xi,5Z)-1,5-Octadien-3-ol	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0039769	6-Octenal	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0031591	5-Methyl-5-hepten-2-one	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0035242	(S,E)-Filbertone	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0040149	(3E,5Z)-3,5-Octadien-1-ol	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0032403	6-Methyl-3-hepten-2-one, trans-	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0061945	2-Ethyl-2-hexenal	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0032451	4-Octen-3-one	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0031301	2-Octen-4-one	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0035390	5-Octen-2-one	C8H14O	M+FA-H	171.1027	-0.4
	HMDB0013809	(E)-2-octenal	C8H14O	M+FA-H	171.1027	-0.4

	HMDB0169421	2-ethenyl-4,6-diethyl-1,3,5-trioxane	C9H16O3	M-H	171.1027	-0.4
	HMDB0163469	(2Z)-4-hydroxy-2-methyloct-2-enoic acid	C9H16O3	M-H	171.1027	-0.4
	HMDB0163470	2-methyl-3-pentyloxirane-2-carboxylic acid	C9H16O3	M-H	171.1027	-0.4
	HMDB0163468	SCHEMBL7173369	C9H16O3	M-H	171.1027	-0.4
	HMDB0040203	2-Methylpropyl 3-hydroxy-2-methylidenebutanoate	C9H16O3	M-H	171.1027	-0.4
	HMDB0163465	(2Z)-7-hydroxy-2-methyloct-2-enoic acid	C9H16O3	M-H	171.1027	-0.4
	HMDB0163466	(2Z)-8-hydroxy-2-methyloct-2-enoic acid	C9H16O3	M-H	171.1027	-0.4
	HMDB0094711	9-oxononanoic acid	C9H16O3	M-H	171.1027	-0.4
	HMDB0036213	cis-3-Hexenyl lactate	C9H16O3	M-H	171.1027	-0.4
	HMDB0036188	Tetrahydrofurfuryl butyrate	C9H16O3	M-H	171.1027	-0.4
	HMDB0040165	Butyl levulinate	C9H16O3	M-H	171.1027	-0.4
	HMDB0060287	4-Hydroperoxy-2-nonenal	C9H16O3	M-H	171.1027	-0.4
	HMDB0059937	6-Pentyl-1,4-dioxan-2-one	C9H16O3	M-H	171.1027	-0.4
	HMDB0040202	Butyl 3-hydroxy-2-methylidenebutanoate	C9H16O3	M-H	171.1027	-0.4
	HMDB0036396	3-Methylbutyl 3-oxobutanoate	C9H16O3	M-H	171.1027	-0.4
	HMDB0179168	3-caproyl propionic acid	C9H16O3	M-H	171.1027	-0.4
	HMDB0062081	9-oxononanoate	C9H15O3	M-H	171.1027	-0.4
	HMDB0059936	5-Pentyl-1,4-dioxan-2-one	C9H16O3	M-H	171.1027	-0.4
	HMDB0163757	3,5-dihydroxy-6-methyloctanoic acid	C9H18O4	M-H20-H	171.1021	2.8
	HMDB0169419	1-(4,6-diethyl-1,3,5-trioxan-2-yl)ethan-1-ol	C9H18O4	M-H20-H	171.1021	2.8
	HMDB0169420	2-(4,6-diethyl-1,3,5-trioxan-2-yl)ethan-1-ol	C9H18O4	M-H20-H	171.1021	2.8
171.1390	HMDB0062015	2,4-dimethylhept-1-ene	C9H18	M+FA-H	171.1391	-0.3
	HMDB0031270	1-Nonene	C9H18	M+FA-H	171.1391	-0.3
	HMDB0038191	Isopropylcyclohexane	C9H18	M+FA-H	171.1391	-0.3
	HMDB0180498	dec-9-ene-1,3-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0180499	dec-9-ene-1,4-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0180500	dec-9-ene-1,5-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0180497	9-Decene-1,2-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0180501	dec-9-ene-1,6-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0180502	dec-9-ene-1,7-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0180503	1-decene-3,-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0180504	8-Oxiranyl-1-octanol	C10H20O2	M-H	171.1391	-0.3
	HMDB0179927	3,7-dimethyl-5-octene-1,7-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0179213	7,8-dihydroxy-p-menthane	C10H20O2	M-H	171.1391	-0.3
	HMDB0179212	2-(4-methylcyclohexyl)propane-1,2-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0094654	propan-2-yl heptanoate	C10H20O2	M-H	171.1391	-0.3
	HMDB0171179	2-(4-methylpent-3-en-1-yl)butane-1,4-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0171178	Citronellol epoxide	C10H20O2	M-H	171.1391	-0.3
	HMDB0171177	3,7-Dimethyl-6-octene-1,5-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0171176	2,6-dimethyloct-2-ene-1,8-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0031264	Methyl nonanoate	C10H20O2	M-H	171.1391	-0.3
	HMDB0032045	Pentyl 3-methylbutanoate	C10H20O2	M-H	171.1391	-0.3
	HMDB0033620	Hexyl butyrate	C10H20O2	M-H	171.1391	-0.3
	HMDB0029760	1,1-Diethoxy-2-hexene	C10H20O2	M-H	171.1391	-0.3
	HMDB0040211	Butyl hexanoate	C10H20O2	M-H	171.1391	-0.3
	HMDB0036145	p-Menthane-3,8-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0041216	2,6-Dimethyl-7-octene-2,6-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0032070	Isooctyl acetate	C10H20O2	M-H	171.1391	-0.3
	HMDB0035595	trans-p-Menthane-1,8-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0040157	3-Methylbutyl 2-methylbutanoate	C10H20O2	M-H	171.1391	-0.3
	HMDB0037849	Hexyl 2-methylpropanoate	C10H20O2	M-H	171.1391	-0.3
	HMDB0040529	3-Methylbutyl pentanoate	C10H20O2	M-H	171.1391	-0.3
	HMDB0031739	7-Hydroxy-3,7-dimethyloctanal	C10H20O2	M-H	171.1391	-0.3
	HMDB0040195	Ethyl octanoate	C10H20O2	M-H	171.1391	-0.3
	HMDB0000511	Capric acid	C10H20O2	M-H	171.1391	-0.3
	HMDB0037387	(1S,3R,4R)-p-Menthane-1,3-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0035723	(1R,2S,3S,4R)-p-Menthane-2,3-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0036136	4-Ethyloctanoic acid	C10H20O2	M-H	171.1391	-0.3
	HMDB0040167	3-Octyl acetate	C10H20O2	M-H	171.1391	-0.3
	HMDB0036228	2-Methylpropyl hexanoate	C10H20O2	M-H	171.1391	-0.3
	HMDB0038038	2-Methylbutyl 3-methylbutanoate	C10H20O2	M-H	171.1391	-0.3
	HMDB0062146	Pentyl pentanoate	C10H20O2	M-H	171.1391	-0.3
	HMDB0034457	Propyl heptanoate	C10H20O2	M-H	171.1391	-0.3
	HMDB0034849	4-Methylnonanoic acid	C10H20O2	M-H	171.1391	-0.3
	HMDB0030029	Isopentyl isopentanoate	C10H20O2	M-H	171.1391	-0.3

	HMDB0061805	(2S)-2-Ethylhexyl acetate	C10H20O2	M-H	171.1391	-0.3
	HMDB0187563	2-(1-hydroxypropan-2-yl)-5-methylcyclohexan-1-ol	C10H20O2	M-H	171.1391	-0.3
	HMDB0061987	2-ethylhexyl acetate	C10H20O2	M-H	171.1391	-0.3
	HMDB0171175	3,7-dimethyloct-6-ene-1,3-diol	C10H20O2	M-H	171.1391	-0.3
	HMDB0180097	Isocaproic acid	C10H20O2	M-H	171.1391	-0.3
	HMDB0038602	Octyl acetate	C10H20O2	M-H	171.1391	-0.3
	HMDB0039218	2-Methylbutyl 2-methylbutanoate	C10H20O2	M-H	171.1391	-0.3
	HMDB0038783	(Z)-1-(1-Ethoxyethoxy)-3-hexene	C10H20O2	M-H	171.1391	-0.3
	HMDB0032315	Hexanal butane-2,3-diol acetal	C10H20O2	M-H	171.1391	-0.3
	HMDB0032302	Heptanal propyleneglycol acetal	C10H20O2	M-H	171.1391	-0.3
	HMDB0032264	Ethyl 2-ethylhexanoate	C10H20O2	M-H	171.1391	-0.3
	HMDB0032155	Acetaldehyde 1,3-octanediol acetal	C10H20O2	M-H	171.1391	-0.3
173.0604	HMDB0133477	(3Z)-3-hydroxy-4-(3-methoxyphenyl)but-3-en-2-one	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0151223	AC1L67O8	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0133534	1-hydroxy-4-(3-methoxyphenyl)but-3-en-2-one	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0137170	2-[(1E)-3-methylbuta-1,3-dien-1-yl]benzene-1,3,5-triol	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0146409	3-(3-methoxyphenyl)-2-methylprop-2-enoic acid	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0146436	SCHEMBL7293162	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0146664	2-hydroxyethyl 3-phenylprop-2-enoate	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0146665	3-(3-hydroxy-phenyl)-acrylic acid ethyl ester	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0151226	3-(2-hydroxy-4-methoxyphenyl)-2-methylprop-2-enal	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0151224	2-(hydroxymethyl)-3-(4-methoxyphenyl)prop-2-enal	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0151227	3-(4-methoxyphenyl)-2-methyloxirane-2-carbaldehyde	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0170844	2-hydroxy-4-(prop-2-en-1-yl)phenyl acetate	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0170975	2-hydroxy-4-[(1Z)-prop-1-en-1-yl]phenyl acetate	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0182825	4-methoxybenzyl acrylate	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0133510	4-(3-hydroxy-5-methoxyphenyl)but-3-en-2-one	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0133482	1-(3-methoxyphenyl)butane-2,3-dione	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0126382	5,5-dimethyl-3,6-dioxatricyclo[5.4,undeca-1(11),7,9-trien-11-ol	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0126381	2,2-dimethyl-2H-chromene-5,6-diol	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0126380	2,2-dimethyl-2H-chromene-5,7-diol	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0126383	2-(hydroxymethyl)-2-methyl-2H-chromen-5-ol	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0129370	1-(4-methoxy-1-benzofuran-5-yl)ethan-1-ol	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0035873	Myristicin	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0031623	Ethyl phenylglycidate	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0131282	ethyl (2E)-3-(4-hydroxyphenyl)prop-2-enoate	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0062067	5-[(4-hydroxyphenyl)methyl]oxolan-2-one	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0062066	5-[(3-hydroxyphenyl)methyl]oxolan-2-one	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0133439	4-(4-hydroxy-3-methoxyphenyl)but-3-en-2-one	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0032591	Dehydrozingerone	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0037877	Eugenyl formate	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0030580	(R)-Shinanolone	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0035894	(Z)-4-Methoxy-6-(1-propenyl)-1,3-benzodioxole	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0041007	1'-Hydroxychavicol acetate	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0040446	Benzyl acetoacetate	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0030752	Methyl trans-p-methoxycinnamate	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0035275	Isomyristicin	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0041481	4-(3,4-Methylenedioxyphenyl)-2-butanone	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0040268	Ethyl 3-oxo-3-phenylpropanoate	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0037277	Isoeugenol formate	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0031610	Allyl phenoxyacetate	C11H12O3	M-H2O-H	173.0603	0.8
	HMDB0029751	Naphthalene	C10H8	M+FA-H	173.0608	-2.3
	HMDB0031845	3-Propylidene-1(3H)-isobenzofuranone	C11H10O2	M-H	173.0608	-2.3
	HMDB0166920	Menadiol	C11H10O2	M-H	173.0608	-2.3
	HMDB0032727	4-Methoxy-1-naphthol	C11H10O2	M-H	173.0608	-2.3
	HMDB0164724	4-Hydroxy-4-methylcyclohexanone	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0165094	3-(Hydroxymethyl)cyclohexanone	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0165096	SCHEMBL443446	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0165097	SCHEMBL132855	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0166738	3-butyloxirane-2-carbaldehyde	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0059876	Pantolactone	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0166739	(2E)-7-hydroxyhept-2-enal	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0031593	5-Methyl-2,3-hexanedione	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0033793	4-Heptenoic acid	C7H12O2	M+FA-H	173.0819	-0.8

173.0818	HMDB0038962	Ethyl tiglate	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0165095	3-Hydroxy-3-methylcyclohexan-1-one	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0180322	3-(3-ethyloxiran-2-yl)propanal	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0031500	Methyl 2E-hexenoate	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0031484	2-Heptenoic acid	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0029314	Isopentenyl acetate	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0031477	3,4-Heptanedione	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0031476	2,3-Heptanedione	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0031504	Methyl (Z)-3-hexenoate	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0031603	Ethyl 4-pentenoate	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0040214	cis-3-Hexenyl formate	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0031342	Cyclohexanecarboxylic acid	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0038271	2-Hexenyl formate	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0031174	4-Methyl-5-hexanolide	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0031681	Dihydro-5-propyl-2(3H)-furanone	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0039819	2,4-Dimethyl-2-pentenoic acid	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0030330	1-Methoxy-3-methylene-2-pentanone	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0031351	Cyclohexyl formate	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0180323	(2E)-3-(3-ethyloxiran-2-yl)prop-2-en-1-ol	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0173762	5-methylcyclohex-4-ene-1,3-diol	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0173763	1-methyl-7-oxabicyclo[4.1]heptan-3-ol	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0173761	3-methylcyclohex-3-ene-1,2-diol	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0173760	SCHEMBL14734478	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0166736	4-Hydroxyheptenal	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0166737	6-Hydroxy-2-heptenal	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0029165	1,3-Diacetylpropane	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0040591	Allyl butyrate	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0032460	4-Pentenyl acetate	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0032391	3-Methyl-3-butenyl acetate	C7H12O2	M+FA-H	173.0819	-0.8
	HMDB0041606	Dimethyl adipate	C8H14O4	M-H	173.0819	-0.8
	HMDB0159133	2-hydroxy-2-(4-hydroxycyclohexyl)acetic acid	C8H14O4	M-H	173.0819	-0.8
	HMDB0059727	2,4-Dimethyladipic acid	C8H14O4	M-H	173.0819	-0.8
	HMDB0059757	3-Methylpimelic acid	C8H14O4	M-H	173.0819	-0.8
	HMDB0060684	2-Propylglutaric acid	C8H14O4	M-H	173.0819	-0.8
	HMDB0000893	Suberic acid	C8H14O4	M-H	173.0819	-0.8
	HMDB0002023	Ethyladipic acid	C8H14O4	M-H	173.0819	-0.8
	HMDB0033838	Diethyl succinate	C8H14O4	M-H	173.0819	-0.8
	HMDB0031710	1,9-Nonanedithiol	C9H20S2	M-H2O-H	173.0823	-2.6
173.1182	HMDB0013821	2-Methyl-4-heptanone	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0062076	6-Methylheptan-2-one	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0062072	5-methylheptan-2-one	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0061986	2-ethylhexanal	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0061912	3,4-Dimethylcyclohexanol	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0172314	1-OCTEN-2-OL	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0170962	7-Octen-1-ol	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0061913	3,5-Dimethylcyclohexanol	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0031296	(E)-2-Octen-1-ol	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0001140	Octanal	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0037181	xi-7-Octen-2-ol	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0035231	(Z)-3-Octen-1-ol	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0035768	(E)-3-Octen-1-ol	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0031298	(Z)-5-Octen-1-ol	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0031295	Ethyl pentyl ketone	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0029574	2,5-Diethyltetrahydrofuran	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0030030	(R)-Sulcatol	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0031299	(R)-1-Octen-3-ol	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0031300	(E)-2-Octen-4-ol	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0032450	trans-3-Octen-2-ol	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0031294	2-Octanone	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0032402	2-Methyl-3-heptanone	C8H16O	M+FA-H	173.1183	-0.7
	HMDB0170940	2-hydroxynonanoic acid	C9H18O3	M-H	173.1183	-0.7
	HMDB0179172	1,5-dihydroxynonan-4-one	C9H18O3	M-H	173.1183	-0.7
	HMDB0179997	SCHEMBL3537	C9H18O3	M-H	173.1183	-0.7
	HMDB0179999	2-hydroxy-7-methyloctanoic acid	C9H18O3	M-H	173.1183	-0.7
	HMDB0179998	SCHEMBL9379	C9H18O3	M-H	173.1183	-0.7

	HMDB0179169	1,8-dihydroxynonan-4-one	C9H18O3	M-H	173.1183	-0.7
	HMDB0179170	SCHEMBL1635	C9H18O3	M-H	173.1183	-0.7
	HMDB0179171	1,3-dihydroxynonan-4-one	C9H18O3	M-H	173.1183	-0.7
	HMDB0170938	8-hydroxy-nonanoic acid	C9H18O3	M-H	173.1183	-0.7
	HMDB0034040	2,4,6-Triethyl-1,3,5-trioxane	C9H18O3	M-H	173.1183	-0.7
	HMDB0031513	3-Hydroxynonanoic acid	C9H18O3	M-H	173.1183	-0.7
	HMDB0170939	9-Hydroxynonanoic acid	C9H18O3	M-H	173.1183	-0.7
174.0411	HMDB0003470	N-Formyl-L-glutamic acid	C6H9NO5	M-H	174.0408	1.7
	HMDB0039163	D-N-(Carboxyacetyl)alanine	C6H9NO5	M-H	174.0408	1.7
	HMDB0000812	N-Acetyl-L-aspartic acid	C6H9NO5	M-H	174.0408	1.7
	HMDB0060273	2-Amino-3-oxoadipate	C6H9NO5	M-H	174.0408	1.7
	HMDB0062585	(3R,5S)-1-pyrroline-3-hydroxy-5-carboxylic acid	C5H7NO3	M+FA-H	174.0408	1.8
	HMDB0000267	Pyroglutamic acid	C5H7NO3	M+FA-H	174.0408	1.8
	HMDB0000805	Pyrrolidonecarboxylic acid	C5H7NO3	M+FA-H	174.0408	1.8
	HMDB0060262	Pyrrolidonecarboxylic acid	C5H7NO3	M+FA-H	174.0408	1.8
	HMDB0001369	Pyrroline hydroxycarboxylic acid	C5H7NO3	M+FA-H	174.0408	1.8
	HMDB0001843	N-Acryloylglycine	C5H7NO3	M+FA-H	174.0408	1.8
	HMDB0002234	1-Pyrroline-4-hydroxy-2-carboxylate	C5H7NO3	M+FA-H	174.0408	1.8
176.9360	HMDB0061093	dimethadione	C5H7NO3	M+FA-H	174.0408	1.8
	HMDB0000250	Pyrophosphate	H4O7P2	M-H	176.9360	0.3
	HMDB0155221	Pyrophosphate	H4O7P2	M-H	176.9360	0.3
177.0340	HMDB0028838	Glycyl-Cysteine	C5H10N2O3S	M-H	177.0339	0.4
	HMDB0028775	2-[(2-amino-1-hydroxy-3-sulfanylpropylidene)amino]acetic acid	C5H10N2O3S	M-H	177.0339	0.4
	HMDB0000078	Cysteinyglycine	C5H10N2O3S	M-H	177.0339	0.4
177.0920	HMDB0061996	(2-methylprop-2-en-1-yl)benzene	C10H12	M+FA-H	177.0921	-0.6
	HMDB0062046	4-ethenyl-1,2-dimethylbenzene	C10H12	M+FA-H	177.0921	-0.6
	HMDB0062142	1-methyl-2-(prop-1-en-2-yl)benzene	C10H12	M+FA-H	177.0921	-0.6
	HMDB0029641	p-Mentha-1,3,5,8-tetraene	C10H12	M+FA-H	177.0921	-0.6
	HMDB0163596	2-hydroxy-3-methyl-2-phenylbutanal	C11H14O2	M-H	177.0921	-0.6
	HMDB0133181	4-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C11H14O2	M-H	177.0921	-0.6
	HMDB0132981	1-(4-hydroxyphenyl)pentan-3-one	C11H14O2	M-H	177.0921	-0.6
	HMDB0151221	3-(4-methoxyphenyl)-2-methylpropanal	C11H14O2	M-H	177.0921	-0.6
	HMDB0133687	1-hydroxy-3-methyl-4-phenylbutan-2-one	C11H14O2	M-H	177.0921	-0.6
	HMDB0133469	4-(3-methoxyphenyl)butan-2-one	C11H14O2	M-H	177.0921	-0.6
	HMDB0133683	4-hydroxy-3-methyl-4-phenylbutan-2-one	C11H14O2	M-H	177.0921	-0.6
	HMDB0133682	3-hydroxy-3-methyl-4-phenylbutan-2-one	C11H14O2	M-H	177.0921	-0.6
	HMDB0133684	4-(3-hydroxyphenyl)-3-methylbutan-2-one	C11H14O2	M-H	177.0921	-0.6
	HMDB0133686	3-benzyl-4-hydroxybutan-2-one	C11H14O2	M-H	177.0921	-0.6
	HMDB0126449	2-[(1E)-3-methylbut-1-en-1-yl]benzene-1,3-diol	C11H14O2	M-H	177.0921	-0.6
	HMDB0126149	2-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C11H14O2	M-H	177.0921	-0.6
	HMDB0151222	3-(4-methoxyphenyl)-2-methylprop-2-en-1-ol	C11H14O2	M-H	177.0921	-0.6
	HMDB0163598	SCHEMBL9714564	C11H14O2	M-H	177.0921	-0.6
	HMDB0163594	4-hydroxy-3-methyl-2-phenylbutanal	C11H14O2	M-H	177.0921	-0.6
	HMDB0163597	SCHEMBL9714781	C11H14O2	M-H	177.0921	-0.6
	HMDB0163592	38-94-9	C11H14O2	M-H	177.0921	-0.6
	HMDB0163593	SCHEMBL11476137	C11H14O2	M-H	177.0921	-0.6
	HMDB0133685	4-(4-hydroxyphenyl)-3-methylbutan-2-one	C11H14O2	M-H	177.0921	-0.6
	HMDB0040287	1-Phenylethyl propanoate	C11H14O2	M-H	177.0921	-0.6
	HMDB0037708	p-Tolyl isobutyrate	C11H14O2	M-H	177.0921	-0.6
	HMDB0040356	Osmorhizole	C11H14O2	M-H	177.0921	-0.6
	HMDB0036235	alpha, alpha-Dimethylphenethyl formate	C11H14O2	M-H	177.0921	-0.6
	HMDB0031864	Methyleugenol	C11H14O2	M-H	177.0921	-0.6
	HMDB0031250	Phenylmethyl 2-methylpropanoate	C11H14O2	M-H	177.0921	-0.6
	HMDB0033376	Phenylmethyl butanoate	C11H14O2	M-H	177.0921	-0.6
	HMDB0033386	3-Phenylpropyl acetate	C11H14O2	M-H	177.0921	-0.6
	HMDB0040583	2-Methylpropyl benzoate	C11H14O2	M-H	177.0921	-0.6
	HMDB0033597	4-(4-Methoxyphenyl)-2-butanone	C11H14O2	M-H	177.0921	-0.6
	HMDB0036385	Methyl 4-phenylbutanoate	C11H14O2	M-H	177.0921	-0.6
	HMDB0040425	Propyl phenylacetate	C11H14O2	M-H	177.0921	-0.6
	HMDB0041553	Methylisoeugenol	C11H14O2	M-H	177.0921	-0.6
	HMDB0002043	5-Phenylvaleric acid	C11H14O2	M-H	177.0921	-0.6
	HMDB0035013	2-Phenylethyl propanoate	C11H14O2	M-H	177.0921	-0.6

	HMDB0038179	3-(2-Hydroxy-4-methylphenyl)-2-butanone	C11H14O2	M-H	177.0921	-0.6
	HMDB0040800	2-Ethoxy-5-(1-propenyl)phenol	C11H14O2	M-H	177.0921	-0.6
	HMDB0040411	Ethyl 3-phenylpropanoate	C11H14O2	M-H	177.0921	-0.6
	HMDB0037680	2-Methylphenyl 2-methylpropanoate	C11H14O2	M-H	177.0921	-0.6
	HMDB0040426	Isopropyl phenylacetate	C11H14O2	M-H	177.0921	-0.6
	HMDB0037734	Isobutyl 2-furanpropionate	C11H16O3	M-H2O-H	177.0916	2.5
	HMDB0037725	Hexyl 2-furoate	C11H16O3	M-H2O-H	177.0916	2.5
	HMDB0179541	3-methoxy-2-methyl-5-(propan-2-yl)benzene-1,4-diol	C11H16O3	M-H2O-H	177.0916	2.5
	HMDB0179545	3-methoxy-5-methyl-2-(propan-2-yl)benzene-1,4-diol	C11H16O3	M-H2O-H	177.0916	2.5
	HMDB0036226	2,6-Dimethoxy-4-propylphenol	C11H16O3	M-H2O-H	177.0916	2.5
	HMDB0135672	4-(3-hydroxybutyl)-2-methoxyphenol	C11H16O3	M-H2O-H	177.0916	2.5
179.0461	HMDB0164043	[(2-aminophenyl)(hydroxy)methylidene]carbamic acid	C8H8N2O3	M-H	179.0462	-0.6
	HMDB0176142	SCHEMBL6994749	C8H8N2O3	M-H	179.0462	-0.6
	HMDB0059766	Picolinoylglycine	C8H8N2O3	M-H	179.0462	-0.6
	HMDB0041912	Isonicotinylglycine	C8H8N2O3	M-H	179.0462	-0.6
	HMDB0003269	Nicotinuric acid	C8H8N2O3	M-H	179.0462	-0.6
	HMDB0015188	Mimosine	C8H10N2O4	M-H2O-H	179.0457	2.4
179.0560	HMDB0158455	ethyl glycerol ether	C5H10O4	M+FA-H	179.0561	-0.6
	HMDB0001292	1-Deoxy-D-xylulose	C5H10O4	M+FA-H	179.0561	-0.6
	HMDB0003224	Deoxyribose	C5H10O4	M+FA-H	179.0561	-0.6
	HMDB0012485	(R)-glycerol 1-acetate	C5H10O4	M+FA-H	179.0561	-0.6
	HMDB0012141	(R)-2,3-Dihydroxy-isovalerate	C5H10O4	M+FA-H	179.0561	-0.6
	HMDB0127615	3-hydroxy-2-(hydroxymethyl)-2-methylpropanoic acid	C5H10O4	M+FA-H	179.0561	-0.6
	HMDB0029576	2,3-Dihydroxy-2-methylbutanoic acid	C5H10O4	M+FA-H	179.0561	-0.6
	HMDB0158453	SCHEMBL8384843	C5H10O4	M+FA-H	179.0561	-0.6
	HMDB0158454	SCHEMBL36647	C5H10O4	M+FA-H	179.0561	-0.6
	HMDB0000421	2,3-Dihydroxyvaleric acid	C5H10O4	M+FA-H	179.0561	-0.6
	HMDB0167973	2-deoxypentose	C5H10O4	M+FA-H	179.0561	-0.6
	HMDB0062138	muco-Inositol	C6H12O6	M-H	179.0561	-0.6
	HMDB0062113	(3R,4R,5S)-5-[(1R)-1,2-dihydroxyethyl]-3,4-dihydroxyoxolan-2-olate	C6H11O6	M-H	179.0561	-0.6
	HMDB0033704	alpha-L-galactose	C6H12O6	M-H	179.0561	-0.6
	HMDB0062100	(3R,4R,5S)-5-[(1R)-1,2-dihydroxyethyl]oxolane-2,3,4-triol	C6H12O6	M-H	179.0561	-0.6
	HMDB0166371	SCHEMBL14339418	C6H12O6	M-H	179.0561	-0.6
	HMDB0240208	neo-inositol	C6H12O6	M-H	179.0561	-0.6
	HMDB0240210	cis-inositol	C6H12O6	M-H	179.0561	-0.6
	HMDB0003418	D-Tagatose	C6H12O6	M-H	179.0561	-0.6
	HMDB0125599	2,5-bis(hydroxymethyl)oxolane-2,3,4-triol	C6H12O6	M-H	179.0561	-0.6
	HMDB0001151	Allose	C6H12O6	M-H	179.0561	-0.6
	HMDB0001266	L-Sorbose	C6H12O6	M-H	179.0561	-0.6
	HMDB0003345	alpha-D-Glucose	C6H12O6	M-H	179.0561	-0.6
	HMDB0061922	alpha-D-Glucose	C6H12O6	M-H	179.0561	-0.6
	HMDB0003449	Beta-D-Galactose	C6H12O6	M-H	179.0561	-0.6
	HMDB0240207	epi-Inositol	C6H12O6	M-H	179.0561	-0.6
	HMDB0012326	L-Gulose	C6H12O6	M-H	179.0561	-0.6
	HMDB0155830	Inositol	C6H12O6	M-H	179.0561	-0.6
	HMDB0240209	D-chiro-Inositol	C6H12O6	M-H	179.0561	-0.6
	HMDB0032222	Dihydroxyacetone (dimer)	C6H12O6	M-H	179.0561	-0.6
	HMDB0000660	D-Fructose	C6H12O6	M-H	179.0561	-0.6
	HMDB0000122	Beta-D-Glucose	C6H12O6	M-H	179.0561	-0.6
	HMDB0062170	Beta-D-Glucose	C6H12O6	M-H	179.0561	-0.6
	HMDB0000516	Beta-D-Glucose	C6H12O6	M-H	179.0561	-0.6
	HMDB0006088	scyllo-Inositol	C6H12O6	M-H	179.0561	-0.6
	HMDB0000143	D-Galactose	C6H12O6	M-H	179.0561	-0.6
	HMDB0000211	myo-Inositol	C6H12O6	M-H	179.0561	-0.6
	HMDB0000346	3-Deoxyarabinohexonic acid	C6H12O6	M-H	179.0561	-0.6
	HMDB0062538	Fructose-1P	C6H12O6	M-H	179.0561	-0.6
	HMDB0062473	Glycoprotein-phospho-D-mannose	C6H12O6	M-H	179.0561	-0.6
	HMDB0240211	allo-Inositol	C6H12O6	M-H	179.0561	-0.6
	HMDB0034220	Levoinositol	C6H12O6	M-H	179.0561	-0.6
	HMDB0000169	Alpha-D-Mannose	C6H12O6	M-H	179.0561	-0.6
	HMDB0062086	beta-D-galactofuranose	C6H12O6	M-H	179.0561	-0.6
	HMDB0155309	keto-D-fructose	C6H12O6	M-H	179.0561	-0.6
	HMDB0062048	3,5-Dimethylbenzaldehyde	C9H10O	M+FA-H	179.0714	-0.9

HMDB0059601	Indan-1-ol	C9H10O	M+FA-H	179.0714	-0.9
HMDB0173827	Benzenemethanol,4-methyl-a-methylene-	C9H10O	M+FA-H	179.0714	-0.9
HMDB0175242	beta-Methylenephenethyl alcohol	C9H10O	M+FA-H	179.0714	-0.9
HMDB0032623	1-Phenyl-1-propanone	C9H10O	M+FA-H	179.0714	-0.9
HMDB0032608	4'-Methylacetophenone	C9H10O	M+FA-H	179.0714	-0.9
HMDB0032142	2,4-Dimethylbenzaldehyde	C9H10O	M+FA-H	179.0714	-0.9
HMDB0032386	1-(2-methylphenyl)ethan-1-one	C9H10O	M+FA-H	179.0714	-0.9
HMDB0059895	m-Methylacetophenone	C9H10O	M+FA-H	179.0714	-0.9
HMDB0061984	2-ethylbenzaldehyde	C9H10O	M+FA-H	179.0714	-0.9
HMDB0061970	phenylacetone	C9H10O	M+FA-H	179.0714	-0.9
HMDB0061961	1-ethenyl-3-methoxybenzene	C9H10O	M+FA-H	179.0714	-0.9
HMDB0029698	trans-Cinnamyl alcohol	C9H10O	M+FA-H	179.0714	-0.9
HMDB0033716	3-Phenylpropanal	C9H10O	M+FA-H	179.0714	-0.9
HMDB0034107	Chavicol	C9H10O	M+FA-H	179.0714	-0.9
HMDB0034563	7-Nonene-3,5-diyne-1-ol	C9H10O	M+FA-H	179.0714	-0.9
HMDB0029639	(4-Methylphenyl)acetaldehyde	C9H10O	M+FA-H	179.0714	-0.9
HMDB0029697	Cinnamyl alcohol	C9H10O	M+FA-H	179.0714	-0.9
HMDB0031626	2-Phenylpropanal	C9H10O	M+FA-H	179.0714	-0.9
HMDB0036441	o-Vinylanisole	C9H10O	M+FA-H	179.0714	-0.9
HMDB0030839	(Z)-4-(1-Propenyl)phenol	C9H10O	M+FA-H	179.0714	-0.9
HMDB0032024	4-Ethylbenzaldehyde	C9H10O	M+FA-H	179.0714	-0.9
HMDB0135646	[3-(4-methoxyphenyl)oxiran-2-yl]methanol	C10H12O3	M-H	179.0714	-0.9
HMDB0135740	3-hydroxy-3-(4-methoxyphenyl)propanal	C10H12O3	M-H	179.0714	-0.9
HMDB0160084	4-Hydroxy-4-phenyl-butyric acid	C10H12O3	M-H	179.0714	-0.9
HMDB0134065	3-(2-hydroxy-3-methoxyphenyl)propanal	C10H12O3	M-H	179.0714	-0.9
HMDB0134076	2-(3-hydroxyprop-1-en-1-yl)-6-methoxyphenol	C10H12O3	M-H	179.0714	-0.9
HMDB0135241	2-methoxy-4-[(oxiran-2-yl)methyl]phenol	C10H12O3	M-H	179.0714	-0.9
HMDB0135739	2-hydroxy-3-(4-methoxyphenyl)propanal	C10H12O3	M-H	179.0714	-0.9
HMDB0135242	2-methoxy-4-(prop-2-en-1-yl)benzene-1,3-diol	C10H12O3	M-H	179.0714	-0.9
HMDB0135243	4-methoxy-6-(prop-2-en-1-yl)benzene-1,3-diol	C10H12O3	M-H	179.0714	-0.9
HMDB0135645	2-(3-hydroxyprop-1-en-1-yl)-5-methoxyphenol	C10H12O3	M-H	179.0714	-0.9
HMDB0062773	-hydroxy-(2E,8E)-decadien-4-ynoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0135240	3-methoxy-5-(prop-2-en-1-yl)benzene-1,2-diol	C10H12O3	M-H	179.0714	-0.9
HMDB0160086	4-(4-HYDROXYPHENYL)BUTANOIC ACID	C10H12O3	M-H	179.0714	-0.9
HMDB0133505	4-(3,4-dihydroxyphenyl)butan-2-one	C10H12O3	M-H	179.0714	-0.9
HMDB0129958	2-(4-methoxyphenyl)propanoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0182822	4-hydroxybenzyl propionate	C10H12O3	M-H	179.0714	-0.9
HMDB0175292	3-(2-hydroxyphenyl)propyl formate	C10H12O3	M-H	179.0714	-0.9
HMDB0175293	3-hydroxy-3-phenylpropyl formate	C10H12O3	M-H	179.0714	-0.9
HMDB0175291	2-hydroxy-3-phenylpropyl formate	C10H12O3	M-H	179.0714	-0.9
HMDB0170984	SCHEMBL12699	C10H12O3	M-H	179.0714	-0.9
HMDB0170983	3-methoxy-5-[(1Z)-prop-1-en-1-yl]benzene-1,2-diol	C10H12O3	M-H	179.0714	-0.9
HMDB0170982	4-methoxy-6-[(1Z)-prop-1-en-1-yl]benzene-1,3-diol	C10H12O3	M-H	179.0714	-0.9
HMDB0170981	2-methoxy-4-[(1Z)-prop-1-en-1-yl]benzene-1,3-diol	C10H12O3	M-H	179.0714	-0.9
HMDB0168431	Benzenethanol, 3-hydroxy-, 1-acetate	C10H12O3	M-H	179.0714	-0.9
HMDB0168433	Acetic acid, hydroxy-, 2-phenylethyl ester	C10H12O3	M-H	179.0714	-0.9
HMDB0168430	beta-Hydroxyphenethyl acetate	C10H12O3	M-H	179.0714	-0.9
HMDB0166637	638-48-8	C10H12O3	M-H	179.0714	-0.9
HMDB0175294	3-(3-hydroxyphenyl)propyl formate	C10H12O3	M-H	179.0714	-0.9
HMDB0175295	Formic acid 3-(4-hydroxyphenyl)propyl ester	C10H12O3	M-H	179.0714	-0.9
HMDB0179728	4-[3-(methoxymethyl)oxiran-2-yl]phenol	C10H12O3	M-H	179.0714	-0.9
HMDB0179726	4-[(1E)-3-methoxyprop-1-en-1-yl]benzene-1,3-diol	C10H12O3	M-H	179.0714	-0.9
HMDB0179727	MolPort19-937-164	C10H12O3	M-H	179.0714	-0.9
HMDB0179464	4-methyl-1-(propan-2-yl)-7-oxabicyclo[4.1]hept-3-ene-2,5-dione	C10H12O3	M-H	179.0714	-0.9
HMDB0179463	2-(2-hydroxypropan-2-yl)-5-methylcyclohexa-2,5-diene-1,4-dione	C10H12O3	M-H	179.0714	-0.9
HMDB0179466	2-(1-hydroxypropan-2-yl)-5-methylcyclohexa-2,5-diene-1,4-dione	C10H12O3	M-H	179.0714	-0.9
HMDB0179465	1-methyl-4-(propan-2-yl)-7-oxabicyclo[4.1]hept-3-ene-2,5-dione	C10H12O3	M-H	179.0714	-0.9
HMDB0179462	2-(hydroxymethyl)-5-(propan-2-yl)cyclohexa-2,5-diene-1,4-dione	C10H12O3	M-H	179.0714	-0.9
HMDB0177511	1-hydroxy-1-(4-methoxyphenyl)propan-2-one	C10H12O3	M-H	179.0714	-0.9
HMDB0177512	2-Hydroxy-1-(4-methoxyphenyl)propan-1-one	C10H12O3	M-H	179.0714	-0.9

HMDB0177507	1-(4-methoxyphenyl)prop-1-ene-1,2-diol	C10H12O3	M-H	179.0714	-0.9
HMDB0166612	1,3-Benzodioxole-5-propanol	C10H12O3	M-H	179.0714	-0.9
HMDB0160085	4-(3-Hydroxyphenyl)butanoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0160087	2-hydroxy-4-phenylbutanoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0142085	dimethoxy-4-vinyl phenol	C10H12O3	M-H	179.0714	-0.9
HMDB0141179	4-hydroxy-4-(4-hydroxyphenyl)butan-2-one	C10H12O3	M-H	179.0714	-0.9
HMDB0141159	1-hydroxy-4-(4-hydroxyphenyl)butan-2-one	C10H12O3	M-H	179.0714	-0.9
HMDB0141138	4-(2,4-dihydroxyphenyl)butan-2-one	C10H12O3	M-H	179.0714	-0.9
HMDB0141118	3-hydroxy-4-(4-hydroxyphenyl)butan-2-one	C10H12O3	M-H	179.0714	-0.9
HMDB0141021	3-(4-hydroxyphenyl)butanoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0141023	2-hydroxy-3-phenylbutanoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0141022	4-hydroxy-3-phenylbutanoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0141020	3-hydroxy-3-phenylbutanoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0145926	5-ethenyl-2,3-dimethoxyphenol	C10H12O3	M-H	179.0714	-0.9
HMDB0160083	3-hydroxy-4-phenylbutanoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0157136	2-hydroxyphenylbutanoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0157135	2-hydroxy-2-phenylbutanoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0157133	4-hydroxy-2-phenylbutanoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0157132	a-methyltropic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0147386	BRN 31128	C10H12O3	M-H	179.0714	-0.9
HMDB0146624	2-(3-hydroxyprop-1-en-1-yl)-3-methoxyphenol	C10H12O3	M-H	179.0714	-0.9
HMDB0146625	4-(3-hydroxyprop-1-en-1-yl)-3-methoxyphenol	C10H12O3	M-H	179.0714	-0.9
HMDB0146623	3-hydroxy-3-(2-methoxyphenyl)propanal	C10H12O3	M-H	179.0714	-0.9
HMDB0146626	[3-(2-methoxyphenyl)oxiran-2-yl]methanol	C10H12O3	M-H	179.0714	-0.9
HMDB0146622	2-hydroxy-3-(2-methoxyphenyl)propanal	C10H12O3	M-H	179.0714	-0.9
HMDB0141019	3-(2-hydroxyphenyl)butanoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0146632	3-(2-methoxyphenyl)propanoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0031240	2-Phenyl-1,3-dioxolane-4-methanol	C10H12O3	M-H	179.0714	-0.9
HMDB0029685	4-Ethoxy-3-methoxybenzaldehyde	C10H12O3	M-H	179.0714	-0.9
HMDB0032640	Ethyl p-anisate	C10H12O3	M-H	179.0714	-0.9
HMDB0037733	Propyl 2-furanacrylate	C10H12O3	M-H	179.0714	-0.9
HMDB0032128	1-(2,4-Dihydroxyphenyl)-1-butanone	C10H12O3	M-H	179.0714	-0.9
HMDB0032574	Propylparaben	C10H12O3	M-H	179.0714	-0.9
HMDB0037602	4-Hydroxy-2,6,6-trimethyl-3-oxo-1,4-cyclohexadiene-1-carboxaldehyde	C10H12O3	M-H	179.0714	-0.9
HMDB0011751	3-Methoxybenzenepropanoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0033761	4-Methoxybenzyl acetate	C10H12O3	M-H	179.0714	-0.9
HMDB0032174	Benzaldehyde glyceryl acetal	C10H12O3	M-H	179.0714	-0.9
HMDB0131174	3-(4-methoxyphenyl)propanoic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0060734	3-(3-Hydroxyphenyl)-2-methylpropionic acid	C10H12O3	M-H	179.0714	-0.9
HMDB0012915	Coniferyl alcohol	C10H12O3	M-H	179.0714	-0.9
HMDB0166652	Coniferyl alcohol	C10H12O3	M-H	179.0714	-0.9
HMDB0168432	p-HPEA-AC	C10H12O3	M-H	179.0714	-0.9
HMDB0127492	4-ethenyl-2,6-dimethoxyphenol	C10H12O3	M-H	179.0714	-0.9
HMDB0059779	2,3-Methylene suberic acid	C10H14O4	M-H2O-H	179.0708	2.1
HMDB0059768	3,4-Methylene suberic acid	C10H14O4	M-H2O-H	179.0708	2.1
HMDB0030991	5-(3E-Pentenyl)tetrahydro-2-oxo-3-furancarboxylic acid	C10H14O4	M-H2O-H	179.0708	2.1
HMDB0033093	3-(4-Hydroxy-3-methoxyphenyl)-1,2-propanediol	C10H14O4	M-H2O-H	179.0708	2.1
HMDB0034099	(2E,4E)-2,7-Dimethyl-2,4-octadienedioic acid	C10H14O4	M-H2O-H	179.0708	2.1
HMDB0131265	2,3,5-trimethoxy-6-methylphenol	C10H14O4	M-H2O-H	179.0708	2.1
HMDB0177594	1-(3,4-dimethoxyphenyl)ethane-1,2-diol	C10H14O4	M-H2O-H	179.0708	2.1
HMDB0004998	Guaifenesin	C10H14O4	M-H2O-H	179.0708	2.1
HMDB0135755	4-ethyl-2,6-dimethoxybenzene-1,3-diol	C10H14O4	M-H2O-H	179.0708	2.1
HMDB0163241	(2E,5Z)-7-hydroxyundeca-2,5-dienoic acid	C11H18O3	M-H2O-H	179.1072	1.1
HMDB0163238	(2E,5Z)--hydroxyundeca-2,5-dienoic acid	C11H18O3	M-H2O-H	179.1072	1.1
HMDB0163239	(2E,5Z)-11-hydroxyundeca-2,5-dienoic acid	C11H18O3	M-H2O-H	179.1072	1.1
HMDB0163242	3-[(2Z)-oct-2-en-1-yl]oxirane-2-carboxylic acid	C11H18O3	M-H2O-H	179.1072	1.1
HMDB0178768	methyl (4Z,8Z)-2-hydroxydeca-4,8-dienoate	C11H18O3	M-H2O-H	179.1072	1.1
HMDB0179397	methyl 3-[(1Z)-hept-1-en-1-yl]oxirane-2-carboxylate	C11H18O3	M-H2O-H	179.1072	1.1
HMDB0179396	methyl (2E,4Z)-9-hydroxydeca-2,4-dienoate	C11H18O3	M-H2O-H	179.1072	1.1
HMDB0179395	methyl (4Z)-6-hydroxydeca-2,4-dienoate	C11H18O3	M-H2O-H	179.1072	1.1
HMDB0178763	methyl (4Z,8Z)--hydroxydeca-4,8-dienoate	C11H18O3	M-H2O-H	179.1072	1.1
HMDB0178766	methyl (4Z)-7-(3-methyloxiran-2-yl)hept-4-enoate	C11H18O3	M-H2O-H	179.1072	1.1
HMDB0179399	methyl (2E,4Z)--hydroxydeca-2,4-dienoate	C11H18O3	M-H2O-H	179.1072	1.1

179.1074	HMDB0179398	methyl (2E)-3-(3-pentylloxiran-2-yl)prop-2-enoate	C11H18O3	M-H2O-H	179.1072	1.1
	HMDB0178764	methyl (4Z,8Z)-3-hydroxydeca-4,8-dienoate	C11H18O3	M-H2O-H	179.1072	1.1
	HMDB0178765	methyl (4Z,8Z)-6-hydroxydeca-4,8-dienoate	C11H18O3	M-H2O-H	179.1072	1.1
	HMDB0163243	(2E)-4-(3-pentylloxiran-2-yl)but-2-enoic acid	C11H18O3	M-H2O-H	179.1072	1.1
	HMDB0178767	methyl 3-{3-[(3Z)-pent-3-en-1-yl]oxiran-2-yl}propanoate	C11H18O3	M-H2O-H	179.1072	1.1
	HMDB0178762	methyl (4Z,8Z)-7-hydroxydeca-4,8-dienoate	C11H18O3	M-H2O-H	179.1072	1.1
	HMDB0061787	(3E,5E)-2,6-Dimethyl-1,3,5,7-octatetraene	C10H14	M+FA-H	179.1078	-2.0
	HMDB0037051	1-Isopropyl-3-methylbenzene	C10H14	M+FA-H	179.1078	-2.0
	HMDB0032627	1-Methyl-2-propylbenzene	C10H14	M+FA-H	179.1078	-2.0
	HMDB0059812	Butylbenzene	C10H14	M+FA-H	179.1078	-2.0
	HMDB0037013	p-Mentha-1,3,8-triene	C10H14	M+FA-H	179.1078	-2.0
	HMDB0037050	1-Isopropyl-2-methylbenzene	C10H14	M+FA-H	179.1078	-2.0
	HMDB0059890	2-Ethyl-p-xylene	C10H14	M+FA-H	179.1078	-2.0
	HMDB0059821	m-Propyltoluene	C10H14	M+FA-H	179.1078	-2.0
	HMDB0005805	p-Cymene	C10H14	M+FA-H	179.1078	-2.0
	HMDB0059832	4-Ethyl-o-xylene	C10H14	M+FA-H	179.1078	-2.0
	HMDB0059823	Prehnitene	C10H14	M+FA-H	179.1078	-2.0
	HMDB0036669	(+)-Myrtenyl formate	C11H16O2	M-H	179.1078	-2.0
	HMDB0163605	2-(1-hydroxy-3-methylbutan-2-yl)phenol	C11H16O2	M-H	179.1078	-2.0
	HMDB0163603	SCHEMBL182446	C11H16O2	M-H	179.1078	-2.0
	HMDB0163602	3-methyl-2-phenylbutane-1,2-diol	C11H16O2	M-H	179.1078	-2.0
	HMDB0163600	2-methyl-3-phenylbutane-1,4-diol	C11H16O2	M-H	179.1078	-2.0
	HMDB0163604	SCHEMBL12872219	C11H16O2	M-H	179.1078	-2.0
	HMDB0163240	(2E,5Z)-undeca-2,5,-trienoic acid	C11H16O2	M-H	179.1078	-2.0
	HMDB0163599	3-methyl-2-phenylbutane-1,3-diol	C11H16O2	M-H	179.1078	-2.0
	HMDB0176253	3-methyl-1-phenylbutane-1,3-diol	C11H16O2	M-H	179.1078	-2.0
	HMDB0176252	AKO231874	C11H16O2	M-H	179.1078	-2.0
	HMDB0036817	Norecasantalic acid	C11H16O2	M-H	179.1078	-2.0
	HMDB0039159	Bovolide	C11H16O2	M-H	179.1078	-2.0
	HMDB0176254	3-(3-hydroxy-3-methylbutyl)phenol	C11H16O2	M-H	179.1078	-2.0
	HMDB0030007	2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]nona-3,8-diene	C11H16O2	M-H	179.1078	-2.0
	HMDB0035240	Dihydroactinidiolide	C11H16O2	M-H	179.1078	-2.0
	HMDB0039957	4-(Butoxymethyl)phenol	C11H16O2	M-H	179.1078	-2.0
	HMDB0030039	Jasmolone	C11H16O2	M-H	179.1078	-2.0
	HMDB0032468	2-Phenylpropionaldehyde dimethyl acetal	C11H16O2	M-H	179.1078	-2.0
	HMDB0176256	2-(3-hydroxy-3-methylbutyl)phenol	C11H16O2	M-H	179.1078	-2.0
	HMDB0176255	4-(3-hydroxy-3-methylbutyl)phenol	C11H16O2	M-H	179.1078	-2.0
	HMDB0151242	3-(4-methoxyphenyl)-2-methylpropan-1-ol	C11H16O2	M-H	179.1078	-2.0
	HMDB0164135	4-(4-methoxyphenyl)butan-2-ol	C11H16O2	M-H	179.1078	-2.0
	HMDB0059925	3-tert-Butyl-4-hydroxyanisole	C11H16O2	M-H	179.1078	-2.0
	HMDB0059926	2-tert-Butyl-4-hydroxyanisole	C11H16O2	M-H	179.1078	-2.0
180.0665	HMDB0062068	5-Acetyl-2-methylpyridine	C8H9NO	M+FA-H	180.0666	-0.6
	HMDB0040008	2,3-Dihydro-1H-pyrrolizine-5-carboxaldehyde	C8H9NO	M+FA-H	180.0666	-0.6
	HMDB0040222	2-Acetyl-5-methylpyridine	C8H9NO	M+FA-H	180.0666	-0.6
	HMDB0037071	2-Acetyl-4-methylpyridine	C8H9NO	M+FA-H	180.0666	-0.6
	HMDB0040223	4-Acetyl-2-methylpyridine	C8H9NO	M+FA-H	180.0666	-0.6
	HMDB0037072	2-Acetyl-6-methylpyridine	C8H9NO	M+FA-H	180.0666	-0.6
	HMDB0170598	p-hydroxystyrylamine	C8H9NO	M+FA-H	180.0666	-0.6
	HMDB0001250	N-Acetylarlyamine	C8H9NO	M+FA-H	180.0666	-0.6
	HMDB0032628	2-Aminoacetophenone	C8H9NO	M+FA-H	180.0666	-0.6
	HMDB0010715	2-Phenylacetamide	C8H9NO	M+FA-H	180.0666	-0.6
	HMDB0032630	2'-Aminoacetophenone	C8H9NO	M+FA-H	180.0666	-0.6
	HMDB0040224	4-Acetyl-3-methylpyridine	C8H9NO	M+FA-H	180.0666	-0.6
	HMDB0040013	5-(2-Furanyl)-3,4-dihydro-2H-pyrrole	C8H9NO	M+FA-H	180.0666	-0.6
	HMDB0162086	8-methyl-1H,3H,4H-pyrano[3,4-c]pyridine-1,4-diol	C9H11NO3	M-H	180.0666	-0.6
	HMDB0162085	8-(hydroxymethyl)-1H,3H,4H-pyrano[3,4-c]pyridin-1-ol	C9H11NO3	M-H	180.0666	-0.6
	HMDB0164039	ethyl 2-(hydroxyamino)benzoate	C9H11NO3	M-H	180.0666	-0.6
	HMDB0185178	4-(2-amino-1-hydroxyprop-2-en-1-yl)benzene-1,2-diol	C9H11NO3	M-H	180.0666	-0.6
	HMDB0164040	SCHEMBL62116	C9H11NO3	M-H	180.0666	-0.6
	HMDB0059720	Meta-Tyrosine	C9H11NO3	M-H	180.0666	-0.6
	HMDB0060280	4,6,7-Trihydroxy-1,2,3,4-tetrahydroisoquinoline	C9H11NO3	M-H	180.0666	-0.6
	HMDB0000158	L-Tyrosine	C9H11NO3	M-H	180.0666	-0.6
	HMDB0164171	L-Tyrosine	C9H11NO3	M-H	180.0666	-0.6

	HMDB0006050	o-Tyrosine	C9H11NO3	M-H	180.0666	-0.6
	HMDB0003831	Beta-Tyrosine	C9H11NO3	M-H	180.0666	-0.6
	HMDB0002184	L-Threo-3-Phenylserine	C9H11NO3	M-H	180.0666	-0.6
	HMDB0001119	4-Hydroxy-4-(3-pyridyl)-butanoic acid	C9H11NO3	M-H	180.0666	-0.6
	HMDB0185177	SCHEMBL05	C9H13NO4	M-H2O-H	180.0661	2.4
	HMDB0155115	5-[1-hydroxy-2-(methylamino)ethyl]benzene-1,2,3-triol	C9H13NO4	M-H2O-H	180.0661	2.4
	HMDB0155853	2-(2-amino-1-hydroxyethyl)-5-methoxybenzene-1,4-diol	C9H13NO4	M-H2O-H	180.0661	2.4
	HMDB0035177	2-Acetyl-1,5,6,7-tetrahydro-6-hydroxy-7-(hydroxymethyl)-4H-azepine-4-one	C9H13NO4	M-H2O-H	180.0661	2.4
	HMDB0155116	4-[1-hydroxy-2-(methylamino)ethyl]benzene-1,2,3-triol	C9H13NO4	M-H2O-H	180.0661	2.4
	HMDB0185176	5-(2-amino-1-hydroxypropyl)benzene-1,2,4-triol	C9H13NO4	M-H2O-H	180.0661	2.4
	HMDB0185175	4-(2-amino-1-hydroxypropyl)benzene-1,2,3-triol	C9H13NO4	M-H2O-H	180.0661	2.4
	HMDB0185174	5-(2-amino-1-hydroxypropyl)benzene-1,2,3-triol	C9H13NO4	M-H2O-H	180.0661	2.4
	HMDB0155114	1,2,4-Benzenetriol, 5-[1-hydroxy-2-(methylamino)ethyl]-	C9H13NO4	M-H2O-H	180.0661	2.4
	HMDB0030009	3,6-Dihydro-4-(4-methyl-3-pentenyl)-1,2-dithiin	C10H16S2	M-H2O-H	181.0510	-0.3
181.0509	HMDB0127495	3,5-dimethoxybenzoic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0171318	methyl 2-hydroxy-3-methoxybenzoate	C9H10O4	M-H	181.0506	1.5
	HMDB0125533	3,5-Dihydroxyphenylpropionic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0140294	2-hydroxy-2-(4-methoxyphenyl)acetic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0134043	3-(2,5-dihydroxyphenyl)propanoic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0137483	4-[(E)-2-hydroxyethenyl]-6-methoxybenzene-1,3-diol	C9H10O4	M-H	181.0506	1.5
	HMDB0140892	2-hydroxy-3-(3-hydroxyphenyl)propanoic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0159058	SCHEMBL173817	C9H10O4	M-H	181.0506	1.5
	HMDB0161054	(2-hydroxy-3-methoxyphenyl)acetic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0168687	4-Ethoxy-2-hydroxybenzoic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0168686	4-(2-hydroxyethoxy)benzoic Acid	C9H10O4	M-H	181.0506	1.5
	HMDB0168688	4-Ethoxy-3-hydroxybenzoic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0171694	4-(Hydroxymethyl)phenoxyacetic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0171695	SCHEMBL146957	C9H10O4	M-H	181.0506	1.5
	HMDB0172128	1-(furan-3-yl)-3-hydroxypentane-1,4-dione	C9H10O4	M-H	181.0506	1.5
	HMDB0172129	1-(furan-3-yl)-5-hydroxypentane-1,4-dione	C9H10O4	M-H	181.0506	1.5
	HMDB0133788	2-(2,4-dihydroxyphenyl)propanoic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0133494	2-hydroxy-2-(3-methoxyphenyl)acetic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0131428	2-(3-hydroxy-5-methoxyphenyl)acetic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0062595	meta-hydroxyphenylhydracrylic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0124923	3-hydroxy-3-(4-hydroxyphenyl)propanoic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0125591	4-ethenyl-6-methoxybenzene-1,2,3-triol	C9H10O4	M-H	181.0506	1.5
	HMDB0129348	2-(3,4-dihydroxyphenyl)propanoic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0000118	Homovanillic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0029273	2,6-Dimethoxybenzoic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0033624	2-Hydroxy-3-(2-hydroxyphenyl)propanoic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0059763	3,4-Dimethoxybenzoic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0126386	3-(2,4-dihydroxyphenyl)propanoic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0029232	3-Hydroxyphenyllactate	C9H10O4	M-H	181.0506	1.5
	HMDB0037274	Maltol propionate	C9H10O4	M-H	181.0506	1.5
	HMDB0029646	2',6'-Dihydroxy-4'-methoxyacetophenone	C9H10O4	M-H	181.0506	1.5
	HMDB0000333	Isohomovanillic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0000423	3,4-Dihydroxyhydrocinnamic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0000755	Hydroxyphenyllactic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0002643	3-(3-Hydroxyphenyl)-3-hydroxypropanoic acid	C9H10O4	M-H	181.0506	1.5
	HMDB0004061	3-Methoxy-4-hydroxyphenylglycolaldehyde	C9H10O4	M-H	181.0506	1.5
	HMDB0134042	3-(2,3-Dihydroxyphenyl)propanoate	C9H10O4	M-H	181.0506	1.5
	HMDB0041270	2',4'-Dihydroxy-6'-methoxyacetophenone	C9H10O4	M-H	181.0506	1.5
	HMDB0240266	Methyl vanillate	C9H10O4	M-H	181.0506	1.5
	HMDB0125595	5-ethenyl-3-methoxybenzene-1,2,4-triol	C9H10O4	M-H	181.0506	1.5
	HMDB0040638	3-(3-Furanyl)-2-methyl-2-propenal	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0167830	4'-Hydroxyacetophenone	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0038176	alpha-Methyl-2-furanacrolein	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0033766	2-Methoxybenzaldehyde	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0033968	Methyl benzoate	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0029635	4-Methylbenzoic acid	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0033128	4-(2-Furanyl)-3-buten-2-one	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0041485	Benzyl formate	C8H8O2	M+FA-H	181.0506	1.5

	HMDB0032568	2'-Hydroxyacetophenone	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0029686	4-Methoxybenzaldehyde	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0003767	4-Hydroxyphenylacetaldehyde	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0002340	2-Methylbenzoic acid	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0031459	3-Methoxybenzaldehyde	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0040733	Phenyl acetate	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0032400	3-(5-Methyl-2-furyl)prop-2-enal	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0000209	Phenylacetic acid	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0032603	2-Hydroxy-4-methylbenzaldehyde	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0062810	m-toluic acid	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0125535	5-ethenylbenzene-1,3-diol	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0167829	1-(3-hydroxyphenyl)ethan-1-one	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0126385	4-ethenylbenzene-1,3-diol	C8H8O2	M+FA-H	181.0506	1.5
	HMDB0183895	phenylacetate	C8H7O2	M+FA-H	181.0506	1.5
	HMDB0124942	4-ethenylbenzene-1,2-diol	C8H8O2	M+FA-H	181.0506	1.5
181.0718	HMDB0000765	Mannitol	C6H14O6	M-H	181.0718	0.2
	HMDB0011632	L-Iditol	C6H14O6	M-H	181.0718	0.2
	HMDB0000107	Galactitol	C6H14O6	M-H	181.0718	0.2
	HMDB0000247	Sorbitol	C6H14O6	M-H	181.0718	0.2
	HMDB0062269	Pentaerithrityl	C5H12O4	M+FA-H	181.0718	0.2
	HMDB0062440	Pentaerithrityl	C5H12O4	M+FA-H	181.0718	0.2
	HMDB0041486	1-Deoxy-D-ribitol	C5H12O4	M+FA-H	181.0718	0.2
	HMDB0011659	2-Methylerythritol	C5H12O4	M+FA-H	181.0718	0.2
	HMDB0033919	2-Deoxy-D-ribitol	C5H12O4	M+FA-H	181.0718	0.2
	HMDB0031201	3-Deoxy-D-arabinitol	C5H12O4	M+FA-H	181.0718	0.2
	HMDB0032441	Nona-2,4,6-trienal	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0031446	p-Isopropylphenol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0032544	2,4,6-Trimethylphenol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0038984	4-Ethyl-2-methylphenol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0038987	2-Ethyl-5-methylphenol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0032029	2-Isopropylphenol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0032149	1-Methoxy-2,4-dimethylbenzene	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0032625	4-Propylphenol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0029667	2,3,6-Trimethylphenol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0169117	alpha, alpha-Dimethylbenzyl alcohol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0125105	1-ethyl-3-methoxybenzene	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0169118	3-(propan-2-yl)phenol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0059896	6-Ethyl-o-cresol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0039782	2-(1-Pentenyl)furan	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0031312	Benzyl ethyl ether	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0033962	3-Phenyl-1-propanol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0031627	1-Phenyl-1-propanol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0034378	1-(4-Methylphenyl)ethanol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0031628	2-Phenyl-1-propanol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0038985	3-Ethyl-5-methylphenol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0032624	2-Propylphenol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0038986	3-Ethyl-4-methylphenol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0038988	2-Ethyl-4-methylphenol	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0032621	(2-Methoxyethyl)benzene	C9H12O	M+FA-H	181.0870	-0.6
	HMDB0179481	4427-54-7	C10H14O3	M-H	181.0870	-0.7
	HMDB0179471	2-(1-hydroxypropan-2-yl)-5-methylcyclohex-2-ene-1,4-dione	C10H14O3	M-H	181.0870	-0.7
	HMDB0179476	5-(1-hydroxypropan-2-yl)-2-methylcyclohex-2-ene-1,4-dione	C10H14O3	M-H	181.0870	-0.7
	HMDB0179478	2-hydroxy-2-isopropyl-5-methylcyclohex-5-ene-1,4-dione	C10H14O3	M-H	181.0870	-0.7
	HMDB0179475	1-methyl-4-(propan-2-yl)-7-oxabicyclo[4.1]heptane-2,5-dione	C10H14O3	M-H	181.0870	-0.7
	HMDB0179477	6-hydroxy-2-methyl-5-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M-H	181.0870	-0.7
	HMDB0179483	2-(1-hydroxypropan-2-yl)-5-methylbenzene-1,4-diol	C10H14O3	M-H	181.0870	-0.7
	HMDB0179482	6-methyl-3-(propan-2-yl)benzene-1,2,4-triol	C10H14O3	M-H	181.0870	-0.7
	HMDB0179480	2,5-dihydroxy-4-isopropylbenzyl alcohol	C10H14O3	M-H	181.0870	-0.7
	HMDB0179479	CTK8G51	C10H14O3	M-H	181.0870	-0.7

181.0869

HMDB0181694	3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M-H	181.0870	-0.7
HMDB0181695	2-(hydroxymethyl)-3-methyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M-H	181.0870	-0.7
HMDB0181696	5-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M-H	181.0870	-0.7
HMDB0181697	1-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M-H	181.0870	-0.7
HMDB0179474	5-(2-hydroxypropan-2-yl)-2-methylcyclohex-2-ene-1,4-dione	C10H14O3	M-H	181.0870	-0.7
HMDB0179473	2-(hydroxymethyl)-5-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M-H	181.0870	-0.7
HMDB0179467	5-(hydroxymethyl)-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M-H	181.0870	-0.7
HMDB0179472	6-hydroxy-5-methyl-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M-H	181.0870	-0.7
HMDB0142086	4-ethyl-2,3-dimethoxyphenol	C10H14O3	M-H	181.0870	-0.7
HMDB0145930	SCHEMBL83728	C10H14O3	M-H	181.0870	-0.7
HMDB0163112	3-[(1Z,4Z)-hepta-1,4-dien-1-yl]oxirane-2-carboxylic acid	C10H14O3	M-H	181.0870	-0.7
HMDB0163114	(2E,4Z)-6-(3-ethyloxiran-2-yl)hexa-2,4-dienoic acid	C10H14O3	M-H	181.0870	-0.7
HMDB0163113	(2E)-3-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}prop-2-enoic acid	C10H14O3	M-H	181.0870	-0.7
HMDB0163111	(2E,7Z)-9-hydroxydeca-2,4,7-trienoic acid	C10H14O3	M-H	181.0870	-0.7
HMDB0163115	(2E,4Z,7Z)-hydroxydeca-2,4,7-trienoic acid	C10H14O3	M-H	181.0870	-0.7
HMDB0179469	2-(2-hydroxypropan-2-yl)-5-methylcyclohex-2-ene-1,4-dione	C10H14O3	M-H	181.0870	-0.7
HMDB0179468	5-hydroxy-5-methyl-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M-H	181.0870	-0.7
HMDB0038181	Peperinic acid	C10H14O3	M-H	181.0870	-0.7
HMDB0032607	threo-Anethole glycol	C10H14O3	M-H	181.0870	-0.7
HMDB0038354	2-Ethoxy-4-(methoxymethyl)phenol	C10H14O3	M-H	181.0870	-0.7
HMDB0059891	Isoamyl 2-furoate	C10H14O3	M-H	181.0870	-0.7
HMDB0039874	Furfuryl isovalerate	C10H14O3	M-H	181.0870	-0.7
HMDB0029456	Amyl 2-furoate	C10H14O3	M-H	181.0870	-0.7
HMDB0037641	4-(Ethoxymethyl)-2-methoxyphenol	C10H14O3	M-H	181.0870	-0.7
HMDB0037727	Furfuryl pentanoate	C10H14O3	M-H	181.0870	-0.7
HMDB0036522	Verimol J	C10H14O3	M-H	181.0870	-0.7
HMDB0179470	4-methyl-1-(propan-2-yl)-7-oxabicyclo[4.1]heptane-2,5-dione	C10H14O3	M-H	181.0870	-0.7
HMDB0033394	4-Ethyl-2,6-dimethoxyphenol	C10H14O3	M-H	181.0870	-0.7
HMDB0034491	Camphoric acid	C10H16O4	M-H2O-H	181.0865	2.4
HMDB0170504	SCHEMBL4585236	C10H16O4	M-H2O-H	181.0865	2.4
HMDB0000603	cis-4-Decenedioic acid	C10H16O4	M-H2O-H	181.0865	2.4
HMDB0061295	526-51-6	C10H16O4	M-H2O-H	181.0865	2.4
HMDB0013227	cis-5-Decenedioic acid	C10H16O4	M-H2O-H	181.0865	2.4
HMDB0030989	5-Pentyltetrahydro-2-oxo-3-furancarboxylic acid	C10H16O4	M-H2O-H	181.0865	2.4
HMDB0034971	(1R,2R,3S,1'R)-Nepetalinic acid	C10H16O4	M-H2O-H	181.0865	2.4
HMDB0030990	alpha-Carboxy-delta-nonolactone	C10H16O4	M-H2O-H	181.0865	2.4
HMDB0036715	Matsutakic acid A	C10H16O4	M-H2O-H	181.0865	2.4
HMDB0032463	5-Pentyl-3h-furan-2-one	C11H18O2	M-H	181.1234	0.5
HMDB0032050	alpha-Terpineol formate	C11H18O2	M-H	181.1234	0.5
HMDB0038279	cis-3-Hexenyl tiglate	C11H18O2	M-H	181.1234	0.5
HMDB0038245	Bornyl formate	C11H18O2	M-H	181.1234	0.5
HMDB0038068	(3E,6Z)-Nonadien-1-yl acetate	C11H18O2	M-H	181.1234	0.5
HMDB0034708	Methyl 4,8-decadienoate	C11H18O2	M-H	181.1234	0.5
HMDB0030006	2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]non-3-ene	C11H18O2	M-H	181.1234	0.5
HMDB0036215	Ethyl octynecarboxylate	C11H18O2	M-H	181.1234	0.5
HMDB0059816	Methyl geranate	C11H18O2	M-H	181.1234	0.5
HMDB0038079	(2E,6Z)-2,6-Nonadien-1-Yl acetate	C11H18O2	M-H	181.1234	0.5
HMDB0163225	(2E)-4-(3-pentyloxiran-2-yl)but-2-enal	C11H18O2	M-H	181.1234	0.5
HMDB0037829	6-(3-Hexenyl)tetrahydro-2H-pyran-2-one	C11H18O2	M-H	181.1234	0.5
HMDB0163221	(2E,5Z)-undeca-2,5-dienoic acid	C11H18O2	M-H	181.1234	0.5
HMDB0163226	(2E,5Z)-11-hydroxyundeca-2,5-dienal	C11H18O2	M-H	181.1234	0.5
HMDB0036191	4-Hydroxy-4-methyl-7-decenoic acid gamma-lactone	C11H18O2	M-H	181.1234	0.5

181.1235

HMDB0035156	Neryl formate	C11H18O2	M-H	181.1234	0.5
HMDB0163223	(2E,5Z)--hydroxyundeca-2,5-dienal	C11H18O2	M-H	181.1234	0.5
HMDB0163222	(2E,5Z)-7-hydroxyundeca-2,5-dienal	C11H18O2	M-H	181.1234	0.5
HMDB0038005	xi-2-Hexyl-5-methyl-3(2H)-furanone	C11H18O2	M-H	181.1234	0.5
HMDB0163224	3-[(2Z)-oct-2-en-1-yl]oxirane-2-carbaldehyde	C11H18O2	M-H	181.1234	0.5
HMDB0030424	Linalyl formate	C11H18O2	M-H	181.1234	0.5
HMDB0037388	Tsibulin 2	C11H18O2	M-H	181.1234	0.5
HMDB0034730	Methyl (2E,4Z)-decadienoate	C11H18O2	M-H	181.1234	0.5
HMDB0040595	Allyl cyclohexylacetate	C11H18O2	M-H	181.1234	0.5
HMDB0041634	(-)-beta-Phellandrene	C10H16	M+FA-H	181.1234	0.5
HMDB0041574	Artemisiatriene	C10H16	M+FA-H	181.1234	0.5
HMDB0041633	(-)-beta-phellandrene	C10H16	M+FA-H	181.1234	0.5
HMDB0006525	(+)-alpha-Pinene	C10H16	M+FA-H	181.1234	0.5
HMDB0032473	Polylimonene	C10H16	M+FA-H	181.1234	0.5
HMDB0036081	beta-Phellandrene	C10H16	M+FA-H	181.1234	0.5
HMDB0034697	(+)-alpha-Carene	C10H16	M+FA-H	181.1234	0.5
HMDB0035087	(+)-alpha-Carene	C10H16	M+FA-H	181.1234	0.5
HMDB0037046	Sylveterpinolene	C10H16	M+FA-H	181.1234	0.5
HMDB0036997	beta-Terpinene	C10H16	M+FA-H	181.1234	0.5
HMDB0034928	(-)-4()-Thujene	C10H16	M+FA-H	181.1234	0.5
HMDB0035851	(R)-alpha-Phellandrene	C10H16	M+FA-H	181.1234	0.5
HMDB0062156	4()-Thujene	C10H16	M+FA-H	181.1234	0.5
HMDB0035619	alpha-Carene	C10H16	M+FA-H	181.1234	0.5
HMDB0036995	alpha-Terpinene	C10H16	M+FA-H	181.1234	0.5
HMDB0038121	1,7,7-Trimethyltricyclo[2.2.12,6]heptane	C10H16	M+FA-H	181.1234	0.5
HMDB0036559	(-)-beta-Pinene	C10H16	M+FA-H	181.1234	0.5
HMDB0036560	(-)-beta-Pinene	C10H16	M+FA-H	181.1234	0.5
HMDB0038150	p-Mentha-2,4-diene	C10H16	M+FA-H	181.1234	0.5
HMDB0004321	(-)-Limonene	C10H16	M+FA-H	181.1234	0.5
HMDB0003375	d-Limonene	C10H16	M+FA-H	181.1234	0.5
HMDB0005806	gamma-Terpinene	C10H16	M+FA-H	181.1234	0.5
HMDB0038169	7-Methyl-3-methylene-1,6-octadiene	C10H16	M+FA-H	181.1234	0.5
HMDB0036116	(-)-3-Thujene	C10H16	M+FA-H	181.1234	0.5
HMDB0035625	(-)-7,7-Dimethyl-2-methylenebicyclo[2.2.1]heptane	C10H16	M+FA-H	181.1234	0.5
HMDB0030089	trans-Ocimen	C10H16	M+FA-H	181.1234	0.5
HMDB0033200	5-Isosylveterpinolene	C10H16	M+FA-H	181.1234	0.5
HMDB0036104	(Z)-3,7-Dimethyl-1,3,7-octatriene	C10H16	M+FA-H	181.1234	0.5
HMDB0035850	alpha-Phellandrene	C10H16	M+FA-H	181.1234	0.5
HMDB0036994	Terpinolene	C10H16	M+FA-H	181.1234	0.5
HMDB0034970	(S)-alpha-Phellandrene	C10H16	M+FA-H	181.1234	0.5
HMDB0035658	(-)-alpha-Pinene	C10H16	M+FA-H	181.1234	0.5
HMDB0061793	Isolimonene	C10H16	M+FA-H	181.1234	0.5
HMDB0061791	2,7,7-Trimethyl-bicyclo[2.2.1]hept-2-ene	C10H16	M+FA-H	181.1234	0.5
HMDB0061792	3-Methylene-1,5,5-trimethylcyclohexene	C10H16	M+FA-H	181.1234	0.5
HMDB0061978	1,5,5-Trimethyl-6-methylene-cyclohexene	C10H16	M+FA-H	181.1234	0.5
HMDB0062083	alpha-Myrcene	C10H16	M+FA-H	181.1234	0.5
HMDB0062101	Decatriene	C10H16	M+FA-H	181.1234	0.5
HMDB0062126	(3E)-2,6-dimethylocta-1,3,7-triene	C10H16	M+FA-H	181.1234	0.5
HMDB0061790	Santolina triene	C10H16	M+FA-H	181.1234	0.5
HMDB0036076	(+)-sabinene	C10H16	M+FA-H	181.1234	0.5
HMDB0061789	2,6-Dimethyl-2,4,6-octatriene	C10H16	M+FA-H	181.1234	0.5
HMDB0061938	Isoterpinolene	C10H16	M+FA-H	181.1234	0.5
HMDB0062128	Isoterpinolene	C10H16	M+FA-H	181.1234	0.5
HMDB0030088	cis-Ocimene	C10H16	M+FA-H	181.1234	0.5
HMDB0059839	Camphene	C10H16	M+FA-H	181.1234	0.5
HMDB0059726	(+)-4-Carene	C10H16	M+FA-H	181.1234	0.5
HMDB0062124	Sylvestrine	C10H16	M+FA-H	181.1234	0.5
HMDB0059884	2-Carene	C10H16	M+FA-H	181.1234	0.5
HMDB0240350	4-(2-Hydroxyethoxy)-2-methoxyphenol	C9H12O4	M-H	183.0663	1.2
HMDB0151525	4-(hydroxymethyl)-5-methoxy-6-methylbenzene-1,3-diol	C9H12O4	M-H	183.0663	1.2
HMDB0180894	4-(1-hydroxyethyl)-5-methoxybenzene-1,3-diol	C9H12O4	M-H	183.0663	1.2
HMDB0151526	5-methoxy-4,6-dimethylbenzene-1,2,3-triol	C9H12O4	M-H	183.0663	1.2
HMDB0131234	4,6-dimethoxy-3-methylbenzene-1,2-diol	C9H12O4	M-H	183.0663	1.2
HMDB0131235	dimethoxy-methyl-hydroquinone	C9H12O4	M-H	183.0663	1.2

183.0665

HMDB0131233	2-(hydroxymethyl)-3,5-dimethoxyphenol	C9H12O4	M-H	183.0663	1.2
HMDB0126620	6-methoxy-3,5-dimethylbenzene-1,2,4-triol	C9H12O4	M-H	183.0663	1.2
HMDB0126619	4-(hydroxymethyl)-5-methoxy-2-methylbenzene-1,3-diol	C9H12O4	M-H	183.0663	1.2
HMDB0126618	2-(hydroxymethyl)-5-methoxy-4-methylbenzene-1,3-diol	C9H12O4	M-H	183.0663	1.2
HMDB0125597	5-ethyl-3-methoxybenzene-1,2,4-triol	C9H12O4	M-H	183.0663	1.2
HMDB0125593	4-ethyl-6-methoxybenzene-1,2,3-triol	C9H12O4	M-H	183.0663	1.2
HMDB0035056	1-(3-Hydroxy-4-methoxyphenyl)-1,2-ethanediol	C9H12O4	M-H	183.0663	1.2
HMDB0036072	Genipic acid	C9H12O4	M-H	183.0663	1.2
HMDB0059730	3,4-Methylenepimelic acid	C9H12O4	M-H	183.0663	1.2
HMDB0039650	4-Formyl-3-(formylmethyl)-4-hexenoic acid	C9H12O4	M-H	183.0663	1.2
HMDB0040603	threo-1-(4-Hydroxyphenyl)-1,2,3-propanetriol	C9H12O4	M-H	183.0663	1.2
HMDB0180032	syringyl alcohol	C9H12O4	M-H	183.0663	1.2
HMDB0001490	Vanylglycol	C9H12O4	M-H	183.0663	1.2
HMDB0166105	2-Methoxybenzyl alcohol	C8H10O2	M+FA-H	183.0663	1.2
HMDB0125590	5-ethylbenzene-1,3-diol	C8H10O2	M+FA-H	183.0663	1.2
HMDB0029671	1,4-Dimethoxybenzene	C8H10O2	M+FA-H	183.0663	1.2
HMDB0168417	1-phenylethane-1,2-diol	C8H10O2	M+FA-H	183.0663	1.2
HMDB0041607	2-Phenoxyethanol	C8H10O2	M+FA-H	183.0663	1.2
HMDB0039802	1-(2-Furanyl)-1-butanone	C8H10O2	M+FA-H	183.0663	1.2
HMDB0168418	3-(2-Hydroxyethyl)phenol	C8H10O2	M+FA-H	183.0663	1.2
HMDB0004284	Tyrosol	C8H10O2	M+FA-H	183.0663	1.2
HMDB0032137	2,6-Dimethyl-1,4-benzenediol	C8H10O2	M+FA-H	183.0663	1.2
HMDB0040174	4-Ethyl-1,2-benzenediol	C8H10O2	M+FA-H	183.0663	1.2
HMDB0040177	3-Ethyl-1,2-benzenediol	C8H10O2	M+FA-H	183.0663	1.2
HMDB0032139	1,2-Dimethoxybenzene	C8H10O2	M+FA-H	183.0663	1.2
HMDB0032036	4-Ethoxyphenol	C8H10O2	M+FA-H	183.0663	1.2
HMDB0029672	1,3-Dimethoxybenzene	C8H10O2	M+FA-H	183.0663	1.2
HMDB0034241	4-Methoxybenzyl alcohol	C8H10O2	M+FA-H	183.0663	1.2
HMDB0126388	4-ethylbenzene-1,3-diol	C8H10O2	M+FA-H	183.0663	1.2
HMDB0032136	2-Methoxy-4-methylphenol	C8H10O2	M+FA-H	183.0663	1.2
HMDB0029563	3-Acetyl-2,5-dimethylfuran	C8H10O2	M+FA-H	183.0663	1.2
HMDB0168448	2-hydroxyphenylethanol	C8H10O2	M+FA-H	183.0663	1.2
HMDB0032159	2-Acetyl-3,5-dimethylfuran	C8H10O2	M+FA-H	183.0663	1.2
HMDB0032290	1-(2-Furyl)butan-3-one	C8H10O2	M+FA-H	183.0663	1.2
HMDB0180424	Nona-trans-2-trans-4-dien-1-al	C9H14O	M+FA-H	183.1027	-0.9
HMDB0167046	SCHEMBL19577743	C9H14O	M+FA-H	183.1027	-0.9
HMDB0031152	(3Z,6Z)-3,6-Nonadienal	C9H14O	M+FA-H	183.1027	-0.9
HMDB0033857	Violet-leaf aldehyde	C9H14O	M+FA-H	183.1027	-0.9
HMDB0031261	(2E,6E)-2,6-Nonadienal	C9H14O	M+FA-H	183.1027	-0.9
HMDB0013824	2-Pentylfuran	C9H14O	M+FA-H	183.1027	-0.9
HMDB0031084	2-Pentylfuran	C9H14O	M+FA-H	183.1027	-0.9
HMDB0031685	2,4-Nonadienal	C9H14O	M+FA-H	183.1027	-0.9
HMDB0035929	(R)-Cryptone	C9H14O	M+FA-H	183.1027	-0.9
HMDB0036069	Pulegone	C9H14O	M+FA-H	183.1027	-0.9
HMDB0036091	exo-5,6-Dimethylbicyclo[2.2.1]hept-5-en-2-ol	C9H14O	M+FA-H	183.1027	-0.9
HMDB0036092	exo-2-Methyl-3-methylenebicyclo[2.2.1]heptan-2-ol	C9H14O	M+FA-H	183.1027	-0.9
HMDB0033434	4-Acetyl-1-methylcyclohexene	C9H14O	M+FA-H	183.1027	-0.9
HMDB0031195	3,5,5-Trimethyl-2-cyclohexen-1-one	C9H14O	M+FA-H	183.1027	-0.9
HMDB0035229	5-Isopropylbicyclo[3.1]hexan-2-one	C9H14O	M+FA-H	183.1027	-0.9
HMDB0040338	3,5,5-Trimethyl-3-cyclohexen-1-one	C9H14O	M+FA-H	183.1027	-0.9
HMDB0178774	3-{3-[(3Z)-pent-3-en-1-yl]oxiran-2-yl}propanoic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0178773	(4Z)-7-(3-methyloxiran-2-yl)hept-4-enoic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0178775	(4Z,8Z)-2-hydroxydeca-4,8-dienoic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0179400	(4Z)-6-hydroxydeca-2,4-dienoic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0179401	(2E,4Z)-9-hydroxydeca-2,4-dienoic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0179402	3-[(1Z)-hept-1-en-1-yl]oxirane-2-carboxylic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0179404	(2E,4Z)--hydroxydeca-2,4-dienoic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0179403	SCHEMBL12833	C10H16O3	M-H	183.1027	-0.9
HMDB0182629	SCHEMBL5986763	C10H16O3	M-H	183.1027	-0.9
HMDB0182628	2-[3-(hydroxymethyl)-2,2-dimethylcyclopent-3-en-1-yl]acetic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0182627	2-[2-(hydroxymethyl)-2,3-dimethylcyclopent-3-en-1-yl]acetic acid	C10H16O3	M-H	183.1027	-0.9

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HMDB0182631	SCHEMBL59867	C10H16O3	M-H	183.1027	-0.9
HMDB0182630	2-{1,2,2-trimethyl-6-oxabicyclo[3.1]hexan-3-yl}acetic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0178772	(4Z,8Z)-6-hydroxydeca-4,8-dienoic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0178770	(4Z,8Z)--hydroxydeca-4,8-dienoic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0178771	(4Z,8Z)-3-hydroxydeca-4,8-dienoic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0131084	(5E)-2,2,5-trimethyl-7-oxohept-5-enoic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0176282	6-hydroxy-1-(hydroxymethyl)-7,7-dimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M-H	183.1027	-0.9
HMDB0176283	1-Methyl-6-hydroxy-7-methyl-7-(hydroxymethyl)norbornane-2-one	C10H16O3	M-H	183.1027	-0.9
HMDB0176285	5,6-dihydroxy-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M-H	183.1027	-0.9
HMDB0176286	3,6-dihydroxy-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M-H	183.1027	-0.9
HMDB0176284	6,6-dihydroxy-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O3	M-H	183.1027	-0.9
HMDB0178769	(4Z,8Z)-7-hydroxydeca-4,8-dienoic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0040883	(E)--Oxo-8-decenoic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0036117	(1'R)-Nepetalic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0036998	(S)-Oleuropeic acid	C10H16O3	M-H	183.1027	-0.9
HMDB0039710	1-Acetylcyclohexyl acetate	C10H16O3	M-H	183.1027	-0.9
HMDB0039052	(4S,8R)-8,9-Dihydroxy-p-menth-1(6)-en-2-one	C10H16O3	M-H	183.1027	-0.9
HMDB0031510	R-2-Hydroxy-3-methylbutanoic acid 3-Methylbutanoyl	C10H18O4	M-H2O-H	183.1021	2.1
HMDB0040196	Oxalic acid dibutyl ester	C10H18O4	M-H2O-H	183.1021	2.1
HMDB0059754	3-Methylazelaic acid	C10H18O4	M-H2O-H	183.1021	2.1
HMDB0059719	Heptylmalonic acid	C10H18O4	M-H2O-H	183.1021	2.1
HMDB0059708	2-Ethylsuberic acid	C10H18O4	M-H2O-H	183.1021	2.1
HMDB0062180	(2S,5S)-2-[(2R)-butan-2-yl]-5-hydroxy-4-oxohexanoic acid	C10H18O4	M-H2O-H	183.1021	2.1
HMDB0000792	Sebacic acid	C10H18O4	M-H2O-H	183.1021	2.1
HMDB0061992	7-methyl-3-methylene-1,6-octadiene	C10H18	M+FA-H	183.1391	-0.3
HMDB0061796	cis-Carane	C10H18	M+FA-H	183.1391	-0.3
HMDB0062091	cis-Carane	C10H18	M+FA-H	183.1391	-0.3
HMDB0062153	3,7-dimethylocta-1,6-diene	C10H18	M+FA-H	183.1391	-0.3
HMDB0062025	2,7-dimethylocta-3,5-diene	C10H18	M+FA-H	183.1391	-0.3
HMDB0061800	1-(3-Methylbutyl)-cyclopentene	C10H18	M+FA-H	183.1391	-0.3
HMDB0061801	3-(2-Methylpropyl)-cyclohexene	C10H18	M+FA-H	183.1391	-0.3
HMDB0061797	2-Menthene	C10H18	M+FA-H	183.1391	-0.3
HMDB0061798	1-Methyl-3-(2-methyl-1-propenyl)cyclopentane	C10H18	M+FA-H	183.1391	-0.3
HMDB0061795	(S)-3,7-Dimethyl-1,6-octadiene	C10H18	M+FA-H	183.1391	-0.3
HMDB0061799	1-Methyl-3-(2-methyl-2-propenyl)-cyclopentane	C10H18	M+FA-H	183.1391	-0.3
HMDB0037213	xi-p-Menth-3-ene	C10H18	M+FA-H	183.1391	-0.3
HMDB0175165	SCHEMBL15641446	C11H20O2	M-H	183.1391	-0.3
HMDB0163852	8-hydroxyundec--en-2-one	C11H20O2	M-H	183.1391	-0.3
HMDB0163856	4-hydroxyundec--en-2-one	C11H20O2	M-H	183.1391	-0.3
HMDB0163854	6-hydroxyundec--en-2-one	C11H20O2	M-H	183.1391	-0.3
HMDB0163855	5-hydroxyundec--en-2-one	C11H20O2	M-H	183.1391	-0.3
HMDB0163853	7-hydroxyundec--en-2-one	C11H20O2	M-H	183.1391	-0.3
HMDB0163858	9-(oxiran-2-yl)nonan-2-one	C11H20O2	M-H	183.1391	-0.3
HMDB0163859	3-hydroxyundec--en-2-one	C11H20O2	M-H	183.1391	-0.3
HMDB0163857	SCHEMBL11481214	C11H20O2	M-H	183.1391	-0.3
HMDB0163860	1-hydroxyundec--en-2-one	C11H20O2	M-H	183.1391	-0.3
HMDB0180766	(2E)-11-hydroxyundec-2-enal	C11H20O2	M-H	183.1391	-0.3
HMDB0180764	(2E)--hydroxyundec-2-enal	C11H20O2	M-H	183.1391	-0.3
HMDB0180765	3-octyloxirane-2-carbaldehyde	C11H20O2	M-H	183.1391	-0.3
HMDB0180763	4-Hydroxy-2-undecenal	C11H20O2	M-H	183.1391	-0.3
HMDB0163245	5Z-undecenoic acid	C11H20O2	M-H	183.1391	-0.3
HMDB0163237	(2E,5Z)-undeca-2,5-diene-1,11-diol	C11H20O2	M-H	183.1391	-0.3
HMDB0163235	{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}methanol	C11H20O2	M-H	183.1391	-0.3
HMDB0163230	4-(3-pentyloxiran-2-yl)butanal	C11H20O2	M-H	183.1391	-0.3
HMDB0163228	(5Z)-4-hydroxyundec-5-enal	C11H20O2	M-H	183.1391	-0.3
HMDB0163229	(5Z)--hydroxyundec-5-enal	C11H20O2	M-H	183.1391	-0.3
HMDB0163227	(5Z)-7-hydroxyundec-5-enal	C11H20O2	M-H	183.1391	-0.3
HMDB0163232	(5Z)-2-hydroxyundec-5-enal	C11H20O2	M-H	183.1391	-0.3

183.1390	HMDB0163231	(5Z)-11-hydroxyundec-5-enal	C11H20O2	M-H	183.1391	-0.3
	HMDB0163234	(2E,5Z)-undeca-2,5-diene-1,-diol	C11H20O2	M-H	183.1391	-0.3
	HMDB0163233	(2E,5Z)-undeca-2,5-diene-1,7-diol	C11H20O2	M-H	183.1391	-0.3
	HMDB0163236	(2E)-4-(3-pentyloxiran-2-yl)but-2-en-1-ol	C11H20O2	M-H	183.1391	-0.3
	HMDB0031062	(Z)-3-Methyl-3-decenoic acid	C11H20O2	M-H	183.1391	-0.3
	HMDB0036784	6-Hexyltetrahydro-2H-pyran-2-one	C11H20O2	M-H	183.1391	-0.3
	HMDB0034428	Cyclohexyl 3-methylbutanoate	C11H20O2	M-H	183.1391	-0.3
	HMDB0037225	Methyl citronellate	C11H20O2	M-H	183.1391	-0.3
	HMDB0033724	Undecylenic acid	C11H20O2	M-H	183.1391	-0.3
	HMDB0038277	cis-3-Hexenyl 2-methylbutanoate	C11H20O2	M-H	183.1391	-0.3
	HMDB0040593	2-Propenyl octanoate	C11H20O2	M-H	183.1391	-0.3
	HMDB0037185	Rhodinyl formate	C11H20O2	M-H	183.1391	-0.3
	HMDB0032396	Methyl 2-decenoate	C11H20O2	M-H	183.1391	-0.3
	HMDB0032453	cis-3-Octenyl propionate	C11H20O2	M-H	183.1391	-0.3
	HMDB0032320	3-Hexenyl 2-methylbutyrate	C11H20O2	M-H	183.1391	-0.3
	HMDB0032534	trans-2-Hexenyl 2-methylbutyrate	C11H20O2	M-H	183.1391	-0.3
	HMDB0032461	Pent-2-enyl hexanoate	C11H20O2	M-H	183.1391	-0.3
	HMDB0032404	6-Methyl-5-hepten-2-one propyleneglycol acetal	C11H20O2	M-H	183.1391	-0.3
	HMDB0032308	(E)-3-Heptenyl 2-methylpropanoate	C11H20O2	M-H	183.1391	-0.3
	HMDB0038278	cis-3-Hexenyl 3-methylbutanoate	C11H20O2	M-H	183.1391	-0.3
	HMDB0038273	2-Hexenyl valerate	C11H20O2	M-H	183.1391	-0.3
	HMDB0031272	Ethyl (E)-2-nonenoate	C11H20O2	M-H	183.1391	-0.3
	HMDB0031063	(Z)-3-Methyl-4-decenoic acid	C11H20O2	M-H	183.1391	-0.3
	HMDB0031087	trans-2-Hexyl-1-cyclopropaneacetic acid	C11H20O2	M-H	183.1391	-0.3
	HMDB0033371	Citronellyl formate	C11H20O2	M-H	183.1391	-0.3
	HMDB0037106	(x)-1-Nonen-3-yl acetate	C11H20O2	M-H	183.1391	-0.3
	HMDB0036140	5-Hexyldihydro-5-methyl-2(3H)-furanone	C11H20O2	M-H	183.1391	-0.3
	HMDB0031691	cis-3-Hexenyl pentanoate	C11H20O2	M-H	183.1391	-0.3
	HMDB0038311	xi-gamma-Undecalactone	C11H20O2	M-H	183.1391	-0.3
	HMDB0031406	Ethyl 3-cyclohexylpropionate	C11H20O2	M-H	183.1391	-0.3
	HMDB0038906	5-Octenyl propanoate	C11H20O2	M-H	183.1391	-0.3
	HMDB0037309	5-Hexyldihydro-4-methyl-2(3H)-furanone	C11H20O2	M-H	183.1391	-0.3
	HMDB0031843	2,3-Undecanedione	C11H20O2	M-H	183.1391	-0.3
	HMDB0038274	2-Hexenyl isovalerate	C11H20O2	M-H	183.1391	-0.3
	HMDB0032489	Prenyl caproate	C11H20O2	M-H	183.1391	-0.3
	HMDB0034429	Cyclohexyl pentanoate	C11H20O2	M-H	183.1391	-0.3
	HMDB0062090	butyl cyclohexanecarboxylate	C11H20O2	M-H	183.1391	-0.3
	HMDB0183924	4-hydroxy-4,8-dimethylnonanoic acid	C11H22O3	M-H2O-H	183.1385	2.7
	HMDB0183925	8-hydroxy-4,8-dimethylnonanoic acid	C11H22O3	M-H2O-H	183.1385	2.7
	HMDB0183926	4-(hydroxymethyl)-8-methylnonanoic acid	C11H22O3	M-H2O-H	183.1385	2.7
	HMDB0183927	9-hydroxy-4,8-dimethylnonanoic acid	C11H22O3	M-H2O-H	183.1385	2.7
	HMDB0183928	2-hydroxy-4,8-dimethylnonanoic acid	C11H22O3	M-H2O-H	183.1385	2.7
	HMDB0175164	2-hydroxy-9-methyldecanoic acid	C11H22O3	M-H2O-H	183.1385	2.7
	HMDB0061654	3-hydroxyundecanoic acid	C11H22O3	M-H2O-H	183.1385	2.7
	HMDB0032443	3-Hydroxynonyl acetate	C11H22O3	M-H2O-H	183.1385	2.7
	HMDB0059736	2-Hydroxyundecanoate	C11H22O3	M-H2O-H	183.1385	2.7
	HMDB0166977	Methyl -hydroxydecanoate	C11H22O3	M-H2O-H	183.1385	2.7
	HMDB0175163	SCHEMBL8984439	C11H22O3	M-H2O-H	183.1385	2.7
	HMDB0175162	SCHEMBL9794217	C11H22O3	M-H2O-H	183.1385	2.7
	HMDB0166976	Methyl 9-hydroxydecanoate	C11H22O3	M-H2O-H	183.1385	2.7
184.0018	HMDB0000272	Phosphoserine	C3H8NO6P	M-H	184.0016	0.8
	HMDB0001721	DL-O-Phosphoserine	C3H8NO6P	M-H	184.0016	0.8
185.0569	HMDB0061890	Pyroglutamylglycine	C7H10N2O4	M-H	185.0568	0.6
	HMDB0004988	Pi-Methylimidazoleacetic acid	C6H8N2O2	M+FA-H	185.0568	0.7
	HMDB0002144	1,3-Dimethyluracil	C6H8N2O2	M+FA-H	185.0568	0.7
	HMDB0002820	Methylimidazoleacetic acid	C6H8N2O2	M+FA-H	185.0568	0.7
	HMDB0002271	Imidazolepropionic acid	C6H8N2O2	M+FA-H	185.0568	0.7
185.0818	HMDB0037625	Allyl tiglate	C8H12O2	M+FA-H	185.0819	-0.7
	HMDB0036176	3-Ethyl-2-hydroxy-4-methyl-2-cyclopenten-1-one	C8H12O2	M+FA-H	185.0819	-0.7
	HMDB0039652	2-Hydroxy-3,4,5-trimethyl-2-cyclopenten-1-one	C8H12O2	M+FA-H	185.0819	-0.7
	HMDB0039680	3,5,5-Trimethyl-1,2-cyclopentanedione	C8H12O2	M+FA-H	185.0819	-0.7
	HMDB0039651	3-Propyl-1,2-cyclopentanedione	C8H12O2	M+FA-H	185.0819	-0.7
	HMDB0039673	4-Ethyl-2-hydroxy-3-methyl-2-cyclopenten-1-one	C8H12O2	M+FA-H	185.0819	-0.7
	HMDB0040463	Ethyl sorbate	C8H12O2	M+FA-H	185.0819	-0.7
	HMDB0040526	3,4,4-Trimethyl-1,2-cyclopentanedione	C8H12O2	M+FA-H	185.0819	-0.7

103.0010	HMDB0039681	3-Isopropyl-1,2-cyclopentanedione	C8H12O2	M+FA-H	185.0819	-0.7
	HMDB0037196	Ethyl 2-methyl-3,4-pentadienoate	C8H12O2	M+FA-H	185.0819	-0.7
	HMDB0037167	3-Ethyl-5-methyl-1,2-cyclopentanedione	C8H12O2	M+FA-H	185.0819	-0.7
	HMDB0032311	2,4-Hexadienyl acetate	C8H12O2	M+FA-H	185.0819	-0.7
	HMDB0060682	2-Propyl-2,4-pentadienoic acid	C8H12O2	M+FA-H	185.0819	-0.7
	HMDB0030992	5-Butyltetrahydro-2-oxo-3-furancarboxylic acid	C9H14O4	M-H	185.0819	-0.7
	HMDB0030988	5-(2-Methylpropyl)tetrahydro-2-oxo-3-furancarboxylic acid	C9H14O4	M-H	185.0819	-0.7
185.1182	HMDB0059828	3-Nonen-5-one	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0062671	(3E)-2,3,4-trimethylhex-3-enal	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0167031	Violet alcohol	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0032535	trans-4-Nonenal	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0037001	Santene hydrate	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0031834	2,6-Dimethyl-5-heptenal	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0037150	2-Ethyl-2-heptenal	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0034764	3-Nonen-2-one	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0031269	2-Nonenal	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0034845	2,4-Nonadien-1-ol	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0033794	2,2,6-Trimethylcyclohexanone	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0035926	8-Nonen-2-one	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0038067	(3E,6Z)-3,6-Nonadien-1-ol	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0030957	(3Z,6Z)-3,6-Nonadien-1-ol	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0035927	1-Nonen-4-one	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0034758	8-Nonen-3-one	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0031262	2,6-Nonadien-1-ol	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0038400	(2xi,4xi)-2,4-Nonadien-1-ol	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0037170	3-Methylene-2-octanone	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0030958	(Z)-6-Nonenal	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0034761	5-Nonen-2-one	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0033554	2-Methyl-2-octenal	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0035916	(E)-2-Nonen-4-one	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0039461	7-Methyl-3-octen-2-one	C9H16O	M+FA-H	185.1183	-0.6
	HMDB0040205	3-Methylbutyl 3-hydroxy-2-methylidenebutanoate	C10H18O3	M-H	185.1183	-0.6
	HMDB0040204	2-Methylbutyl 3-hydroxy-2-methylidenebutanoate	C10H18O3	M-H	185.1183	-0.6
	HMDB0030367	Ethyl (3R,5Z)-3-hydroxy-5-octenoate	C10H18O3	M-H	185.1183	-0.6
	HMDB0038978	(1beta,2beta,5beta)-p-Menth-3-ene-1,2,5-triol	C10H18O3	M-H	185.1183	-0.6
	HMDB0041545	(1R,2R,4R)-1,8-Epoxy-p-menthane-2,4-diol	C10H18O3	M-H	185.1183	-0.6
	HMDB0030369	3-Hydroxy-5Z-octenyl acetate	C10H18O3	M-H	185.1183	-0.6
	HMDB0180054	(6E)-9-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M-H	185.1183	-0.6
	HMDB0180055	(6E)-2-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M-H	185.1183	-0.6
	HMDB0180148	1-(hydroxymethyl)-3,3-dimethyl-2-oxabicyclo[2.2.2]octan-6-ol	C10H18O3	M-H	185.1183	-0.6
	HMDB0180505	3-hydroxy-9-decenoic acid	C10H18O3	M-H	185.1183	-0.6
	HMDB0180508	6-hydroxydec-9-enoic acid	C10H18O3	M-H	185.1183	-0.6
	HMDB0180506	4-hydroxydec-9-enoic acid	C10H18O3	M-H	185.1183	-0.6
	HMDB0180507	5-hydroxydec-9-enoic acid	C10H18O3	M-H	185.1183	-0.6
	HMDB0180510	8-hydroxy-9-decenoic acid	C10H18O3	M-H	185.1183	-0.6
	HMDB0180511	Oxiraneoctanoic acid	C10H18O3	M-H	185.1183	-0.6
	HMDB0180512	2-hydroxydec-9-enoic acid	C10H18O3	M-H	185.1183	-0.6
	HMDB0180053	5-[3-(propan-2-yl)oxiran-2-yl]pentanoic acid	C10H18O3	M-H	185.1183	-0.6
	HMDB0180052	(6E)-5-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M-H	185.1183	-0.6
	HMDB0180051	(6E)-8-hydroxy-8-methylnon-6-enoic acid	C10H18O3	M-H	185.1183	-0.6
	HMDB0041376	exo,exo-1,8-Epoxy-p-menthane-2,6-diol	C10H18O3	M-H	185.1183	-0.6
	HMDB0039533	(E)--Hydroxy-8-decenoic acid	C10H18O3	M-H	185.1183	-0.6
	HMDB0033010	(1S,2S,4S,5R)-1,8-Epoxy-p-menthane-2,5-diol	C10H18O3	M-H	185.1183	-0.6
	HMDB0010724	3-Oxodecanoic acid	C10H18O3	M-H	185.1183	-0.6
	HMDB0164896	6,7-dihydroxy-7-methyl-3-methylideneoctanal	C10H18O3	M-H	185.1183	-0.6
	HMDB0164962	1-(2-hydroxypropan-2-yl)-4-methylbicyclo[3.1]hexane-2,4-diol	C10H18O3	M-H	185.1183	-0.6
	HMDB0180509	7-hydroxydec-9-enoic acid	C10H18O3	M-H	185.1183	-0.6
	HMDB0038692	6-Methyl-2-methylene-6-octene-1,3,8-triol	C10H18O3	M-H	185.1183	-0.6
	HMDB0039587	5-Hexyl-1,4-dioxan-2-one	C10H18O3	M-H	185.1183	-0.6
	HMDB0163825	5-(1,2-dihydroxypropan-2-yl)-2-methylcyclohexan-1-one	C10H18O3	M-H	185.1183	-0.6
	HMDB0039582	6-Hexyl-1,4-dioxan-2-one	C10H18O3	M-H	185.1183	-0.6

	HMDB0039974	(1S,2S,4R,8R)-p-Menthane-1,2,8,9-tetrol	C10H20O4	M-H2O-H	185.1178	2.3
	HMDB0033642	(2xi,3xi,6E)-3,7-Dimethyl-6-octene-1,2,3,8-tetrol	C10H20O4	M-H2O-H	185.1178	2.3
	HMDB0033217	(2xi,6xi)-7-Methyl-3-methylene-1,2,6,7-octanetetrol	C10H20O4	M-H2O-H	185.1178	2.3
	HMDB0039053	(1alpha,2alpha,4betaH,6alpha,8R)-p-Menthane-2,6,8,9-tetrol	C10H20O4	M-H2O-H	185.1178	2.3
	HMDB0035133	3,7-Dimethyl-3-octene-1,2,6,7-tetrol	C10H20O4	M-H2O-H	185.1178	2.3
185.1546	HMDB0061804	m-Menthane	C10H20	M+FA-H	185.1547	-0.6
	HMDB0041402	Butylcyclohexane	C10H20	M+FA-H	185.1547	-0.6
	HMDB0061803	cis-3-Decene	C10H20	M+FA-H	185.1547	-0.6
	HMDB0094652	(2E)-3,7-dimethyloct-2-ene	C10H20	M+FA-H	185.1547	-0.6
	HMDB0031455	p-Menthane	C10H20	M+FA-H	185.1547	-0.6
	HMDB0035141	1-Isopropyl-2,3-dimethylcyclopentane	C10H20	M+FA-H	185.1547	-0.6
	HMDB0061951	(2Z)-3,7-dimethyloct-2-ene	C10H20	M+FA-H	185.1547	-0.6
	HMDB0062092	(1R,2S)-1-methyl-2-propylcyclohexane	C10H20	M+FA-H	185.1547	-0.6
	HMDB0059860	2-Methylbutyl hexanoate	C11H22O2	M-H	185.1547	-0.6
	HMDB0180760	(2E)-undec-2-ene-1,-diol	C11H22O2	M-H	185.1547	-0.6
	HMDB0180762	(2E)-undec-2-ene-1,11-diol	C11H22O2	M-H	185.1547	-0.6
	HMDB0165570	1-HYDROXYUNDECAN-2-ONE	C11H22O2	M-H	185.1547	-0.6
	HMDB0165571	3-Hydroxy-2-undecanone	C11H22O2	M-H	185.1547	-0.6
	HMDB0165569	11-hydroxy-2-undecanone	C11H22O2	M-H	185.1547	-0.6
	HMDB0165568	SCHEMBL117411	C11H22O2	M-H	185.1547	-0.6
	HMDB0094659	tert-butyl heptanoate	C11H22O2	M-H	185.1547	-0.6
	HMDB0180761	3-octyloxiranemethanol	C11H22O2	M-H	185.1547	-0.6
	HMDB0180759	(2E)-undec-2-ene-1,4-diol	C11H22O2	M-H	185.1547	-0.6
	HMDB0033848	Methyl decanoate	C11H22O2	M-H	185.1547	-0.6
	HMDB0034458	Isobutyl enanthate	C11H22O2	M-H	185.1547	-0.6
	HMDB0040171	Heptyl 2-methylpropanoate	C11H22O2	M-H	185.1547	-0.6
	HMDB0040266	Nonyl acetate	C11H22O2	M-H	185.1547	-0.6
	HMDB0041559	Butyl heptanoate	C11H22O2	M-H	185.1547	-0.6
	HMDB0034460	Heptyl butanoate	C11H22O2	M-H	185.1547	-0.6
	HMDB0034134	Octyl propanoate	C11H22O2	M-H	185.1547	-0.6
	HMDB0039215	Hexyl 2-methylbutanoate	C11H22O2	M-H	185.1547	-0.6
	HMDB0034456	9-Methyldecanoic acid	C11H22O2	M-H	185.1547	-0.6
	HMDB0033618	3-Methylbutyl hexanoate	C11H22O2	M-H	185.1547	-0.6
	HMDB0038237	xi-8-Methyldecanoic acid	C11H22O2	M-H	185.1547	-0.6
	HMDB0002373	4,6-Dimethylnonanoic acid	C11H22O2	M-H	185.1547	-0.6
	HMDB0000947	Undecanoic acid	C11H22O2	M-H	185.1547	-0.6
	HMDB0036034	6,6-Dimethoxy-2,5,5-trimethyl-2-hexene	C11H22O2	M-H	185.1547	-0.6
	HMDB0032044	Hexyl 3-methylbutanoate	C11H22O2	M-H	185.1547	-0.6
	HMDB0038267	7,7-Diethoxy-3-heptene	C11H22O2	M-H	185.1547	-0.6
	HMDB0062119	Hexyl valerate	C11H22O2	M-H	185.1547	-0.6
	HMDB0059831	Propyl octanoate	C11H22O2	M-H	185.1547	-0.6
	HMDB0032325	2-Hexyl-4,5-dimethyl-1,3-dioxolane	C11H22O2	M-H	185.1547	-0.6
	HMDB0032448	Octanal propyleneglycol acetal	C11H22O2	M-H	185.1547	-0.6
	HMDB0036229	Pentyl hexanoate	C11H22O2	M-H	185.1547	-0.6
	HMDB0040193	Ethyl nonanoate	C11H22O2	M-H	185.1547	-0.6
186.8844	HMDB0031258	Lenthionine	C2H4S5	M-H	186.8844	0.1
187.0613	HMDB0157323	3-(4-carboxybutyl)oxirane-2-carboxylic acid	C8H12O5	M-H	187.0612	0.6
	HMDB0157322	SCHEMBL4732887	C8H12O5	M-H	187.0612	0.6
	HMDB0157320	(2E)-5-hydroxyoct-2-enedioic acid	C8H12O5	M-H	187.0612	0.6
	HMDB0157321	(2E)-6-hydroxyoct-2-enedioic acid	C8H12O5	M-H	187.0612	0.6
	HMDB0157324	(2E)-7-hydroxyoct-2-enedioic acid	C8H12O5	M-H	187.0612	0.6
	HMDB0059767	Tetrahydro-2,5-furan-diacetic acid	C8H12O5	M-H	187.0612	0.6
	HMDB0172015	4-methoxy-5-methyl-2-methylideneoxolan-3-one	C7H10O3	M+FA-H	187.0612	0.6
	HMDB0163404	5-ethyl-4-methyloxolane-2,3-dione	C7H10O3	M+FA-H	187.0612	0.6
	HMDB0180324	(2E)-3-(3-ethyloxiran-2-yl)prop-2-enoic acid	C7H10O3	M+FA-H	187.0612	0.6
	HMDB0180325	(2E)-4,5-dihydroxyhepta-2,4-dienal	C7H10O3	M+FA-H	187.0612	0.6
	HMDB0033551	5-Ethyl-3-hydroxy-4-methyl-2(5H)-furanone	C7H10O3	M+FA-H	187.0612	0.6
	HMDB0165787	2-ethyl-5-methyloxolane-3,4-dione	C7H10O3	M+FA-H	187.0612	0.6
	HMDB0164727	4,6-dihydroxy-4-methylcyclohex-2-en-1-one	C7H10O3	M+FA-H	187.0612	0.6
	HMDB0164726	5-hydroxy-5-methyl-7-oxabicyclo[4.1]heptan-2-one	C7H10O3	M+FA-H	187.0612	0.6
	HMDB0164725	4-hydroxy-4-(hydroxymethyl)cyclohex-2-en-1-one	C7H10O3	M+FA-H	187.0612	0.6
	HMDB0041427	Erinapyrone B	C7H10O3	M+FA-H	187.0612	0.6
	HMDB0041426	Erinapyrone A	C7H10O3	M+FA-H	187.0612	0.6
	HMDB0033736	Homofureanol	C7H10O3	M+FA-H	187.0612	0.6

187.0727	HMDB0034230	Mesifurane	C7H10O3	M+FA-H	187.0612	0.6
	HMDB0038791	2,4,6-Triethyl-1,3,5-oxadithiane	C9H18OS2	M-H2O-H	187.0615	-1.2
	HMDB0006029	N-Acetylglutamine	C7H12N2O4	M-H	187.0724	1.4
	HMDB0011173	Glycylhydroxyproline	C7H12N2O4	M-H	187.0724	1.4
	HMDB0028842	Glycyl-Hydroxyproline	C7H12N2O4	M-H	187.0724	1.4
187.0975	HMDB0145363	1-[(carboxyamino)methyl]-3,4-dihydro-2H-pyrrol-1-ium	C6H11N2O2	M+FA-H	187.0724	1.4
	HMDB0240650	ectoine	C6H10N2O2	M+FA-H	187.0724	1.4
	HMDB0062077	6-methylheptan-2,4-dione	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0062166	Vinyl hexanoate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0163316	(3E)-7-hydroxyoct-3-en-2-one	C8H14O2	M+FA-H	187.0976	-0.4
187.0975	HMDB0163317	Ethanone, 1-(3-butyloxiranyl)-	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0163318	(E)-8-Hydroxy-3-octene-2-one	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0163315	SCHEMBL17867	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0163319	(3E)-1-hydroxyoct-3-en-2-one	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0031293	2,3-Octanedione	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0029761	Ethyl 2-methyl-4-pentenoate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0031403	Cyclohexaneacetic acid	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0031352	Cyclohexyl acetate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0031343	Methyl cyclohexanecarboxylate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0036212	2-Methylpropyl (2E)-butenoate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0032533	trans-3-Hexenyl acetate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0035422	4-Butyl-gamma-butyrolactone	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0240301	3-Octenoic acid	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0032164	Allyl valerate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0032278	Ethyl trans-2-methyl-2-pentenoate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0037624	Isopropyl tiglate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0032266	Ethyl (E)-3-hexenoate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0000392	2-Octenoic acid	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0038036	2-Propenyl 3-methylbutanoate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0039793	(E)-4-Octenoic acid	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0037630	xi-Tetrahydro-3-propyl-2H-pyran-2-one	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0038310	xi-Tetrahydro-6-propyl-2H-pyran-2-one	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0039872	Methyl 2-heptenoate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0001568	trans-2-Octenoic acid	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0037622	Ethyl 2-methyl-3-pentenoate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0040215	cis-3-Hexenyl acetate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0040212	2-Hexenyl acetate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0032268	Ethyl 2E-hexenoate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0036236	2-Methylallyl butyrate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0032207	cis-5-Octenoic acid	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0013904	(3E)-2-Propylpent-3-enoic acid	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0013902	2-ene-Valproic acid	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0059908	Ethyl-3-hexanoate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0032267	Ethyl 5-hexenoate	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0013903	(3Z)-2-Propylpent-3-enoic acid	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0061342	(3Z)-2-Propylpent-3-enoic acid	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0013897	4-ene-Valproic acid	C8H14O2	M+FA-H	187.0976	-0.4
	HMDB0059879	Diethyl glutarate	C9H16O4	M-H	187.0976	-0.4
	HMDB0000784	Azelaic acid	C9H16O4	M-H	187.0976	-0.4
	HMDB0179175	2-hydroxy-4-oxononanoic acid	C9H16O4	M-H	187.0976	-0.4
	HMDB0179176	3-hydroxy-4-oxononanoic acid	C9H16O4	M-H	187.0976	-0.4
	HMDB0179174	9-hydroxy-4-oxononanoic acid	C9H16O4	M-H	187.0976	-0.4
	HMDB0179177	5-hydroxy-4-oxononanoic acid	C9H16O4	M-H	187.0976	-0.4
	HMDB0179173	8-hydroxy-4-oxononanoic acid	C9H16O4	M-H	187.0976	-0.4
	HMDB0011717	Nonate	C9H16O4	M-H	187.0976	-0.4
	HMDB0059814	Diethyl methylsuccinate	C9H16O4	M-H	187.0976	-0.4
	HMDB0059783	3-Methylsuberic acid	C9H16O4	M-H	187.0976	-0.4
	HMDB0059760	2,4-Dimethylpimelic acid	C9H16O4	M-H	187.0976	-0.4
	HMDB0032200	cis- and trans-Ethyl 2,4-dimethyl-1,3-dioxolane-2-acetate	C9H16O4	M-H	187.0976	-0.4
	HMDB0032387	(+/-)-Methyl 5-acetoxylhexanoate	C9H16O4	M-H	187.0976	-0.4
	HMDB0032258	(+/-)-Ethyl 3-acetoxy-2-methylbutyrate	C9H16O4	M-H	187.0976	-0.4
	HMDB0036233	Butyl ethyl malonate	C9H16O4	M-H	187.0976	-0.4
	HMDB0167930	8-Nonen-2-ol	C9H18O	M+FA-H	187.1340	-0.4

187.1339	HMDB0167929	Nonen-2-ol	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0059887	(E)-6-Nonenol	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0040581	(Z)-6-Nonen-1-ol	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0030959	(Z)-3-Nonen-1-ol	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0034152	1-Nonen-3-ol	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0163453	ZINC1986326	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0041601	(E)-3-Nonen-1-ol	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0041499	(Z)-2-Nonen-1-ol	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0031267	3-Nonanone	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0031730	3,5,5-Trimethylhexanal	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0031268	Amyl propyl ketone	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0031417	2,6-Dimethyl-4-heptanone	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0059835	Nonanal	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0037304	2,6-Dimethyl-6-hepten-1-ol	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0031684	2-Methyloctanal	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0031266	2-Nonanone	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0029557	Dihydroisophorol	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0041498	2-Nonen-1-ol	C9H18O	M+FA-H	187.1340	-0.4
	HMDB0179928	(5E)-3,7-dimethyloct-5-ene-1,3,7-triol	C10H20O3	M-H	187.1340	-0.4
	HMDB0180586	8-hydroxy-4-methylnonanoic acid	C10H20O3	M-H	187.1340	-0.4
	HMDB0180585	AKO19123491	C10H20O3	M-H	187.1340	-0.4
	HMDB0180589	SCHEMBL45681	C10H20O3	M-H	187.1340	-0.4
	HMDB0094656	2s-hydroxy-decanoic acid	C10H20O3	M-H	187.1340	-0.4
	HMDB0002203	3-Hydroxycapric acid	C10H20O3	M-H	187.1340	-0.4
	HMDB0041600	Ethyl 3-hydroxyoctanoate	C10H20O3	M-H	187.1340	-0.4
	HMDB0179931	(3E)-2,6-dimethyloct-3-ene-1,2,8-triol	C10H20O3	M-H	187.1340	-0.4
	HMDB0180106	SCHEMBL4626344	C10H20O3	M-H	187.1340	-0.4
	HMDB0180104	8-Hydroxy-8-methylnonanoic acid	C10H20O3	M-H	187.1340	-0.4
	HMDB0179929	(5E)-3,7-dimethyloct-5-ene-1,4,7-triol	C10H20O3	M-H	187.1340	-0.4
	HMDB0179930	4-[3-(2-hydroxypropan-2-yl)oxiran-2-yl]-3-methylbutan-1-ol	C10H20O3	M-H	187.1340	-0.4
	HMDB0180588	9-hydroxy-4-methylnonanoic acid	C10H20O3	M-H	187.1340	-0.4
	HMDB0180587	4-(hydroxymethyl)nonanoic acid	C10H20O3	M-H	187.1340	-0.4
	HMDB0180105	9-hydroxy-8-methylnonanoic acid	C10H20O3	M-H	187.1340	-0.4
	HMDB0179932	(5E)-3-(hydroxymethyl)-7-methyloct-5-ene-1,7-diol	C10H20O3	M-H	187.1340	-0.4
	HMDB0010725	(R)-3-Hydroxydecanoic acid	C10H20O3	M-H	187.1340	-0.4
	HMDB0034783	cis-p-Menthane-1,7,8-triol	C10H20O3	M-H	187.1340	-0.4
	HMDB0039669	2-Hexyl-1,3-dioxolane-4-methanol	C10H20O3	M-H	187.1340	-0.4
	HMDB0033640	7-Methyl-3-methylene-1,6,7-octanetriol	C10H20O3	M-H	187.1340	-0.4
	HMDB0038186	2,6-Dimethyl-7-octene-2,3,6-triol	C10H20O3	M-H	187.1340	-0.4
	HMDB0033201	9-Hydroxydecanoic acid	C10H20O3	M-H	187.1340	-0.4
	HMDB0039668	2-Hexyl-1,3-dioxan-5-ol	C10H20O3	M-H	187.1340	-0.4
	HMDB0039470	(1S,2S,4R,8R)-p-Menthane-1,2,9-triol	C10H20O3	M-H	187.1340	-0.4
	HMDB0039893	(1R,2R,4S)-p-Menthane-1,2,8-triol	C10H20O3	M-H	187.1340	-0.4
	HMDB0033574	(1R,2R,4R,8R)-p-Menthane-2,8,9-triol	C10H20O3	M-H	187.1340	-0.4
	HMDB0040329	xi-5-Hydroxydecanoic acid	C10H20O3	M-H	187.1340	-0.4
189.0767	HMDB0163403	5-ethyl-3-hydroxy-4-methyloxolan-2-one	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0180835	pentyl 2-oxoacetate	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0180326	(2E)-3-[3-(1-hydroxyethyl)oxiran-2-yl]prop-2-en-1-ol	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0180327	(2E)-3-[3-(2-hydroxyethyl)oxiran-2-yl]prop-2-en-1-ol	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0172013	4-methoxy-2,5-dimethyloxolan-3-one	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0166745	(2E)-6-hydroxyhept-2-enoic acid	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0166746	ACMC-mulz	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0166747	SCHEMBL088	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0166744	(2E)-4-hydroxyhept-2-enoic acid	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0166501	(4Z)-2-hydroxyhept-4-enoic acid	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0166500	SCHEMBL26282	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0166498	(4Z)-3-hydroxyhept-4-enoic acid	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0166499	SCHEMBL7994854	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0166497	(4Z)-6-hydroxyhept-4-enoic acid	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0165786	2(5)-ethyl-4-hydroxy-5(2)-methyl-3(2H)-furanone (ethylfuranol)	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0164728	4-hydroxy-4-(hydroxymethyl)cyclohexan-1-one	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0164729	2,4-dihydroxy-4-methylcyclohexan-1-one	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0061990	2-hydroxycyclohexanecarboxylic acid	C7H12O3	M+FA-H	189.0768	-0.8

	HMDB0031176	Tetrahydrofurfuryl acetate	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0040433	Ethyl levulinate	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0036594	Botryodiplodin	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0001988	4-Hydroxycyclohexylcarboxylic acid	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0037114	Methyl (R)-3-methyl-2-oxopentanoate	C7H12O3	M+FA-H	189.0768	-0.8
	HMDB0157325	SCHEMBL596	C8H14O5	M-H	189.0768	-0.8
	HMDB0000325	3-Hydroxysuberlic acid	C8H14O5	M-H	189.0768	-0.8
	HMDB0157326	2-hydroxyoctanedioic Acid	C8H14O5	M-H	189.0768	-0.8
	HMDB0061681	6-(2-Hydroxyethoxy)-6-oxohexanoic acid	C8H14O5	M-H	189.0768	-0.8
	HMDB0166861	SCHEMBL846	C8H14O5	M-H	189.0768	-0.8
	HMDB0040220	Diethyl L-malate	C8H14O5	M-H	189.0768	-0.8
	HMDB0033942	Dambonitol	C8H16O6	M-H2O-H	189.0763	2.1
	HMDB0029968	Ethyl beta-D-glucopyranoside	C8H16O6	M-H2O-H	189.0763	2.1
	HMDB0041862	D-Glucaro-1,4-lactone	C6H8O7	M-H	191.0197	0.4
	HMDB0149524	ACMC-mker	C6H8O7	M-H	191.0197	0.4
191.0198	HMDB0000094	Citric acid	C6H8O7	M-H	191.0197	0.4
	HMDB0000193	Isocitric acid	C6H8O7	M-H	191.0197	0.4
	HMDB0001874	D-threo-Isocitric acid	C6H8O7	M-H	191.0197	0.4
	HMDB0005971	Diketogulonic acid	C6H8O7	M-H	191.0197	0.4
	HMDB0006511	2,3-Diketo-L-gulonate	C6H8O7	M-H	191.0197	0.4
	HMDB0062803	4,5,6-trihydroxy-2,3-dioxohexanoic acid	C6H8O7	M-H	191.0197	0.4
	HMDB0033717	(1R,2R)-Isocitric acid	C6H8O7	M-H	191.0197	0.4
	HMDB0161318	893-18-9	C5H6O5	M+FA-H	191.0197	0.4
	HMDB0161317	(2E)-2-(hydroxymethyl)but-2-enedioic acid	C5H6O5	M+FA-H	191.0197	0.4
	HMDB0160653	Pentadic acid, 2,3-anhydro-4-deoxy- (9CI)	C5H6O5	M+FA-H	191.0197	0.4
	HMDB0160654	SCHEMBL3125276	C5H6O5	M+FA-H	191.0197	0.4
	HMDB0013701	3-Oxoglutaric acid	C5H6O5	M+FA-H	191.0197	0.4
	HMDB0164700	3,4-dihydroxy-5-(hydroxymethyl)-2,5-dihydrofuran-2-one	C5H6O5	M+FA-H	191.0197	0.4
	HMDB0000208	Oxoglutaric acid	C5H6O5	M+FA-H	191.0197	0.4
191.1074	HMDB0032797	Jasmonic acid	C12H18O3	M-H2O-H	191.1072	1.0
	HMDB0037735	Isoamyl 2-furonpropionate	C12H18O3	M-H2O-H	191.1072	1.0
	HMDB0033102	Dihydro-3-(2-octenyl)-2,5-furandione	C12H18O3	M-H2O-H	191.1072	1.0
	HMDB0037642	4-(Butoxymethyl)-2-methoxyphenol	C12H18O3	M-H2O-H	191.1072	1.0
	HMDB0041573	3-Ethenyl-2,5-dimethyl-4-oxohex-5-en-2-yl acetate	C12H18O3	M-H2O-H	191.1072	1.0
	HMDB0037104	(R)-8-Acetoxycarvotanacetone	C12H18O3	M-H2O-H	191.1072	1.0
	HMDB0037135	1-Benzyloxy-1-(2-methoxyethoxy)ethane	C12H18O3	M-H2O-H	191.1072	1.0
	HMDB0032871	Sedanonic acid	C12H18O3	M-H2O-H	191.1072	1.0
	HMDB0037816	Dihydro-3-(1-octenyl)-2,5-furandione	C12H18O3	M-H2O-H	191.1072	1.0
	HMDB0061808	(3-Methyl-2-butenyl)-benzene	C11H14	M+FA-H	191.1078	-1.8
	HMDB0037709	4-Methylphenyl 3-methylbutanoate	C12H16O2	M-H	191.1078	-1.9
	HMDB0039496	2-Ethoxy-1-methoxy-4-(1-propenyl)benzene	C12H16O2	M-H	191.1078	-1.9
	HMDB0031618	Ethyl 4-phenylbutanoate	C12H16O2	M-H	191.1078	-1.9
	HMDB0035014	2-Phenylethyl butanoate	C12H16O2	M-H	191.1078	-1.9
	HMDB0040427	Butyl phenylacetate	C12H16O2	M-H	191.1078	-1.9
	HMDB0038180	2-(2-Hydroxy-4-methylphenyl)-3-pentanone	C12H16O2	M-H	191.1078	-1.9
	HMDB0036734	11,12,13-Trinor-1()-spirovetivene-2,7-dione	C12H16O2	M-H	191.1078	-1.9
	HMDB0172371	(3E)-3-butyldiene-1,3,3a,4,5,7a-hexahydro-2-benzofuran-1-one	C12H16O2	M-H	191.1078	-1.9
	HMDB0171338	5-hydroxy-4-(4-methylphenyl)pentan-2-one	C12H16O2	M-H	191.1078	-1.9
	HMDB0171340	1-hydroxy-4-(4-methylphenyl)pentan-2-one	C12H16O2	M-H	191.1078	-1.9
	HMDB0171341	3-hydroxy-4-(4-methylphenyl)pentan-2-one	C12H16O2	M-H	191.1078	-1.9
	HMDB0171336	4-hydroxy-4-(p-tolyl)-2-pentanone	C12H16O2	M-H	191.1078	-1.9
	HMDB0171337	4-[4-(hydroxymethyl)phenyl]pentan-2-one	C12H16O2	M-H	191.1078	-1.9
	HMDB0132979	(1E)-1-(4-methoxyphenyl)pent-1-en-3-ol	C12H16O2	M-H	191.1078	-1.9
	HMDB0132971	1-(4-methoxyphenyl)pentan-3-one	C12H16O2	M-H	191.1078	-1.9
	HMDB0132942	1-(4-hydroxyphenyl)-4-methylpentan-3-one	C12H16O2	M-H	191.1078	-1.9
	HMDB0031571	2-Methyl-1-phenyl-2-propenyl acetate	C12H16O2	M-H	191.1078	-1.9
	HMDB0035015	2-Phenylethyl 2-methylpropanoate	C12H16O2	M-H	191.1078	-1.9
	HMDB0037792	1-Ethoxy-2-methoxy-4-(1-propenyl)benzene	C12H16O2	M-H	191.1078	-1.9
	HMDB0037716	1-Phenylethyl isobutyrate	C12H16O2	M-H	191.1078	-1.9
	HMDB0035447	5-Isopropyl-2-methylphenol acetate	C12H16O2	M-H	191.1078	-1.9
	HMDB0037165	4-Methyl-2-(1-phenylethyl)-1,3-dioxolane, 9CI	C12H16O2	M-H	191.1078	-1.9
	HMDB0035010	2-Methylpropyl phenylacetate	C12H16O2	M-H	191.1078	-1.9
	HMDB0039841	2-Benzyl-4,5-dimethyl-1,3-dioxolane	C12H16O2	M-H	191.1078	-1.9

	HMDB0039643	11,12,13-Trinor-1,3,5-bisabolatrien--oic acid	C12H16O2	M-H	191.1078	-1.9
	HMDB0032043	Benzyl 3-methylbutanoate	C12H16O2	M-H	191.1078	-1.9
	HMDB0036388	3-Phenylpropyl propanoate	C12H16O2	M-H	191.1078	-1.9
	HMDB0033380	3-Methylbutyl benzoate	C12H16O2	M-H	191.1078	-1.9
	HMDB0037717	1-Phenylethyl butyrate	C12H16O2	M-H	191.1078	-1.9
	HMDB0031614	4-Phenyl-2-butyl acetate	C12H16O2	M-H	191.1078	-1.9
193.0870	HMDB0061997	2-Methyl-3-phenylpropanal	C10H12O	M+FA-H	193.0870	-0.1
	HMDB0133593	(2E)-2-methyl-3-phenylprop-2-en-1-ol	C10H12O	M+FA-H	193.0870	-0.1
	HMDB0133746	4-phenylbutan-2-one	C10H12O	M+FA-H	193.0870	-0.1
	HMDB0033382	2-(4-Methylphenyl)propanal	C10H12O	M+FA-H	193.0870	-0.1
	HMDB0059845	p-Ethylacetophenone	C10H12O	M+FA-H	193.0870	-0.1
	HMDB0032140	2',4'-Dimethylacetophenone	C10H12O	M+FA-H	193.0870	-0.1
	HMDB0032017	3,4,5-Trimethylbenzaldehyde	C10H12O	M+FA-H	193.0870	-0.1
	HMDB0032015	Duryl aldehyde	C10H12O	M+FA-H	193.0870	-0.1
	HMDB0032014	2,3,6-Trimethylbenzaldehyde	C10H12O	M+FA-H	193.0870	-0.1
	HMDB0032016	2,4,6-Trimethylbenzaldehyde	C10H12O	M+FA-H	193.0870	-0.1
	HMDB0180475	SCHEMBL295411	C10H12O	M+FA-H	193.0870	-0.1
	HMDB0034121	1-Methoxy-4-(2-propenyl)benzene	C10H12O	M+FA-H	193.0870	-0.1
	HMDB0031616	4-Phenyl-3-buten-2-ol	C10H12O	M+FA-H	193.0870	-0.1
	HMDB0002214	Cuminaldehyde	C10H12O	M+FA-H	193.0870	-0.1
	HMDB0030837	Anethole	C10H12O	M+FA-H	193.0870	-0.1
	HMDB0182834	4-hydroxybenzyl butyrate	C11H14O3	M-H	193.0870	-0.1
	HMDB0171010	cis-4-Propenylsyringol	C11H14O3	M-H	193.0870	-0.1
	HMDB0126466	2-[(1E)-4-hydroxy-3-methylbut-1-en-1-yl]benzene-1,3-diol	C11H14O3	M-H	193.0870	-0.1
	HMDB0166268	76773-99-4	C11H14O3	M-H	193.0870	-0.1
	HMDB0163607	4-hydroxy-3-methyl-2-phenylbutanoic acid	C11H14O3	M-H	193.0870	-0.1
	HMDB0151230	3-hydroxy-2-[(4-methoxyphenyl)methyl]propanal	C11H14O3	M-H	193.0870	-0.1
	HMDB0146411	3-(3-Methoxyphenyl)-2-methylpropanoic acid	C11H14O3	M-H	193.0870	-0.1
	HMDB0141323	4-hydroxy-4-(3-methoxyphenyl)butan-2-one	C11H14O3	M-H	193.0870	-0.1
	HMDB0133538	1-hydroxy-4-(3-methoxyphenyl)butan-2-one	C11H14O3	M-H	193.0870	-0.1
	HMDB0133515	4-(3-hydroxy-5-methoxyphenyl)butan-2-one	C11H14O3	M-H	193.0870	-0.1
	HMDB0133484	3-hydroxy-4-(3-methoxyphenyl)butan-2-one	C11H14O3	M-H	193.0870	-0.1
	HMDB0133463	4-(3-hydroxybut-1-en-1-yl)-2-methoxyphenol	C11H14O3	M-H	193.0870	-0.1
	HMDB0133194	4-[(3,3-dimethyloxiran-2-yl)methyl]benzene-1,3-diol	C11H14O3	M-H	193.0870	-0.1
	HMDB0151228	3-hydroxy-3-(4-methoxyphenyl)-2-methylpropanal	C11H14O3	M-H	193.0870	-0.1
	HMDB0151229	3-(4-methoxyphenyl)-2-methylpropanoic acid	C11H14O3	M-H	193.0870	-0.1
	HMDB0151232	2-hydroxy-3-(4-methoxyphenyl)-2-methylpropanal	C11H14O3	M-H	193.0870	-0.1
	HMDB0163609	2-hydroxy-3-methyl-2-phenylbutanoic acid	C11H14O3	M-H	193.0870	-0.1
	HMDB0163606	3-hydroxy-3-methyl-2-phenylbutanoic acid	C11H14O3	M-H	193.0870	-0.1
	HMDB0151235	2-(3-hydroxy-2-methylprop-1-en-1-yl)-5-methoxyphenol	C11H14O3	M-H	193.0870	-0.1
	HMDB0163610	SCHEMBL8733687	C11H14O3	M-H	193.0870	-0.1
	HMDB0151236	[3-(4-methoxyphenyl)-2-methyloxiran-2-yl]methanol	C11H14O3	M-H	193.0870	-0.1
	HMDB0163612	AKO229142	C11H14O3	M-H	193.0870	-0.1
	HMDB0151233	2-(4-methoxybenzylidene)propane-1,3-diol	C11H14O3	M-H	193.0870	-0.1
	HMDB0163611	2-(4-hydroxyphenyl)-3-methylbutanoic acid	C11H14O3	M-H	193.0870	-0.1
	HMDB0164132	(4r)-hydroxy-4-(4'-methoxyphenyl)-butan-2-one	C11H14O3	M-H	193.0870	-0.1
	HMDB0133190	4-[(2E)-4-hydroxy-3-methylbut-2-en-1-yl]benzene-1,3-diol	C11H14O3	M-H	193.0870	-0.1
	HMDB0133193	5-(3-methylbut-2-en-1-yl)benzene-1,2,4-triol	C11H14O3	M-H	193.0870	-0.1
	HMDB0124918	2-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C11H14O3	M-H	193.0870	-0.1
	HMDB0164133	SCHEMBL13742814	C11H14O3	M-H	193.0870	-0.1
	HMDB0164134	2-Butanone, 4-hydroxy-4-(4-methoxyphenyl)-	C11H14O3	M-H	193.0870	-0.1
	HMDB0126162	3-(3-methylbut-2-en-1-yl)benzene-1,2,4-triol	C11H14O3	M-H	193.0870	-0.1
	HMDB0126161	2-(4-hydroxy-3-methylbut-2-en-1-yl)benzene-1,3-diol	C11H14O3	M-H	193.0870	-0.1
	HMDB0126163	2-[(3,3-dimethyloxiran-2-yl)methyl]benzene-1,3-diol	C11H14O3	M-H	193.0870	-0.1
	HMDB0133192	4-(3-methylbut-2-en-1-yl)benzene-1,2,3-triol	C11H14O3	M-H	193.0870	-0.1
	HMDB0133191	4-(4-hydroxy-3-methylbut-2-en-1-yl)benzene-1,3-diol	C11H14O3	M-H	193.0870	-0.1
	HMDB0132270	5-(4-hydroxyphenyl)pentanoic acid	C11H14O3	M-H	193.0870	-0.1
	HMDB0126464	2-[(1E)-3-methylbut-1-en-1-yl]benzene-1,3,5-triol	C11H14O3	M-H	193.0870	-0.1
	HMDB0126463	3-[(1E)-3-methylbut-1-en-1-yl]benzene-1,2,4-triol	C11H14O3	M-H	193.0870	-0.1
	HMDB0126465	2-[3-(propan-2-yl)oxiran-2-yl]benzene-1,3-diol	C11H14O3	M-H	193.0870	-0.1
	HMDB0126462	2-[(1E)-3-hydroxy-3-methylbut-1-en-1-yl]benzene-1,3-diol	C11H14O3	M-H	193.0870	-0.1

HMDB0126262	2-[(2E)-4-hydroxy-3-methylbut-2-en-1-yl]benzene-1,3-diol	C11H14O3	M-H	193.0870	-0.1
HMDB0059898	Ethyl 4-ethoxybenzoate	C11H14O3	M-H	193.0870	-0.1
HMDB0062055	4-hydroxy-5-phenylpentanoic acid	C11H14O3	M-H	193.0870	-0.1
HMDB0036432	Isobutyl salicylate	C11H14O3	M-H	193.0870	-0.1
HMDB0041506	2-Benzyl-5-hydroxymethyl-1,3-dioxolane	C11H14O3	M-H	193.0870	-0.1
HMDB0032590	Zingerone	C11H14O3	M-H	193.0870	-0.1
HMDB0037271	2,6-Dimethoxy-4-(1-propenyl)phenol	C11H14O3	M-H	193.0870	-0.1
HMDB0040730	Butyl salicylate	C11H14O3	M-H	193.0870	-0.1
HMDB0041505	5-Hydroxy-2-benzyl-1,3-dioxane	C11H14O3	M-H	193.0870	-0.1
HMDB0034990	4-Methoxybenzyl propanoate	C11H14O3	M-H	193.0870	-0.1
HMDB0032575	Butylparaben	C11H14O3	M-H	193.0870	-0.1
HMDB0034206	Ethyl 4-methylphenoxyacetate	C11H14O3	M-H	193.0870	-0.1
HMDB0041194	Methoxyeugenol	C11H14O3	M-H	193.0870	-0.1
HMDB0031984	2,5-Dimethoxy-4-(2-propenyl)phenol	C11H14O3	M-H	193.0870	-0.1
HMDB0179740	gamma-Methoxyisoeugenol	C11H14O3	M-H	193.0870	-0.1
HMDB0059942	[2-(4-Methylphenyl)-1,3-dioxolan-4-yl]methanol	C11H14O3	M-H	193.0870	-0.1
HMDB0059944	2-(3-Methylphenyl)-1,3-dioxan-5-ol	C11H14O3	M-H	193.0870	-0.1
HMDB0059943	2-(2-Methylphenyl)-1,3-dioxan-5-ol	C11H14O3	M-H	193.0870	-0.1
HMDB0059945	2-(4-Methylphenyl)-1,3-dioxan-5-ol	C11H14O3	M-H	193.0870	-0.1
HMDB0059941	[2-(3-Methylphenyl)-1,3-dioxolan-4-yl]methanol	C11H14O3	M-H	193.0870	-0.1
HMDB0059940	[2-(2-Methylphenyl)-1,3-dioxolan-4-yl]methanol	C11H14O3	M-H	193.0870	-0.1
HMDB0041666	3-Hydroxyphenyl-valeric acid	C11H14O3	M-H	193.0870	-0.1
HMDB0031517	(R)-3-Hydroxy-5-phenylpentanoic acid	C11H14O3	M-H	193.0870	-0.1
HMDB0059744	3,4-Methyleneazelaic acid	C11H16O4	M-H2O-H	193.0865	2.8
HMDB0169511	2-(1-hydroxyethyl)-3,5-dimethoxy-6-methylphenol	C11H16O4	M-H2O-H	193.0865	2.8
HMDB0153808	2-(3-hydroxy-3-methylbutyl)benzene-1,3,5-triol	C11H16O4	M-H2O-H	193.0865	2.8
HMDB0030175	Venoterpine	C9H11NO	M+FA-H	194.0823	-0.3
HMDB0040029	2,3-Dihydro-5-methyl-1H-pyrrolizine-7-	C9H11NO	M+FA-H	194.0823	-0.3
HMDB0040016	2-(2-Furanyl)-3,4,5,6-tetrahydropyridine	C9H11NO	M+FA-H	194.0823	-0.3
HMDB0039662	2,3,6,7-Tetrahydrocyclopent[b]azepin-8(1H)-one	C9H11NO	M+FA-H	194.0823	-0.3
HMDB0040043	3-(2-Furanylmethylene)pyrrolidine	C9H11NO	M+FA-H	194.0823	-0.3
HMDB0040051	5-Acetyl-2,3-dihydro-1H-pyrrolizine	C9H11NO	M+FA-H	194.0823	-0.3
HMDB0040050	3,4-Dihydro-5-(5-methyl-2-furanyl)-2H-pyrrole	C9H11NO	M+FA-H	194.0823	-0.3
HMDB0040047	2,3-Dihydro-6-methyl-1H-pyrrolizine-5-	C9H11NO	M+FA-H	194.0823	-0.3
HMDB0166077	2-hydroxyethyl 2-(methylamino)benzoate	C10H13NO3	M-H	194.0823	-0.3
HMDB0185208	4-(2-amino-1-hydroxyprop-2-en-1-yl)-2-methoxyphenol	C10H13NO3	M-H	194.0823	-0.3
HMDB0060065	N-methyl-4,6,7-trihydroxy-1,2,3,4-tetrahydroisoquinoline	C10H13NO3	M-H	194.0823	-0.3
HMDB0041943	N-Acetyldopamine	C10H13NO3	M-H	194.0823	-0.3
HMDB0060351	2-Phenyl-1,3-propanediol monocarbamate	C10H13NO3	M-H	194.0823	-0.3
HMDB0029217	Tyrosine methylester	C10H13NO3	M-H	194.0823	-0.3
HMDB0014903	Metyrosine	C10H13NO3	M-H	194.0823	-0.3
HMDB0185203	2-amino-1-(4-hydroxy-3-methoxyphenyl)propane-1,3-diol	C10H15NO4	M-H2O-H	194.0817	2.5
HMDB0155125	2-[1-hydroxy-2-(methylamino)ethyl]-5-methoxybenzene-1,4-diol	C10H15NO4	M-H2O-H	194.0817	2.5
HMDB0125517	2-(2,6-dihydroxy-3,4-dimethoxycyclohexylidene)acetonitrile	C10H15NO4	M-H2O-H	194.0817	2.5
HMDB0185197	2-(2-amino-1-hydroxypropyl)-5-methoxybenzene-1,4-diol	C10H15NO4	M-H2O-H	194.0817	2.5
HMDB0135276	2-hydroxy-3-phenylpropanal	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0135278	3-(3-hydroxyphenyl)propanal	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0135281	(3-phenyloxiran-2-yl)methanol	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0176419	6-(3-methyloxiran-2-yl)hexa-3,5-dien-1-ol	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0134027	2-(3-hydroxyprop-1-en-1-yl)phenol	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0134026	3-(2-hydroxyphenyl)propanal	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0000764	Hydrocinnamic acid	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0125532	3-ethenyl-5-methoxyphenol	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0062349	4-Chromanol	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0135277	3-hydroxy-3-phenylpropanal	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0135279	3-(4-hydroxyphenyl)propanal	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0135644	4-(3-hydroxyprop-1-en-1-yl)phenol	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0177508	4-(3-methyloxiran-2-yl)phenol	C9H10O2	M+FA-H	195.0663	-0.9

195.0661

HMDB0135239	4-(prop-2-en-1-yl)benzene-1,2-diol	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0032569	2'-Methoxyacetophenone	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0040925	2-(2-Furanyl)-3-methyl-2-butenal	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0038355	2-Ethyl-4-(2-furanyl)-2-propenal	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0037715	1-Phenylethyl formate	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0176418	2-Nonene-4,6-diyne-1,9-diol	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0170980	4-[(1Z)-prop-1-en-1-yl]benzene-1,2-diol	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0170763	4-(oxiran-2-ylmethyl)phenol	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0032617	Methyl phenylacetate	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0011743	2-Phenylpropionate	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0032073	o-Tolyl acetate	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0032075	p-Tolyl acetate	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0033970	4-Ethoxybenzaldehyde	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0033967	Ethyl benzoate	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0031310	Benzyl acetate	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0032592	2'-Hydroxy-5'-methylacetophenone	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0003654	4-Coumaryl alcohol	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0040428	2-Phenylethyl formate	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0059824	4-Hydroxy-3-methylacetophenone	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0002097	4-Ethylbenzoic acid	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0032570	4'-Methoxyacetophenone	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0013744	2-Methoxy-4-vinylphenol	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0002237	3,4-Dimethylbenzoic acid	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0146635	4-vinyl-3-methoxyphenol	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0135280	3-[(1E)-3-hydroxyprop-1-en-1-yl]phenol	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0146657	2-hydroxycinnamyl alcohol	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0002222	3-Methylphenylacetic acid	C9H10O2	M+FA-H	195.0663	-0.9
HMDB0131138	3-(3-hydroxy-4-methoxyphenyl)propanoic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0169508	1-(2,4-dihydroxy-6-methoxy-3-methylphenyl)ethan-1-one	C10H12O4	M-H	195.0663	-0.9
HMDB0125530	3-(3-hydroxy-5-methoxyphenyl)propanoic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0129339	2-(3-hydroxy-4-methoxyphenyl)propanoic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0130895	2-(4-hydroxy-3-methoxyphenyl)propanoic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0131427	2-(3,5-dimethoxyphenyl)acetic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0133490	3-hydroxy-3-(3-methoxyphenyl)propanoic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0146636	3-(4-hydroxy-2-methoxyphenyl)propanoic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0133782	2-(2-hydroxy-4-methoxyphenyl)propanoic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0146633	AKO241634	C10H12O4	M-H	195.0663	-0.9
HMDB0140897	3-(3-hydroxy-2-methoxyphenyl)propanoic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0134100	3-(2-hydroxy-3-methoxyphenyl)propanoic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0140293	3-hydroxy-3-(4-methoxyphenyl)propanoic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0135753	4-ethenyl-2,6-dimethoxybenzene-1,3-diol	C10H12O4	M-H	195.0663	-0.9
HMDB0166066	(4-methoxyphenyl)methyl 2-hydroxyacetate	C10H12O4	M-H	195.0663	-0.9
HMDB0131175	3-(2-hydroxy-4-methoxyphenyl)propanoic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0133530	2-hydroxy-3-(3-methoxyphenyl)propanoic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0177595	AKO153285	C10H12O4	M-H	195.0663	-0.9
HMDB0040256	(S)-2-(4-Methoxyphenoxy)propanoic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0000434	Homoveratric acid	C10H12O4	M-H	195.0663	-0.9
HMDB0032365	Maltyl isobutyrate	C10H12O4	M-H	195.0663	-0.9
HMDB0040637	4-Hydroxy-6-methyl-3-(1-oxobutyl)-2H-pyran-2-one	C10H12O4	M-H	195.0663	-0.9
HMDB0039427	2-Hydroxy-3-(4-methoxyphenyl)propanoic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0029645	Xanthoxylin	C10H12O4	M-H	195.0663	-0.9
HMDB0037177	1-(2,4,5-Trihydroxyphenyl)-1-butanone	C10H12O4	M-H	195.0663	-0.9
HMDB0029648	2,4,5-Trimethoxybenzaldehyde	C10H12O4	M-H	195.0663	-0.9
HMDB0030571	(+)-3-(3,4-Methylenedioxyphenyl)-1,2-propanediol	C10H12O4	M-H	195.0663	-0.9
HMDB0035721	(S)-Batatic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0060735	3-(3,4-Dihydroxyphenyl)-2-methylpropionic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0060733	3-(3-Hydroxyphenyl)-2-methylactic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0060398	5-Hydroxyconiferyl alcohol	C10H12O4	M-H	195.0663	-0.9
HMDB0062121	Dihydroferulic acid	C10H12O4	M-H	195.0663	-0.9
HMDB0169507	CHEMBL56	C10H12O4	M-H	195.0663	-0.9
HMDB0170510	(2E,4E)-7-(hydroxymethyl)-2-methylocta-2,4-dienedioic acid	C10H14O5	M-H2O-H	195.0657	1.9
HMDB0159583	Fareanol	C10H14O5	M-H2O-H	195.0657	1.9

	HMDB0170507	(2E,4E)-6-hydroxy-2,7-dimethylocta-2,4-dienedioic acid	C10H14O5	M-H2O-H	195.0657	1.9
	HMDB0170505	(2E,4E)-7-hydroxy-2,7-dimethylocta-2,4-dienedioic acid	C10H14O5	M-H2O-H	195.0657	1.9
	HMDB0170509	(2E)-3-[3-(2-carboxy-2-methylethyl)oxiran-2-yl]-2-methylprop-2-enoic acid	C10H14O5	M-H2O-H	195.0657	1.9
	HMDB0170508	3-[(1E)-4-carboxy-4-methylbut-1-en-1-yl]-2-methyloxirane-2-carboxylic acid	C10H14O5	M-H2O-H	195.0657	1.9
	HMDB0170506	(2E,4E)-2-(hydroxymethyl)-7-methylocta-2,4-dienedioic acid	C10H14O5	M-H2O-H	195.0657	1.9
195.1027	HMDB0135672	4-(3-hydroxybutyl)-2-methoxyphenol	C11H16O3	M-H	195.1027	0.2
	HMDB0037734	Isobutyl 2-furanpropionate	C11H16O3	M-H	195.1027	0.2
	HMDB0036226	2,6-Dimethoxy-4-propylphenol	C11H16O3	M-H	195.1027	0.2
	HMDB0179541	3-methoxy-2-methyl-5-(propan-2-yl)benzene-1,4-diol	C11H16O3	M-H	195.1027	0.2
	HMDB0179545	3-methoxy-5-methyl-2-(propan-2-yl)benzene-1,4-diol	C11H16O3	M-H	195.1027	0.2
	HMDB0037725	Hexyl 2-furoate	C11H16O3	M-H	195.1027	0.2
	HMDB0133616	2-methyl-3-phenylpropan-1-ol	C10H14O	M+FA-H	195.1027	0.2
	HMDB0163107	(2E,4Z,7Z)-deca-2,4,7,9-tetraen-1-ol	C10H14O	M+FA-H	195.1027	0.2
	HMDB0035591	3-Caren-5-one	C10H14O	M+FA-H	195.1027	0.2
	HMDB0029652	2-(4-Methylphenyl)-2-propanol	C10H14O	M+FA-H	195.1027	0.2
	HMDB0035770	5-Isopropyl-2-methylphenol	C10H14O	M+FA-H	195.1027	0.2
	HMDB0033544	(2E,4Z,7Z)-2,4,7-Decatrienal	C10H14O	M+FA-H	195.1027	0.2
	HMDB0036999	Piperitenone	C10H14O	M+FA-H	195.1027	0.2
	HMDB0035172	2,6,6-Trimethyl-1,4-cyclohexadiene-1-carboxaldehyde	C10H14O	M+FA-H	195.1027	0.2
	HMDB0031570	2-Methyl-1-phenyl-2-propanol	C10H14O	M+FA-H	195.1027	0.2
	HMDB0062147	Perillene	C10H14O	M+FA-H	195.1027	0.2
	HMDB0032213	2-trans-4-trans-7-cis-Decatrienal	C10H14O	M+FA-H	195.1027	0.2
	HMDB0036070	1-Acetyl-4-isopropenylcyclopentene	C10H14O	M+FA-H	195.1027	0.2
	HMDB0035824	Carvone	C10H14O	M+FA-H	195.1027	0.2
	HMDB0001878	Thymol	C10H14O	M+FA-H	195.1027	0.2
	HMDB0003647	Perillyl aldehyde	C10H14O	M+FA-H	195.1027	0.2
	HMDB0004487	(S)-Carvone	C10H14O	M+FA-H	195.1027	0.2
	HMDB0061788	(S)-Carvone	C10H14O	M+FA-H	195.1027	0.2
	HMDB0038913	4,6-Decadiyn-1-ol	C10H14O	M+FA-H	195.1027	0.2
	HMDB0031613	4-Phenyl-2-butanol	C10H14O	M+FA-H	195.1027	0.2
	HMDB0034921	Teresantalal	C10H14O	M+FA-H	195.1027	0.2
	HMDB0035089	(R)-Carvone	C10H14O	M+FA-H	195.1027	0.2
	HMDB0035761	(-)-Pinocarvone	C10H14O	M+FA-H	195.1027	0.2
	HMDB0035250	Myrtenal	C10H14O	M+FA-H	195.1027	0.2
	HMDB0032626	1-Methoxy-4-propylbenzene	C10H14O	M+FA-H	195.1027	0.2
	HMDB0032063	4-tert-Butylphenol	C10H14O	M+FA-H	195.1027	0.2
	HMDB0036089	(R)-Menthofuran	C10H14O	M+FA-H	195.1027	0.2
	HMDB0037561	Linden ether	C10H14O	M+FA-H	195.1027	0.2
	HMDB0031817	Cuminyl alcohol	C10H14O	M+FA-H	195.1027	0.2
	HMDB0034846	2-(4-Methylphenyl)-1-propanol	C10H14O	M+FA-H	195.1027	0.2
	HMDB0036061	Safranal	C10H14O	M+FA-H	195.1027	0.2
	HMDB0030985	alpha-Carboxy-delta-decalactone	C11H18O4	M-H2O-H	195.1021	3.0
	HMDB0030986	2-Carboxy-5,7-dimethyl-4-octanolide	C11H18O4	M-H2O-H	195.1021	3.0
	HMDB0030984	5-Hexyltetrahydro-2-oxo-3-furancarboxylic acid	C11H18O4	M-H2O-H	195.1021	3.0
	HMDB0030944	Cystophorene	C11H18	M+FA-H	195.1391	-0.8
	HMDB0061811	4-Methyl-2-methylene-1-(1-methylethylidene)-cyclohexane	C11H18	M+FA-H	195.1391	-0.8
	HMDB0035792	(E)-4,8-Dimethyl-1,3,7-nonatriene	C11H18	M+FA-H	195.1391	-0.8
	HMDB0032901	Yuzu lactone	C12H20O2	M-H	195.1391	-0.8
	HMDB0038270	cis-3-Hexenyl cis-3-hexenoate	C12H20O2	M-H	195.1391	-0.8
	HMDB0030945	Methyl 2-undecynoate	C12H20O2	M-H	195.1391	-0.8
	HMDB0039522	Linalyl acetate	C12H20O2	M-H	195.1391	-0.8
	HMDB0040725	Fenchyl acetate	C12H20O2	M-H	195.1391	-0.8
	HMDB0036048	Artemisia alcohol acetate	C12H20O2	M-H	195.1391	-0.8
	HMDB0040397	(-)-Bornyl acetate	C12H20O2	M-H	195.1391	-0.8
	HMDB0032051	alpha-Terpeneol acetate	C12H20O2	M-H	195.1391	-0.8
	HMDB0041494	(S)-Santolina acetate	C12H20O2	M-H	195.1391	-0.8
	HMDB0030867	Dihydro-5-(2-octenyl)-2(3H)-furanone	C12H20O2	M-H	195.1391	-0.8
	HMDB0031692	cis-3-Hexenyl trans-4-hexenoate	C12H20O2	M-H	195.1391	-0.8
	HMDB0031030	6-Heptyl-5,6-dihydro-2H-pyran-2-one	C12H20O2	M-H	195.1391	-0.8

195.1389	HMDB0036599	Ethyl 2Z,4E-decadienoic acid	C12H20O2	M-H	195.1391	-0.8
	HMDB0034903	(3R,3aR,7aS)-3-Butylhexahydro-1(3H)-isobenzofuranone	C12H20O2	M-H	195.1391	-0.8
	HMDB0038280	cis-3-Hexenyl trans-2-hexenoate	C12H20O2	M-H	195.1391	-0.8
	HMDB0041469	Dihydrocarveol acetate	C12H20O2	M-H	195.1391	-0.8
	HMDB0032193	alpha-Campholene acetate	C12H20O2	M-H	195.1391	-0.8
	HMDB0040206	Allyl 3-cyclohexylpropionate	C12H20O2	M-H	195.1391	-0.8
	HMDB0040227	Isopulegol acetate	C12H20O2	M-H	195.1391	-0.8
	HMDB0037301	p-Menth-1-en-9-ol acetate	C12H20O2	M-H	195.1391	-0.8
	HMDB0061816	3,7-Dimethyl-2,6-octadien-1-ylacetate	C12H20O2	M-H	195.1391	-0.8
	HMDB0032331	(Z)-4-Hydroxy-6-dodecenoic acid lactone	C12H20O2	M-H	195.1391	-0.8
	HMDB0062144	p-Menth-1-en-4-yl acetate	C12H20O2	M-H	195.1391	-0.8
	HMDB0035157	geranyl acetate	C12H20O2	M-H	195.1391	-0.8
	HMDB0159935	SCHEMBL14224944	C12H22O3	M-H2O-H	195.1385	2.0
	HMDB0159936	(5Z)-2-hydroxydodec-5-enoic acid	C12H22O3	M-H2O-H	195.1385	2.0
	HMDB0159931	(5Z)-7-hydroxydodec-5-enoic acid	C12H22O3	M-H2O-H	195.1385	2.0
	HMDB0159934	4-(3-hexyloxiran-2-yl)butanoic acid	C12H22O3	M-H2O-H	195.1385	2.0
	HMDB0159932	(5Z)-4-hydroxydodec-5-enoic acid	C12H22O3	M-H2O-H	195.1385	2.0
	HMDB0159933	(5Z)-11-hydroxydodec-5-enoic acid	C12H22O3	M-H2O-H	195.1385	2.0
	HMDB0037398	4-Acetoxy-2-hexyltetrahydrofuran	C12H22O3	M-H2O-H	195.1385	2.0
	HMDB0010727	3-Oxododecanoic acid	C12H22O3	M-H2O-H	195.1385	2.0
196.0384	HMDB0000197	Indoleacetic acid	C10H9NO2	M+Na-2H	196.0380	2.1
	HMDB0004073	5-Hydroxyindoleacetaldehyde	C10H9NO2	M+Na-2H	196.0380	2.1
	HMDB0040972	1-Methoxy-1H-indole-3-carboxaldehyde	C10H9NO2	M+Na-2H	196.0380	2.1
	HMDB0038628	Hydroxymethyl indol-3-yl ketone	C10H9NO2	M+Na-2H	196.0380	2.1
	HMDB0162021	7-methylidene-5H,6H,7H-cyclopenta[c]pyridine-4-carboxylic acid	C10H9NO2	M+Na-2H	196.0380	2.1
196.0618	HMDB0038336	2-Hydroxy-3-(3,4-dihydroxyphenyl)propanamide	C9H11NO4	M-H	196.0615	1.4
	HMDB0000609	DL-Dopa	C9H11NO4	M-H	196.0615	1.4
	HMDB0038750	N-Hydroxy-L-tyrosine	C9H11NO4	M-H	196.0615	1.4
	HMDB0000181	L-Dopa	C9H11NO4	M-H	196.0615	1.4
	HMDB0186197	N-(Acetyloxy)benzenamine	C8H9NO2	M+FA-H	196.0615	1.4
	HMDB0029703	Methyl 2-aminobenzoate	C8H9NO2	M+FA-H	196.0615	1.4
	HMDB0001859	Acetaminophen	C8H9NO2	M+FA-H	196.0615	1.4
	HMDB0060680	2-Amino-3-methylbenzoate	C8H9NO2	M+FA-H	196.0615	1.4
	HMDB0176134	4-(Methylamino)benzoic acid	C8H9NO2	M+FA-H	196.0615	1.4
	HMDB0012992	Leukoaminochrome	C8H9NO2	M+FA-H	196.0615	1.4
	HMDB0033903	3alpha,4,7,7alpha-Tetrahydro-1H-isoindole-1,3(2H)-dione	C8H9NO2	M+FA-H	196.0615	1.4
	HMDB0032609	2-(Methylamino)benzoic acid	C8H9NO2	M+FA-H	196.0615	1.4
	HMDB0059846	Ethyl nicotinate	C8H9NO2	M+FA-H	196.0615	1.4
	HMDB0012219	Dopamine quinone	C8H9NO2	M+FA-H	196.0615	1.4
	HMDB0002210	2-Phenylglycine	C8H9NO2	M+FA-H	196.0615	1.4
	HMDB0062129	(Z)-(methyl N-hydroxybenzenecarboximidate)	C8H9NO2	M+FA-H	196.0615	1.4
	HMDB0061919	2'-Hydroxyacetanilide	C8H9NO2	M+FA-H	196.0615	1.4
	HMDB0012245	Kinetin	C10H9N5O	M-H2O-H	196.0623	-2.7
197.0572	HMDB0015188	Mimosine	C8H10N2O4	M-H	197.0568	2.1
	HMDB0168463	2-AMINO-6-HYDROXYBENZAMIDE	C7H8N2O2	M+FA-H	197.0568	2.1
	HMDB0168464	2-AMINO-4-HYDROXYBENZAMIDE	C7H8N2O2	M+FA-H	197.0568	2.1
	HMDB0168465	2-(hydroxyamino)benzene-1-carboximidic acid	C7H8N2O2	M+FA-H	197.0568	2.1
	HMDB0004193	N1-Methyl-2-pyridone-5-carboxamide	C7H8N2O2	M+FA-H	197.0568	2.1
	HMDB0004194	N1-Methyl-4-pyridone-3-carboxamide	C7H8N2O2	M+FA-H	197.0568	2.1
	HMDB0168680	(4-ethoxyphenyl)methanol	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0125537	3-ethyl-5-methoxyphenol	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0150177	3-phenylpropane-1,2-diol	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0146637	4-ETHYL-3-METHOXYPHENOL	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0175240	2-Phenyl-1,2-propanediol	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0032599	3-(4-Hydroxyphenyl)-1-propanol	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0040216	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0039801	1-(2-Furanyl)-1-pentanone	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0036227	2-Propenyl 2,4-hexadienoate	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0039956	4-(Ethoxymethyl)phenol	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0036169	3-(5-Methyl-2-furanyl)butanal	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0041326	(Dimethoxymethyl)benzene	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0040449	2-(Ethoxymethyl)phenol	C9H12O2	M+FA-H	197.0819	-0.7

197.0818	HMDB0175244	4-(1-hydroxypropan-2-yl)phenol	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0175241	2-PHENYL-1,3-PROPANEDIOL	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0175243	SCHEMBL9169343	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0032132	2-Isopropyl-1,4-benzenediol	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0173825	1-[4-(Hydroxymethyl)phenyl]ethanol	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0173826	1-(4-methylphenyl)ethane-1,2-diol	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0059853	3,5-Dimethoxytoluene	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0041804	2-Isopropoxyphenol	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0150180	2-(3-hydroxypropyl)phenol	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0150178	1-Phenylpropane-1,3-diol	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0150179	3-(3-hydroxypropyl)phenol	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0040175	4-Ethyl-2-methoxyphenol	C9H12O2	M+FA-H	197.0819	-0.7
	HMDB0135755	4-ethyl-2,6-dimethoxybenzene-1,3-diol	C10H14O4	M-H	197.0819	-0.7
	HMDB0131265	2,3,5-trimethoxy-6-methylphenol	C10H14O4	M-H	197.0819	-0.7
	HMDB0004998	Guaifenesin	C10H14O4	M-H	197.0819	-0.7
	HMDB0034099	(2E,4E)-2,7-Dimethyl-2,4-octadienedioic acid	C10H14O4	M-H	197.0819	-0.7
	HMDB0033093	3-(4-Hydroxy-3-methoxyphenyl)-1,2-propanediol	C10H14O4	M-H	197.0819	-0.7
	HMDB0030991	5-(3E-Pentenyl)tetrahydro-2-oxo-3-furancarboxylic acid	C10H14O4	M-H	197.0819	-0.7
	HMDB0059768	3,4-Methylene suberic acid	C10H14O4	M-H	197.0819	-0.7
	HMDB0059779	2,3-Methylene suberic acid	C10H14O4	M-H	197.0819	-0.7
	HMDB0177594	1-(3,4-dimethoxyphenyl)ethane-1,2-diol	C10H14O4	M-H	197.0819	-0.7
	HMDB0182561	5-(1-carboxyethyl)-2-hydroxy-2-methylcyclopentane-1-carboxylic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0170513	3-[3-(2-carboxy-2-methylethyl)oxiran-2-yl]-2-methylpropanoic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0170514	(4E)-2-(hydroxymethyl)-7-methyloct-4-enedioic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0170512	(4E)-3-hydroxy-2,7-dimethyloct-4-enedioic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0182565	2-(1-carboxy-2-hydroxyethyl)-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0182564	2-(1-carboxyethyl)-3-hydroxy-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0182566	2-(1-carboxyethyl)-1-hydroxy-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0182563	5-(1-carboxyethyl)-3-hydroxy-2-methylcyclopentane-1-carboxylic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0182560	2-(1-carboxyethyl)-5-(hydroxymethyl)cyclopentane-1-carboxylic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0182562	2-(1-carboxy-1-hydroxyethyl)-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0175348	SCHEMBL1335666	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0175346	5-hydroxy-1,2,2-trimethylcyclopentane-1,3-dicarboxylic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0175347	4-hydroxy-1,2,2-trimethylcyclopentane-1,3-dicarboxylic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0175345	2-(hydroxymethyl)-1,2-dimethylcyclopentane-1,3-dicarboxylic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0175344	1-Hydroxymethyl-2,2-dimethyl-cyclopentane-1,3-dicarboxylic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0170511	(4E)-2-hydroxy-2,7-dimethyloct-4-enedioic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0160552	(4Z)-9-hydroxydec-4-enedioic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0160551	(4Z)-2-hydroxydec-4-enedioic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0160549	(4Z)-3-hydroxydec-4-enedioic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0160547	(4Z)-8-hydroxydec-4-enedioic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0160548	(4Z)-6-hydroxydec-4-enedioic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0160550	5-[3-(2-carboxyethyl)oxiran-2-yl]pentanoic acid	C10H16O5	M-H2O-H	197.0814	2.1
	HMDB0160546	(4Z)-7-hydroxydec-4-enedioic acid	C10H16O5	M-H2O-H	197.0814	2.1
197.0968	HMDB0133178	(2Z)-2-(phenylmethylidene)hept-6-enoic acid	C14H16O2	M-H2O-H	197.0966	0.8
	HMDB0040833	3-[4-Hydroxy-3-(3-methyl-2-butenyl)phenyl]-2-propenal	C14H16O2	M-H2O-H	197.0966	0.8
	HMDB0032078	Dibenzyl ether	C14H14O	M-H	197.0972	-2.0
	HMDB0182523	p-Menth-1(7)-en-2-one	C10H16O	M+FA-H	197.1183	-0.1
	HMDB0187618	isopiperitenol	C10H16O	M+FA-H	197.1183	-0.1
	HMDB0182597	SCHEMBL13931696	C10H16O	M+FA-H	197.1183	-0.1
	HMDB0182548	2-[(1R)-4-methylcyclohexa-2,4-dien-1-yl]propan-1-ol	C10H16O	M+FA-H	197.1183	-0.1

HMDB0182545	(6S)-3-methyl-6-(propan-2-yl)cyclohexa-2,4-dien-1-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0182547	(5S)-2-methyl-5-(propan-2-yl)-7-oxabicyclo[4.1]hept-2-ene	C10H16O	M+FA-H	197.1183	-0.1
HMDB0182544	SCHEMBL4374431	C10H16O	M+FA-H	197.1183	-0.1
HMDB0182546	(4S)-1-methyl-4-(propan-2-yl)-7-oxabicyclo[4.1]hept-2-ene	C10H16O	M+FA-H	197.1183	-0.1
HMDB0182543	(R)-p-Mentha-1,5-diene-8-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0182542	ZINC321828	C10H16O	M+FA-H	197.1183	-0.1
HMDB0181809	2-[(1R)-4-methylidenebicyclo[3.1]hexan-1-yl]propan-1-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0181808	(1S)-4-methylidene-1-(propan-2-yl)bicyclo[3.1]hexan-6-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0181807	(5S)-2-methylidene-5-(propan-2-yl)bicyclo[3.1]hexan-1-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0187619	2-methyl-2-(4-methylcyclohex-3-en-1-yl)oxirane	C10H16O	M+FA-H	197.1183	-0.1
HMDB0181806	(1R)-4-methylidene-1-(propan-2-yl)bicyclo[3.1]hexan-2-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0181805	AC1O5B2Q	C10H16O	M+FA-H	197.1183	-0.1
HMDB0181804	2-[(1R)-4-methylidenebicyclo[3.1]hexan-1-yl]propan-2-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0163091	(4Z,7Z)-deca-4,7-dienal	C10H16O	M+FA-H	197.1183	-0.1
HMDB0163092	SCHEMBL5863926	C10H16O	M+FA-H	197.1183	-0.1
HMDB0041013	Isocyclocitral	C10H16O	M+FA-H	197.1183	-0.1
HMDB0037280	Junione	C10H16O	M+FA-H	197.1183	-0.1
HMDB0036129	Verbenol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0034973	(R)-Campholenic aldehyde	C10H16O	M+FA-H	197.1183	-0.1
HMDB0034985	(+)-Fenchone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0034975	Piperitone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0036128	(-)-trans-Pinocarveol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035744	(-)-Isopinocampone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0036115	(-)-3-Isothujone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0036598	(E,E)-2,4-Decadienal	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035656	3-Pinanone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035737	(R)-Piperitone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035738	(R)-Piperitone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0038290	Photocitral A	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035743	Pinocarveol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035092	cis-Citral	C10H16O	M+FA-H	197.1183	-0.1
HMDB0040766	Anethofuran	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035100	2-Pinen--ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035125	Darwinol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035280	Teresantalol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035078	Geranial	C10H16O	M+FA-H	197.1183	-0.1
HMDB0036083	Carveol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0037008	6,8-Epoxy-p-menth-2-ene	C10H16O	M+FA-H	197.1183	-0.1
HMDB0036082	(-)-cis-Carveol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035158	1,2-Epoxy-p-menth-8-ene	C10H16O	M+FA-H	197.1183	-0.1
HMDB0036087	(R)-p-Mentha-1,8-dien-7-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0036088	(R)-p-Mentha-1,8-dien-7-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0039008	3,4-Epoxy-p-menth-1(7)-ene	C10H16O	M+FA-H	197.1183	-0.1
HMDB0030893	Isocitral	C10H16O	M+FA-H	197.1183	-0.1
HMDB0037024	4-Acetyl-1,4-dimethyl-1-cyclohexene	C10H16O	M+FA-H	197.1183	-0.1
HMDB0034974	(R)-Carvotanacetone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0037025	Hop ether	C10H16O	M+FA-H	197.1183	-0.1
HMDB0032120	2,6-Dimethyl-1,7-octadien-3-one	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035120	Dehydrolinalool	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035600	(S)-Phellandral	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035741	(-)-trans-Isopulegone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0038557	xi-3,6-Dihydro-4-methyl-2-(2-methyl-1-propenyl)-2H-pyran	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035622	(+)-cis-Carveol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0036080	(1S,4S)-Dihydrocarvone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0036114	(-)-3-Thujone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035054	(1S,4R)-p-Mentha-2,8-dien-1-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035077	(1R,4R)-p-Mentha-2,8-dien-1-ol	C10H16O	M+FA-H	197.1183	-0.1

HMDB0003667	Alpha-Pinene-oxide	C10H16O	M+FA-H	197.1183	-0.1
HMDB0003634	Perillyl alcohol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0003450	(-)-trans-Carveol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0037302	xi-p-Mentha-3,8-dien-1-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035203	(S)-9,-Cyclo-p-menth-1-en-4-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0036127	(-)-Pinocamphone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0036044	Marmelo oxide A	C10H16O	M+FA-H	197.1183	-0.1
HMDB0034715	p-Mentha-1(6),8-dien-3-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0037015	p-Mentha-1,8-dien-4-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0037303	xi-p-Mentha-1(7),2-dien-4-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0038251	xi-Pinol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035241	(Z)-2-Methyl-6-methylene-2,7-octadien-1-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0037010	(2S,4R)-p-Mentha-1(7),8-dien-2-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035277	(2S,4R)-p-Mentha-1(7),5-dien-2-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0041631	3-Thujanone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0059608	(+)-trans-Carveol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0032242	(E)-3,7-Dimethyl-1,5,7-octatrien-3-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0032536	2-(trans-2-Pentenyl)cyclopentanone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0059885	p-Menth-1-en-9-al	C10H16O	M+FA-H	197.1183	-0.1
HMDB0059761	4-(1-Methylethyl)-1-cyclohexene-4-carboxaldehyde	C10H16O	M+FA-H	197.1183	-0.1
HMDB0059827	3-Cyclohexene-1-carboxaldehyde, 1,3,4-trimethyl-	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035604	Pulegone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0061794	Pulegone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0061292	SCHEMBL6943113	C10H16O	M+FA-H	197.1183	-0.1
HMDB0059875	Carvotanacetone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0059838	Camphor	C10H16O	M+FA-H	197.1183	-0.1
HMDB0041011	beta-Cyclocitral	C10H16O	M+FA-H	197.1183	-0.1
HMDB0034916	cis-2-Thujen-4-ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0039816	2-Hexylfuran	C10H16O	M+FA-H	197.1183	-0.1
HMDB0036079	Dihydrocarvone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0037009	Terpinolene oxide	C10H16O	M+FA-H	197.1183	-0.1
HMDB0030892	p-Menth-3-en-9-al	C10H16O	M+FA-H	197.1183	-0.1
HMDB0036113	(+)-3-Thujone	C10H16O	M+FA-H	197.1183	-0.1
HMDB0037172	Tetrahydro-5-isopropenyl-2-methyl-2-vinylfuran	C10H16O	M+FA-H	197.1183	-0.1
HMDB0035706	alpha-Cyclocitral	C10H16O	M+FA-H	197.1183	-0.1
HMDB0037017	(R)-p-Mentha-1,8-dien--ol	C10H16O	M+FA-H	197.1183	-0.1
HMDB0031854	3-Methyl-5-propyl-2-cyclohexen-1-one	C10H16O	M+FA-H	197.1183	-0.1
HMDB0036085	Dehydro-1,8-cineole	C10H16O	M+FA-H	197.1183	-0.1
HMDB0179398	methyl (2E)-3-(3-pentyloxiran-2-yl)prop-2-enoate	C11H18O3	M-H	197.1183	-0.1
HMDB0179399	methyl (2E,4Z)--hydroxydeca-2,4-dienoate	C11H18O3	M-H	197.1183	-0.1
HMDB0179397	methyl 3-[(1Z)-hept-1-en-1-yl]oxirane-2-carboxylate	C11H18O3	M-H	197.1183	-0.1
HMDB0179395	methyl (4Z)-6-hydroxydeca-2,4-dienoate	C11H18O3	M-H	197.1183	-0.1
HMDB0178764	methyl (4Z,8Z)-3-hydroxydeca-4,8-dienoate	C11H18O3	M-H	197.1183	-0.1
HMDB0178765	methyl (4Z,8Z)-6-hydroxydeca-4,8-dienoate	C11H18O3	M-H	197.1183	-0.1
HMDB0179396	methyl (2E,4Z)-9-hydroxydeca-2,4-dienoate	C11H18O3	M-H	197.1183	-0.1
HMDB0163238	(2E,5Z)--hydroxyundeca-2,5-dienoic acid	C11H18O3	M-H	197.1183	-0.1
HMDB0178767	methyl 3-{3-[(3Z)-pent-3-en-1-yl]oxiran-2-yl}propanoate	C11H18O3	M-H	197.1183	-0.1
HMDB0178763	methyl (4Z,8Z)--hydroxydeca-4,8-dienoate	C11H18O3	M-H	197.1183	-0.1
HMDB0178768	methyl (4Z,8Z)-2-hydroxydeca-4,8-dienoate	C11H18O3	M-H	197.1183	-0.1
HMDB0163241	(2E,5Z)-7-hydroxyundeca-2,5-dienoic acid	C11H18O3	M-H	197.1183	-0.1
HMDB0163239	(2E,5Z)-11-hydroxyundeca-2,5-dienoic acid	C11H18O3	M-H	197.1183	-0.1
HMDB0163242	3-[(2Z)-oct-2-en-1-yl]oxirane-2-carboxylic acid	C11H18O3	M-H	197.1183	-0.1
HMDB0163243	(2E)-4-(3-pentyloxiran-2-yl)but-2-enoic acid	C11H18O3	M-H	197.1183	-0.1
HMDB0178766	methyl (4Z)-7-(3-methyloxiran-2-yl)hept-4-enoate	C11H18O3	M-H	197.1183	-0.1
HMDB0178762	methyl (4Z,8Z)-7-hydroxydeca-4,8-dienoate	C11H18O3	M-H	197.1183	-0.1
HMDB0000888	Undecanedioic acid	C11H20O4	M-H2O-H	197.1178	2.7
HMDB0037137	Butyl butyryllactate	C11H20O4	M-H2O-H	197.1178	2.7
HMDB0041218	(Z)-1,5-Undecadiene	C11H20	M+FA-H	197.1547	-1.0
HMDB0032712	1,4-Undecadiene	C11H20	M+FA-H	197.1547	-1.0
HMDB0037305	Methyl 9-undecenoate	C12H22O2	M-H	197.1547	-1.0
HMDB0037498	1-Ethenylhexyl butanoate	C12H22O2	M-H	197.1547	-1.0
HMDB0039220	Ethyl 4-decenoate	C12H22O2	M-H	197.1547	-1.0
HMDB0029585	Methyl -undecenoate	C12H22O2	M-H	197.1547	-1.0
HMDB0037742	xi-5-Dodecanolide	C12H22O2	M-H	197.1547	-1.0

197.1545	HMDB0034844	Citronellyl acetate	C12H22O2	M-H	197.1547	-1.0
	HMDB0037329	Ethyl 2-decenoate	C12H22O2	M-H	197.1547	-1.0
	HMDB0040163	Hexyl 2-methyl-4-pentenoate	C12H22O2	M-H	197.1547	-1.0
	HMDB0038924	2-Hexenyl hexanoate	C12H22O2	M-H	197.1547	-1.0
	HMDB0034160	Citronellyl acetate	C12H22O2	M-H	197.1547	-1.0
	HMDB0033378	cis-3-Hexenyl hexanoate	C12H22O2	M-H	197.1547	-1.0
	HMDB0040158	Hexyl 2-methyl-3-pentenoate	C12H22O2	M-H	197.1547	-1.0
	HMDB0029763	Allyl nonanoate	C12H22O2	M-H	197.1547	-1.0
	HMDB0041264	Menthyl acetate	C12H22O2	M-H	197.1547	-1.0
	HMDB0031683	xi-Dihydro-5-octyl-2(3H)-furanone	C12H22O2	M-H	197.1547	-1.0
	HMDB0037813	3-Heptyldihydro-5-methyl-2(3H)-furanone	C12H22O2	M-H	197.1547	-1.0
	HMDB0038269	Hexyl 2E-hexenoate	C12H22O2	M-H	197.1547	-1.0
	HMDB0038895	7-Hexyl-2-oxepanone	C12H22O2	M-H	197.1547	-1.0
	HMDB0036182	5,5-Dibutyl-4,5-dihydro-2(3H)furanone	C12H22O2	M-H	197.1547	-1.0
	HMDB0040361	1,1-Dimethoxy-3,7-dimethyl-2,6-octadiene	C12H22O2	M-H	197.1547	-1.0
	HMDB0038081	2-Octenyl butyrate	C12H22O2	M-H	197.1547	-1.0
	HMDB0037186	Rhodinyl acetate	C12H22O2	M-H	197.1547	-1.0
	HMDB0032214	cis-4-Decenyl acetate	C12H22O2	M-H	197.1547	-1.0
	HMDB0041449	[(3,7-Dimethyl-6-octenyl)oxy]acetaldehyde	C12H22O2	M-H	197.1547	-1.0
	HMDB0032248	11-Dodecenoic acid	C12H22O2	M-H	197.1547	-1.0
	HMDB0032235	2,6-Dimethyl-5-heptenal propyleneglycol acetal	C12H22O2	M-H	197.1547	-1.0
	HMDB0010729	trans-Dodec-2-enoic acid	C12H22O2	M-H	197.1547	-1.0
	HMDB0000529	5Z-Dodecenoic acid	C12H22O2	M-H	197.1547	-1.0
	HMDB0010728	(R)-3-Hydroxydodecanoic acid	C12H24O3	M-H2O-H	197.1542	1.7
	HMDB0000387	(S)-3-hydroxylauric acid	C12H24O3	M-H2O-H	197.1542	1.7
	HMDB0062032	3-hydroxy-2,4,4-trimethylpentyl 2-methylpropanoate	C12H24O3	M-H2O-H	197.1542	1.7
	HMDB0002059	12-Hydroxydodecanoic acid	C12H24O3	M-H2O-H	197.1542	1.7
	HMDB0040169	xi-5-Hydroxydodecanoic acid	C12H24O3	M-H2O-H	197.1542	1.7
197.1908	HMDB0032154	Acetaldehyde hexyl isoamyl acetal	C13H28O2	M-H2O-H	197.1905	1.3
	HMDB0032550	Valeraldehyde dibutyl acetal	C13H28O2	M-H2O-H	197.1905	1.3
	HMDB0034148	2-Tridecanone	C13H26O	M-H	197.1911	-1.5
	HMDB0062117	6,-Dimethylundecan-2-one	C13H26O	M-H	197.1911	-1.5
	HMDB0030928	Tridecanal	C13H26O	M-H	197.1911	-1.5
198.9969	HMDB0171732	4-hydroxy-2H,9H-[1,3]thiazino[6,5-b]indol-2-one	C10H6N2O2S	M-H2O-H	198.9966	1.5
199.0613	HMDB0159571	5-(1,2-dihydroxyethyl)-3-methoxybenzene-1,2-diol	C9H12O5	M-H	199.0612	0.5
	HMDB0033091	(Z)-3-(1-Formyl-1-propenyl)pentanedioic acid	C9H12O5	M-H	199.0612	0.5
	HMDB0131231	5-methoxy-4-methylbenzene-1,3-diol	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0131232	5-methoxy-2-methylbenzene-1,3-diol	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0169080	2-Hydroxy-3-methoxybenzyl alcohol	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0146894	4-Ethylpyrogallol	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0146874	SCHEMBL093	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0125534	5-ethylbenzene-1,2,3-triol	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0131479	2,3-dimethoxyphenol	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0059966	3,5-Dimethoxyphenol	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0037724	Propyl 2-furoate	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0034158	2,6-Dimethoxyphenol	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0037728	2-Furanylmethyl propanoate	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0032012	4-Hydroxy-3-methoxybenzenemethanol	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0030570	Sylvopinol	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0135785	1-(4-hydroxyphenyl)ethane-1,2-diol	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0126617	2,4-dimethylbenzene-1,3,5-triol	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0005784	Hydroxytyrosol	C8H10O3	M+FA-H	199.0612	0.5
	HMDB0180432	3-[(1E)-hex-1-en-1-yl]oxirane-2-carbaldehyde	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0060285	4-Oxo-2-nonenal	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0167038	(2E,6Z)-9-hydroxynona-2,6-dienal	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0036177	3,5,5-Trimethyl-1,2-cyclohexanedione	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0036239	3,5,5-Trimethyl-1,2-cyclohexanedione	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0032442	2-Nonenoic acid gamma-lactone	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0032314	2,4-Hexadienyl propionate	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0167034	(2E,6Z)-8-hydroxynona-2,6-dienal	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0180430	(2E,4E)-6-hydroxynona-2,4-dienal	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0037276	Octahydro-2H-1-benzopyran-2-one	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0031302	Methyl 2-octynoate	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0180431	SCHEMBL179742	C9H14O2	M+FA-H	199.0976	-0.9

199.0974	HMDB0038268	Allyl hexenoate	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0180434	(2E,4E)-9-hydroxynona-2,4-dienal	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0038697	xi-2,2,6-Trimethyl-1,4-cyclohexanedione	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0180433	trans-4,5-Epoxy-(E)-nonenal	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0035135	(E)-2,6-Dimethyl-2,5-heptadienoic acid	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0167037	(2E)-5-(3-ethyloxiran-2-yl)pent-2-enal	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0167035	(2E,6Z)-5-hydroxynona-2,6-dienal	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0040285	Anapear	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0163467	(2Z)-2-methylocta-2,7-dienoic acid	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0164921	1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0167033	(2E,6Z)-4-hydroxynona-2,6-dienal	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0167032	2E,6Z-nonadienoic acid	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0167036	3-[(3Z)-hex-3-en-1-yl]oxirane-2-carbaldehyde	C9H14O2	M+FA-H	199.0976	-0.9
	HMDB0170504	SCHEMBL4585236	C10H16O4	M-H	199.0976	-0.9
	HMDB0000603	cis-4-Decenedioic acid	C10H16O4	M-H	199.0976	-0.9
	HMDB0061295	526-51-6	C10H16O4	M-H	199.0976	-0.9
	HMDB0013227	cis-5-Decenedioic acid	C10H16O4	M-H	199.0976	-0.9
	HMDB0034491	Camphoric acid	C10H16O4	M-H	199.0976	-0.9
	HMDB0030989	5-Pentyltetrahydro-2-oxo-3-furancarboxylic acid	C10H16O4	M-H	199.0976	-0.9
	HMDB0030990	alpha-Carboxy-delta-nonalactone	C10H16O4	M-H	199.0976	-0.9
	HMDB0036715	Matsutakic acid A	C10H16O4	M-H	199.0976	-0.9
	HMDB0034971	(1R,2R,3S,1'R)-Nepetalinic acid	C10H16O4	M-H	199.0976	-0.9
	HMDB0000350	3-Hydroxysebacic acid	C10H18O5	M-H2O-H	199.0970	1.8
	HMDB0029189	5-Hydroxysebacate	C10H18O5	M-H2O-H	199.0970	1.8
	HMDB0000424	2-Hydroxydecanedioic acid	C10H18O5	M-H2O-H	199.0970	1.8
199.1337	HMDB0061802	5-Methyl-2-(1-methylethyl)-cyclohexanone	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0059869	p-tert-Butylcyclohexanone	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0187564	CTK8I1689	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0163116	(4Z,7Z)-deca-4,7-dien-1-ol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0032530	(+)-thujan-3-ol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0035815	(+)-Isoborneol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0041014	4-Decenal	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0036097	Rose oxide	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0037133	Linaloyl oxide	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0037048	m-Menth-1-en-8-ol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0035825	(-)-Dihydrocarveol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0035783	(+)-Menthone	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0037016	p-Menth-1-en-5-ol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0035954	(1R*,3R*,6S*)-3-Caranol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0035820	(R)-Citronellal	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0035842	(R)-Citronellal	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0034848	9-Decenal	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0036993	gamma-Terpineol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0036991	delta-Terpineol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0037215	trans-beta-Terpineol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0037161	2-Isopropyl-5-methyl-2-hexenal	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0035823	(S)-p-Menth-1-en-4-ol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0037006	cis-Isopulegone	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0036100	3,7-Dimethyl-1,6-octadien-3-ol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0032118	2,6-Dimethyl-7-octen-3-one	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0035841	Citronellal	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0037007	p-Menth-1-en-9-ol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0037019	6,8-Epoxy-p-menthane	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0036077	p-Menth-8-en-3-ol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0034976	(-)-Borneol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0035818	(-)-Borneol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0036126	(-)-Pinocampheol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0035819	(-)-Isoborneol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0041034	(4Z,7Z)-4,7-Decadien-1-ol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0031410	3-Decen-2-one	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0037049	(R)-m-Menth-1(6)-en-8-ol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0038025	xi-p-Menth-3-en-1-ol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0035861	trans-(-)-p-Menth-1-en-3-ol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0005812	Geraniol	C10H18O	M+FA-H	199.1340	-1.3
	HMDB0004043	alpha-Terpineol	C10H18O	M+FA-H	199.1340	-1.3

HMDB0036112	(1R,4S,5R)-4-Thujanol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0037047	(-)-trans-m-Menth-8-en-1-ol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0036068	Campholenic alcohol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0035955	(1R*,2S*,3S*,6S*)-2-Caranol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0036196	(2E,4E)-2,4-Decadien-1-ol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0004472	Eucalyptol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0035155	beta-Geraniol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0059881	Ocimenol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0035833	p-Menth-1-en-4-ol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0035272	p-Menthan-2-one	C10H18O	M+FA-H	199.1340	-1.3
HMDB0034932	Fenchol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0035162	(-)-Menthone	C10H18O	M+FA-H	199.1340	-1.3
HMDB0059864	(-)-Menthone	C10H18O	M+FA-H	199.1340	-1.3
HMDB0035838	Piperitol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0036086	(S)-alpha-Terpineol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0038185	Ocimen quintoxide	C10H18O	M+FA-H	199.1340	-1.3
HMDB0040448	2-(1-Methylpropyl)cyclohexanone	C10H18O	M+FA-H	199.1340	-1.3
HMDB0034972	Isomenthone	C10H18O	M+FA-H	199.1340	-1.3
HMDB0030999	2-Decenal	C10H18O	M+FA-H	199.1340	-1.3
HMDB0036041	(R)-Lavandulol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0036101	(R)-3,7-Dimethyl-1,6-octadien-3-ol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0036102	(R)-3,7-Dimethyl-1,6-octadien-3-ol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0036996	cis-beta-Terpineol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0037214	cis-beta-Terpineol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0036096	1,4-Cineole	C10H18O	M+FA-H	199.1340	-1.3
HMDB0036107	Myrcenol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0034969	(-)-Carvomenthone	C10H18O	M+FA-H	199.1340	-1.3
HMDB0036078	(-)-Isopulegol	C10H18O	M+FA-H	199.1340	-1.3
HMDB0032662	(S)-9-Hydroxy--undecenoic acid	C11H20O3	M-H	199.1340	-1.4
HMDB0037179	3-Nonanon-1-yl acetate	C11H20O3	M-H	199.1340	-1.4
HMDB0165691	2-hydroxy--undecenoic acid	C11H20O3	M-H	199.1340	-1.4
HMDB0165690	9-(oxiran-2-yl)nonanoic Acid	C11H20O3	M-H	199.1340	-1.4
HMDB0036029	Clarycet	C11H20O3	M-H	199.1340	-1.4
HMDB0165687	5-hydroxyundec--enoic acid	C11H20O3	M-H	199.1340	-1.4
HMDB0165688	4-hydroxyundec--enoic acid	C11H20O3	M-H	199.1340	-1.4
HMDB0165689	3-hydroxy--undecenoic acid	C11H20O3	M-H	199.1340	-1.4
HMDB0165684	8-hydroxyundec--enoic acid	C11H20O3	M-H	199.1340	-1.4
HMDB0165686	6-hydroxyundec--enoic acid	C11H20O3	M-H	199.1340	-1.4
HMDB0165685	7-hydroxyundec--enoic acid	C11H20O3	M-H	199.1340	-1.4
HMDB0134121	2-benzyl octanal	C15H22O	M-H20-H	199.1487	-2.4
HMDB0134122	(2Z)-2-(phenylmethylidene)octan-1-ol	C15H22O	M-H20-H	199.1487	-2.4
HMDB0094674	1-Phenylnonan-1-one	C15H22O	M-H20-H	199.1487	-2.4
HMDB0035643	beta-Sinensal	C15H22O	M-H20-H	199.1487	-2.4
HMDB0038215	alpha-Sinensal	C15H22O	M-H20-H	199.1487	-2.4
HMDB0036201	(E)-,11-Dihydro-alpha-atlantone	C15H22O	M-H20-H	199.1487	-2.4
HMDB0038187	beta-Atlantone	C15H22O	M-H20-H	199.1487	-2.4
HMDB0036797	Mustakone	C15H22O	M-H20-H	199.1487	-2.4
HMDB0036733	Vulgarone A	C15H22O	M-H20-H	199.1487	-2.4
HMDB0036667	Zerumbone	C15H22O	M-H20-H	199.1487	-2.4
HMDB0036813	alpha-Santalal	C15H22O	M-H20-H	199.1487	-2.4
HMDB0035081	(5alpha,alpha)-3,7(11)-Eudesmadien-2-one	C15H22O	M-H20-H	199.1487	-2.4
HMDB0036718	beta-Santalal	C15H22O	M-H20-H	199.1487	-2.4
HMDB0036109	1,3,5-Bisabolatrien--one	C15H22O	M-H20-H	199.1487	-2.4
HMDB0035747	Patchoulenone	C15H22O	M-H20-H	199.1487	-2.4
HMDB0040686	Isohumbertiol	C15H22O	M-H20-H	199.1487	-2.4
HMDB0038164	Vulgarone B	C15H22O	M-H20-H	199.1487	-2.4
HMDB0037000	alpha-Turmerone	C15H22O	M-H20-H	199.1487	-2.4
HMDB0038195	Xanthorrhizol	C15H22O	M-H20-H	199.1487	-2.4
HMDB0038200	Calamusenone	C15H22O	M-H20-H	199.1487	-2.4
HMDB0038511	Bisacumol	C15H22O	M-H20-H	199.1487	-2.4
HMDB0013687	Nookatone	C15H22O	M-H20-H	199.1487	-2.4
HMDB0035657	Solavetivone	C15H22O	M-H20-H	199.1487	-2.4
HMDB0035786	Valerenal	C15H22O	M-H20-H	199.1487	-2.4
HMDB0037061	(+)-4,11-Eudesmadien-3-one	C15H22O	M-H20-H	199.1487	-2.4
HMDB0035835	Furanoeremophilane	C15H22O	M-H20-H	199.1487	-2.4

199.1482

	HMDB0037068	Curlone	C15H22O	M-H2O-H	199.1487	-2.4
	HMDB0039637	beta-Elementone	C15H22O	M-H2O-H	199.1487	-2.4
	HMDB0036071	Dendrolasin	C15H22O	M-H2O-H	199.1487	-2.4
	HMDB0036443	Rotundone	C15H22O	M-H2O-H	199.1487	-2.4
	HMDB0038201	4,7(11)-Guaiadien-8-one	C15H22O	M-H2O-H	199.1487	-2.4
	HMDB0035082	(5beta,7beta,beta)-3,11-Eudesmadien-2-one	C15H22O	M-H2O-H	199.1487	-2.4
199.1702	HMDB0013693	AC1L1WLS	C15H22O	M-H2O-H	199.1487	-2.4
	HMDB0061812	(E)-5-Undecene	C11H22	M+FA-H	199.1704	-0.8
	HMDB0062070	5-ethylnon-1-ene	C11H22	M+FA-H	199.1704	-0.8
	HMDB0031205	(E)-4-Undecene	C11H22	M+FA-H	199.1704	-0.8
	HMDB0062601	(4E)-7-methyldec-4-ene	C11H22	M+FA-H	199.1704	-0.8
	HMDB0062670	1-ethyl-2-propylcyclohexane	C11H22	M+FA-H	199.1704	-0.8
	HMDB0062668	5-methyldec-1-ene	C11H22	M+FA-H	199.1704	-0.8
	HMDB0029551	1-Undecene	C11H22	M+FA-H	199.1704	-0.8
	HMDB0168121	2-hydroxydodecanal	C12H24O2	M-H	199.1704	-0.8
	HMDB0168119	11-hydroxydodecanal	C12H24O2	M-H	199.1704	-0.8
	HMDB0168120	12-hydroxydodecanal	C12H24O2	M-H	199.1704	-0.8
	HMDB0032440	Nonanal propyleneglycol acetal	C12H24O2	M-H	199.1704	-0.8
	HMDB0032310	2-Heptyl butyrate	C12H24O2	M-H	199.1704	-0.8
	HMDB0034128	Isopropyl nonanoate	C12H24O2	M-H	199.1704	-0.8
	HMDB0034136	Octyl butanoate	C12H24O2	M-H	199.1704	-0.8
	HMDB0036225	Pentyl heptanoate	C12H24O2	M-H	199.1704	-0.8
	HMDB0034137	Octyl 2-methylpropanoate	C12H24O2	M-H	199.1704	-0.8
	HMDB0030998	Ethyl decanoate	C12H24O2	M-H	199.1704	-0.8
	HMDB0040166	Decyl acetate	C12H24O2	M-H	199.1704	-0.8
	HMDB0033619	Hexyl hexanoate	C12H24O2	M-H	199.1704	-0.8
	HMDB0035410	(R)-Dihydrocitronellol acetate	C12H24O2	M-H	199.1704	-0.8
	HMDB0061988	2-ethylhexyl butanoate	C12H24O2	M-H	199.1704	-0.8
	HMDB0059868	Isobutyl octanoate	C12H24O2	M-H	199.1704	-0.8
	HMDB0000638	Dodecanoic acid	C12H24O2	M-H	199.1704	-0.8
	HMDB0040219	8,8-Dimethoxy-2,6-dimethyl-2-octanol	C12H26O3	M-H2O-H	199.1698	2.0
201.0769	HMDB0032306	Diethyl oxalpropionate	C9H14O5	M-H	201.0768	0.3
	HMDB0033092	3-(1-Hydroxymethyl-1-propenyl)pentanedioic acid	C9H14O5	M-H	201.0768	0.3
	HMDB0031101	8-Hydroxy-5,6-octadienoic acid	C8H12O3	M+FA-H	201.0768	0.3
	HMDB0159132	2-(4-oxocyclohexyl)acetic Acid	C8H12O3	M+FA-H	201.0768	0.3
	HMDB0032232	2,5-Dimethyl-4-ethoxy-3(2H)-furanone	C8H12O3	M+FA-H	201.0768	0.3
	HMDB0163454	SCHEMBL11263	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0163455	(2Z)-2-(hydroxymethyl)oct-2-enal	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0163458	2-methyl-3-pentyloxirane-2-carbaldehyde	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0163457	(2Z)-7-hydroxy-2-methyloct-2-enal	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0163456	(2Z)-4-hydroxy-2-methyloct-2-enal	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0163459	(2Z)-8-hydroxy-2-methyloct-2-enal	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0166518	2-(hydroxymethyl)-2,6-dimethylcyclohexan-1-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0166519	6-(hydroxymethyl)-2,2-dimethylcyclohexan-1-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179782	(5E)-7-hydroxynon-5-en-2-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0167040	(6Z)-5-hydroxynon-6-enal	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0167041	5-(3-ethyloxiran-2-yl)pentanal	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179784	(5E)-8-hydroxynon-5-en-2-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179786	(5E)-9-hydroxynon-5-en-2-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179787	(5E)-1-hydroxynon-5-en-2-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179788	(5E)-3-hydroxynon-5-en-2-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179806	(3Z)-9-hydroxynon-3-en-2-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179805	Ethanone, 1-(3-pentyloxiranyl)-	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179804	(3Z)-8-hydroxynon-3-en-2-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179803	(3Z)-5-hydroxynon-3-en-2-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179807	(3Z)-1-hydroxynon-3-en-2-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0180000	7-METHYL-7-OCTENOIC ACID	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0180426	(2E,4E)-nona-2,4-diene-1,8-diol	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0180428	(2E)-3-(3-butyloxiran-2-yl)prop-2-en-1-ol	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0180425	(2E,4E)-nona-2,4-diene-1,6-diol	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0180427	{3-[(1E)-hex-1-en-1-yl]oxiran-2-yl}methanol	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0180429	(2E,4E)-nona-2,4-diene-1,9-diol	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179785	4-(3-propyloxiran-2-yl)butan-2-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179783	4-Hydroxynon-5-en-2-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0167039	(6Z)-8-hydroxynon-6-enal	C9H16O2	M+FA-H	201.1132	-0.7

201.1131	HMDB0167042	(6Z)-9-hydroxynon-6-enal	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0167043	(6Z)-2-hydroxynon-6-enal	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0167045	(2E,6Z)-nona-2,6-diene-1,9-diol	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0167044	(2E,6Z)-nona-2,6-diene-1,8-diol	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0167047	(2E,6Z)-nona-2,6-diene-1,4-diol	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0167048	(2E,6Z)-nona-2,6-diene-1,5-diol	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0167049	{3-[(3Z)-hex-3-en-1-yl]oxiran-2-yl}methanol	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0167050	(2E)-5-(3-ethyloxiran-2-yl)pent-2-en-1-ol	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0167057	6Z-Nonenoic acid	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179750	7-hydroxynon-8-en-3-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179752	7-(oxiran-2-yl)heptan-3-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179754	4-hydroxynon-8-en-3-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179751	2-hydroxynon-8-en-3-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0179753	SCHEMBL18838844	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0031271	2-Nonenoic acid	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0038272	trans-2-Hexenyl propanoate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0036208	2-Propenyl 2-ethylbutanoate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0032413	Methyl 2-octenoate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0032491	Prenyl isobutyrate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0032265	cis-Ethyl 4-heptenoate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0032307	Hept-trans-2-en-1-yl acetate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0059728	Methyl 3-Octenoate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0059817	(Z)-Oak lactone	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0059894	(Z)-Oak lactone	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0059840	(E)-2-Ethyl heptenoate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0060286	3,4-Epoxyxnonanal	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0038275	cis-3-Hexenyl propanoate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0039794	Methyl 4Z-octenoate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0004362	4-Hydroxynonenal	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0035307	Quercuslactone a	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0037618	(E)-3-Heptenyl acetate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0037023	2-Hydroxy-2,6,6-trimethylcyclohexanone	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0031531	Dihydro-5-pentyl-2(3H)-furanone	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0036222	Cyclohexyl propionate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0031263	2,4-Nonanedione	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0034716	4-Oxononanal	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0033167	Ethyl cyclohexanecarboxylate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0040210	2-Propenyl hexanoate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0037496	Methyl (E)-2-octenoate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0031514	6-Butyltetrahydro-2H-pyran-2-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0037629	Isobutyl angelate	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0039736	6-Hydroxy-4,6-dimethyl-3-hepten-2-one	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0170941	8-nonylenic acid	C9H16O2	M+FA-H	201.1132	-0.7
	HMDB0040196	Oxalic acid dibutyl ester	C10H18O4	M-H	201.1132	-0.7
	HMDB0031510	R-2-Hydroxy-3-methylbutanoic acid 3-Methylbutanoyl	C10H18O4	M-H	201.1132	-0.7
	HMDB0000792	Sebacic acid	C10H18O4	M-H	201.1132	-0.7
	HMDB0059754	3-Methylazelaic acid	C10H18O4	M-H	201.1132	-0.7
	HMDB0059719	Heptylmalonic acid	C10H18O4	M-H	201.1132	-0.7
	HMDB0059708	2-Ethylsuberic acid	C10H18O4	M-H	201.1132	-0.7
	HMDB0062180	(2S,5S)-2-[(2R)-butan-2-yl]-5-hydroxy-4-oxohexanoic acid	C10H18O4	M-H	201.1132	-0.7
	HMDB0179809	9-hydroxynonan-2-one	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0179988	Isononanoic acid	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0062123	2-methylpropyl pentanoate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0163472	2-methyl-octanoic acid	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0171041	SCHEMBL926	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0179811	2-nonanon-3-ol	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0179810	1-hydroxy-2-nonanone	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0179808	8-hydroxynonan-2-one	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0179167	1-hydroxynonan-4-one	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0171040	non-8-ene-2,7-diol	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0171042	SCHEMBL7123711	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0163464	(2Z)-2-methyloct-2-ene-1,8-diol	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0163460	2-Hexylidene-1,3-propanediol	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0163461	(2Z)-2-methyloct-2-ene-1,4-diol	C9H18O2	M+FA-H	203.1289	-1.4

203.1286	HMDB0163463	(2-methyl-3-pentylloxiran-2-yl)methanol	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0163462	(2Z)-2-methyloct-2-ene-1,7-diol	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0000798	Oenanthic ether	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0037288	4-Methyl-2-pentyl-1,3-dioxolane	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0036234	3-Methylbutyl 2-methylpropanoate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0038603	Octyl formate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0040295	Butyl pentanoate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0034606	Hexyl propionate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0031291	Methyl caprylate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0034165	Propyl hexanoate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0039216	Butyl 2-methylbutanoate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0034162	Pentyl butanoate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0031480	Heptyl acetate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0039219	1-Methylbutyl butanoate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0031557	4-Methyloctanoic acid	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0030331	xi-2-Ethylheptanoic acid	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0000847	Pelargonic acid	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0037164	3-(Hydroxymethyl)-2-octanone	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0037143	1-Hydroxy-3-nonanone	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0038040	2-Methylpropyl 3-methylbutanoate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0032406	5-Methylhexyl acetate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0032309	3-Heptyl acetate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0032454	3-Octyl formate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0059822	Ethyl 5-methylhexanoate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0040221	Isoamyl butyrate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0032042	Butyl 3-methylbutanoate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0040430	Isopropyl hexanoate	C9H18O2	M+FA-H	203.1289	-1.4
	HMDB0039053	(1alpha,2alpha,4betaH,6alpha,8R)-p-Menthane-2,6,8,9-tetrol	C10H20O4	M-H	203.1289	-1.4
	HMDB0039974	(1S,2S,4R,8R)-p-Menthane-1,2,8,9-tetrol	C10H20O4	M-H	203.1289	-1.4
	HMDB0033642	(2xi,3xi,6E)-3,7-Dimethyl-6-octene-1,2,3,8-tetrol	C10H20O4	M-H	203.1289	-1.4
	HMDB0033217	(2xi,6xi)-7-Methyl-3-methylene-1,2,6,7-octanetetrol	C10H20O4	M-H	203.1289	-1.4
	HMDB0035133	3,7-Dimethyl-3-octene-1,2,6,7-tetrol	C10H20O4	M-H	203.1289	-1.4
205.1597	HMDB0035631	alpha-Irone	C14H22O	M-H	205.1598	-0.4
	HMDB0036024	-Isopropyl-2,7-dimethyl-1-oxaspiro[4.5]deca-3,6-diene	C14H22O	M-H	205.1598	-0.4
	HMDB0013816	2,4-di-tert-Butylphenol	C14H22O	M-H	205.1598	-0.4
	HMDB0035245	1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1-penten-3-one	C14H22O	M-H	205.1598	-0.4
	HMDB0133179	2-benzylheptan-1-ol	C14H22O	M-H	205.1598	-0.4
	HMDB0031737	delta-Methylionone	C14H22O	M-H	205.1598	-0.4
	HMDB0038130	1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one	C14H22O	M-H	205.1598	-0.4
	HMDB0031738	3-Methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	C14H22O	M-H	205.1598	-0.4
	HMDB0036023	Etaspiroene	C14H22O	M-H	205.1598	-0.4
	HMDB0061831	(Z)-alpha-Irone	C14H22O	M-H	205.1598	-0.4
	HMDB0032397	Methyl-delta-ionone	C14H22O	M-H	205.1598	-0.4
	HMDB0013825	4-(1,1,3,3-Tetramethylbutyl)-phenol	C14H22O	M-H	205.1598	-0.4
	HMDB0032528	4-(1,1,3,3-Tetramethylbutyl)-phenol	C14H22O	M-H	205.1598	-0.4
	HMDB0000560	Goshuyic acid	C14H24O2	M-H2O-H	205.1592	2.2
	HMDB0039129	Goshuyic acid	C14H24O2	M-H2O-H	205.1592	2.2
	HMDB0032342	Isobornyl isobutyrate	C14H24O2	M-H2O-H	205.1592	2.2
	HMDB0030427	Linalyl butyrate	C14H24O2	M-H2O-H	205.1592	2.2
	HMDB0038260	Geranyl 2-methylpropanoate	C14H24O2	M-H2O-H	205.1592	2.2
	HMDB0037814	2-Propenyl cyclohexanepentanoate	C14H24O2	M-H2O-H	205.1592	2.2
	HMDB0030426	Linalyl isobutyrate	C14H24O2	M-H2O-H	205.1592	2.2
	HMDB0031015	Ethyl (2E,6Z)-dodecadienoate	C14H24O2	M-H2O-H	205.1592	2.2
	HMDB0038259	Neryl butyrate	C14H24O2	M-H2O-H	205.1592	2.2
	HMDB0032524	Terpinyl isobutyrate	C14H24O2	M-H2O-H	205.1592	2.2
	HMDB0036424	Allyl undecylenate	C14H24O2	M-H2O-H	205.1592	2.2
	HMDB0032053	alpha-Terpineol butanoate	C14H24O2	M-H2O-H	205.1592	2.2
	HMDB0038246	Bornyl butyrate	C14H24O2	M-H2O-H	205.1592	2.2
	HMDB0163191	(2E,4E,7Z)-9-hydroxytrideca-2,4,7-trienal	C13H20O2	M-H	207.1391	0.7
	HMDB0163195	(2E,4E)-6-(3-pentylloxiran-2-yl)hexa-2,4-dienal	C13H20O2	M-H	207.1391	0.7
	HMDB0178135	3-[(2Z)-but-2-en-1-yl]-4-(hydroxymethyl)-2,4-dimethylcyclohex-2-en-1-one	C13H20O2	M-H	207.1391	0.7

207.1392	HMDB0178139	6-[(2Z)-but-2-en-1-yl]-1,5,5-trimethyl-7-oxabicyclo[4.1]heptan-2-one	C13H20O2	M-H	207.1391	0.7
	HMDB0178137	3-[(2Z)-4-hydroxybut-2-en-1-yl]-2,4,4-trimethylcyclohex-2-en-1-one	C13H20O2	M-H	207.1391	0.7
	HMDB0178136	3-[(2Z)-but-2-en-1-yl]-2-(hydroxymethyl)-4,4-dimethylcyclohex-2-en-1-one	C13H20O2	M-H	207.1391	0.7
	HMDB0178138	2,4,4-trimethyl-3-[(3-methyloxiran-2-yl)methyl]cyclohex-2-en-1-one	C13H20O2	M-H	207.1391	0.7
	HMDB0178140	3-[(2Z)-but-2-en-1-yl]-6-hydroxy-2,4,4-trimethylcyclohex-2-en-1-one	C13H20O2	M-H	207.1391	0.7
	HMDB0163196	(2E,4E,7Z)-13-hydroxytrideca-2,4,7-trienal	C13H20O2	M-H	207.1391	0.7
	HMDB0163193	3-[(1E,4Z)-deca-1,4-dien-1-yl]oxirane-2-carbaldehyde	C13H20O2	M-H	207.1391	0.7
	HMDB0163192	(2E,4E,7Z)-12-hydroxytrideca-2,4,7-trienal	C13H20O2	M-H	207.1391	0.7
	HMDB0132947	1-(4-methoxyphenyl)-4-methylpentan-3-ol	C13H20O2	M-H	207.1391	0.7
	HMDB0163190	(2E,4E,7Z)-trideca-2,4,7-trienoic acid	C13H20O2	M-H	207.1391	0.7
	HMDB0163194	(2E)-3-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}prop-2-enal	C13H20O2	M-H	207.1391	0.7
	HMDB0040233	2,3,5,6,8,8a-Hexahydro-2,5,5,8a-tetramethyl-7H-1-benzopyran-7-one	C13H20O2	M-H	207.1391	0.7
	HMDB0036686	2,2,6,7-Tetramethylbicyclo[4.3]nona-1(9),4-diene-7,8-diol	C13H20O2	M-H	207.1391	0.7
	HMDB0038047	Carvyl propionate	C13H20O2	M-H	207.1391	0.7
	HMDB0029668	Eremopetasinorol	C13H20O2	M-H	207.1391	0.7
	HMDB0038529	5,9:6,9-Diepoxy-4-megastigmen-9-one	C13H20O2	M-H	207.1391	0.7
	HMDB0035228	Theaspiron A	C13H20O2	M-H	207.1391	0.7
	HMDB0034984	(5R,6S)-5,6-Epoxy-7-megastigmen-9-one	C13H20O2	M-H	207.1391	0.7
	HMDB0034672	(5alpha,8beta,9beta)-5,9-Epoxy-3,6-megastigmadien-8-ol	C13H20O2	M-H	207.1391	0.7
	HMDB0036824	Acetal R	C13H20O2	M-H	207.1391	0.7
	HMDB0031869	(S,E)-Lyralol propanoate	C13H20O2	M-H	207.1391	0.7
	HMDB0037776	3-Mercaptohexyl hexanoate	C13H20O2	M-H	207.1391	0.7
	HMDB0041636	(3R,8E)-3-Hydroxy-5,8-megastigmadien-7-one	C13H20O2	M-H	207.1391	0.7
	HMDB0036821	Apo-9-zeaxanthinone	C13H20O2	M-H	207.1391	0.7
	HMDB0036759	Pregeijerene	C12H18	M+FA-H	207.1391	0.7
	HMDB0013806	1,3-Diisopropylbenzene	C12H18	M+FA-H	207.1391	0.7
	HMDB0061815	Hexylbenzene	C12H18	M+FA-H	207.1391	0.7
209.0813	HMDB0032496	Propyl propane thiosulfonate	C11H16O5	M-H2O-H	209.0814	-0.4
	HMDB0153812	2-(3,4-dihydroxy-3-methylbutyl)benzene-1,3,5-triol	C11H16O5	M-H2O-H	209.0814	-0.4
	HMDB0153819	2-(1,3-dihydroxy-3-methylbutyl)benzene-1,3,5-triol	C11H16O5	M-H2O-H	209.0814	-0.4
209.1185	HMDB0032871	Sedanonic acid	C12H18O3	M-H	209.1183	0.9
	HMDB0032797	Jasmonic acid	C12H18O3	M-H	209.1183	0.9
	HMDB0037735	Isoamyl 2-furonpropionate	C12H18O3	M-H	209.1183	0.9
	HMDB0033102	Dihydro-3-(2-octenyl)-2,5-furandione	C12H18O3	M-H	209.1183	0.9
	HMDB0037642	4-(Butoxymethyl)-2-methoxyphenol	C12H18O3	M-H	209.1183	0.9
	HMDB0041573	3-Ethenyl-2,5-dimethyl-4-oxohex-5-en-2-yl acetate	C12H18O3	M-H	209.1183	0.9
	HMDB0037104	(R)-8-Acetoxy-carvotanacetone	C12H18O3	M-H	209.1183	0.9
	HMDB0037135	1-Benzyloxy-1-(2-methoxyethoxy)ethane	C12H18O3	M-H	209.1183	0.9
	HMDB0037816	Dihydro-3-(1-octenyl)-2,5-furandione	C12H18O3	M-H	209.1183	0.9
	HMDB0163591	3-methyl-2-phenylbutan-1-ol	C11H16O	M+FA-H	209.1183	0.9
	HMDB0032060	2-Butyl-4-methylphenol	C11H16O	M+FA-H	209.1183	0.9
	HMDB0036719	Norbicycloekasantalal	C11H16O	M+FA-H	209.1183	0.9
	HMDB0035989	Thymol methyl ether	C11H16O	M+FA-H	209.1183	0.9
	HMDB0031311	Benzyl butyl ether	C11H16O	M+FA-H	209.1183	0.9
	HMDB0035601	(Z)-3-Methyl-2-(2-pentenyl)-2-cyclopenten-1-one	C11H16O	M+FA-H	209.1183	0.9
	HMDB0036814	Santalone	C11H16O	M+FA-H	209.1183	0.9
	HMDB0031624	5-Phenyl-1-pentanol	C11H16O	M+FA-H	209.1183	0.9
	HMDB0031625	1-Phenyl-2-pentanol	C11H16O	M+FA-H	209.1183	0.9
	HMDB0031866	2-Methyl-4-phenyl-2-butanol	C11H16O	M+FA-H	209.1183	0.9
	HMDB0036816	Norecasantalal	C11H16O	M+FA-H	209.1183	0.9
	HMDB0031454	trans-Jasmone	C11H16O	M+FA-H	209.1183	0.9
	HMDB0037294	2-Methyl-3-(2-pentenyl)-2-cyclopenten-1-one	C11H16O	M+FA-H	209.1183	0.9
	HMDB0029653	1-(1-Methoxy-1-methylethyl)-4-methylbenzene	C11H16O	M+FA-H	209.1183	0.9
	HMDB0163198	(4E,7Z)-9-hydroxytrideca-4,7-dienal	C13H22O2	M-H	209.1547	0.0
	HMDB0163197	(4E,7Z)-3-hydroxytrideca-4,7-dienal	C13H22O2	M-H	209.1547	0.0
	HMDB0163201	(4E)-6-(3-pentyloxiran-2-yl)hex-4-enal	C13H22O2	M-H	209.1547	0.0
	HMDB0163202	(4E,7Z)-13-hydroxytrideca-4,7-dienal	C13H22O2	M-H	209.1547	0.0

209.1547	HMDB0163199	(4E,7Z)-12-hydroxytrideca-4,7-dienal	C13H22O2	M-H	209.1547	0.0
	HMDB0163200	3-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}propanal	C13H22O2	M-H	209.1547	0.0
	HMDB0178147	3-[(2Z)-but-2-en-1-yl]-6-hydroxy-2,4,4-trimethylcyclohexan-1-one	C13H22O2	M-H	209.1547	0.0
	HMDB0178146	2,4,4-trimethyl-3-[(3-methyloxiran-2-yl)methyl]cyclohexan-1-one	C13H22O2	M-H	209.1547	0.0
	HMDB0178144	3-[(2Z)-4-hydroxybut-2-en-1-yl]-2,4,4-trimethylcyclohexan-1-one	C13H22O2	M-H	209.1547	0.0
	HMDB0182748	63512--3	C13H22O2	M-H	209.1547	0.0
	HMDB0182747	4-[2-(hydroxymethyl)-2-methyl-6-methylidenecyclohexyl]butan-2-one	C13H22O2	M-H	209.1547	0.0
	HMDB0182752	4-(2,2-dimethyl-6-methylidenecyclohexyl)-1-hydroxybutan-2-one	C13H22O2	M-H	209.1547	0.0
	HMDB0182749	4-(1-hydroxy-2,2-dimethyl-6-methylidenecyclohexyl)butan-2-one	C13H22O2	M-H	209.1547	0.0
	HMDB0182750	4-(5-hydroxy-2,2-dimethyl-6-methylidenecyclohexyl)butan-2-one	C13H22O2	M-H	209.1547	0.0
	HMDB0182751	4-(2,2-dimethyl-6-methylidenecyclohexyl)-3-hydroxybutan-2-one	C13H22O2	M-H	209.1547	0.0
	HMDB0178145	3-[(2Z)-1-hydroxybut-2-en-1-yl]-2,4,4-trimethylcyclohexan-1-one	C13H22O2	M-H	209.1547	0.0
	HMDB0178141	3-[(2Z)-but-2-en-1-yl]-4-(hydroxymethyl)-2,4-dimethylcyclohexan-1-one	C13H22O2	M-H	209.1547	0.0
	HMDB0163203	(4E,7Z)-2-hydroxytrideca-4,7-dienal	C13H22O2	M-H	209.1547	0.0
	HMDB0163206	{3-[(1E,4Z)-deca-1,4-dien-1-yl]oxiran-2-yl}methanol	C13H22O2	M-H	209.1547	0.0
	HMDB0163204	(2E,4E,7Z)-trideca-2,4,7-triene-1,9-diol	C13H22O2	M-H	209.1547	0.0
	HMDB0163205	(2E,4E,7Z)-trideca-2,4,7-triene-1,12-diol	C13H22O2	M-H	209.1547	0.0
	HMDB0163209	(2E,4E,7Z)-trideca-2,4,7-triene-1,13-diol	C13H22O2	M-H	209.1547	0.0
	HMDB0163208	(2E,4E)-6-(3-pentyloxiran-2-yl)hexa-2,4-dien-1-ol	C13H22O2	M-H	209.1547	0.0
	HMDB0163207	(2E)-3-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}prop-2-en-1-ol	C13H22O2	M-H	209.1547	0.0
	HMDB0163218	(4E,7Z)-4,7-tridecadienoic acid	C13H22O2	M-H	209.1547	0.0
	HMDB0178143	3-[(2Z)-but-2-en-1-yl]-2-hydroxy-2,4,4-trimethylcyclohexan-1-one	C13H22O2	M-H	209.1547	0.0
	HMDB0182790	4-{2,2,6-trimethyl-7-oxabicyclo[4.1]heptan-1-yl}butan-2-one	C13H22O2	M-H	209.1547	0.0
	HMDB0037390	Tsibulin 1	C13H22O2	M-H	209.1547	0.0
	HMDB0041554	Artemisyl propionate	C13H22O2	M-H	209.1547	0.0
	HMDB0032098	Cepanone	C13H22O2	M-H	209.1547	0.0
	HMDB0040232	Octahydro-2,5,5,8a-tetramethyl-7H-1-benzopyran-7-one	C13H22O2	M-H	209.1547	0.0
	HMDB0030425	Linalyl propionate	C13H22O2	M-H	209.1547	0.0
	HMDB0038291	2-Propenyl cyclohexanebutanoate	C13H22O2	M-H	209.1547	0.0
	HMDB0031014	Methyl (2E,6Z)-dodecadienoate	C13H22O2	M-H	209.1547	0.0
	HMDB0038249	Isobornyl propionate	C13H22O2	M-H	209.1547	0.0
	HMDB0032052	alpha-Terpineol propanoate	C13H22O2	M-H	209.1547	0.0
	HMDB0037286	Citral propylene glycol acetal	C13H22O2	M-H	209.1547	0.0
	HMDB0178142	3-[(2Z)-but-2-en-1-yl]-2-(hydroxymethyl)-4,4-dimethylcyclohexan-1-one	C13H22O2	M-H	209.1547	0.0
	HMDB0037307	Propyl 2,4-decadienoate	C13H22O2	M-H	209.1547	0.0
	HMDB0038258	Neryl propionate	C13H22O2	M-H	209.1547	0.0
	HMDB0036139	Menthone 1,2-glyceryl ketal	C13H24O3	M-H20-H	209.1542	2.6
	HMDB0037212	Menthyl lactate	C13H24O3	M-H20-H	209.1542	2.6
	HMDB0035881	11-Hydroxy-9-tridecenoic acid	C13H24O3	M-H20-H	209.1542	2.6
	HMDB0040004	Menthone 1,3-glyceryl ketal	C13H24O3	M-H20-H	209.1542	2.6
210.0286	HMDB0062567	{[(carboxymethyl)(methyl)azaniumyl](iminiumyl)methyl}(phosphono)azanide	C4H11N3O5P	M-H	210.0285	0.3
	HMDB0001511	Phosphocreatine	C4H10N3O5P	M-H	210.0285	0.3
210.0886	HMDB0015078	Zalcitabine	C9H13N3O3	M-H	210.0884	0.9
	HMDB0240341	N-Acetyl-3-methylhistidine	C9H13N3O3	M-H	210.0884	0.9
	HMDB0240340	N-acetyl-1-methyl-L-histidine	C9H13N3O3	M-H	210.0884	0.9
	HMDB0041448	Dicyclohexyl disulfide	C12H22S2	M-H20-H	211.0979	0.0
	HMDB0059744	3,4-Methyleneazelaic acid	C11H16O4	M-H	211.0976	1.5
	HMDB0169511	2-(1-hydroxyethyl)-3,5-dimethoxy-6-methylphenol	C11H16O4	M-H	211.0976	1.5

211.0979	HMDB0153808	2-(3-hydroxy-3-methylbutyl)benzene-1,3,5-triol	C11H16O4	M-H	211.0976	1.5
	HMDB0179459	5-methyl-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0179460	NSC143559	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0163096	4,5-epoxy-(e,z)-2,7-decadienal	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0163098	(4Z,7Z)--hydroxydeca-2,4,7-trienal	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0163095	3-[(1Z,4Z)-hepta-1,4-dien-1-yl]oxirane-2-carbaldehyde	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0163097	(2E,4Z)-6-(3-ethyloxiran-2-yl)hexa-2,4-dienal	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0163094	(2E,7Z)-9-hydroxydeca-2,4,7-trienal	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0163093	SCHEMBL36924	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0180472	2-(4-methylphenyl)propane-1,2-diol	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0180474	p-Cymene-9,-diol	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0180473	2-[4-(hydroxymethyl)phenyl]propan-1-ol	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0181686	2-(hydroxymethyl)-3-methyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0181689	4-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0181688	1-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0181687	5-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0181685	3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptane-3-carbaldehyde	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0146631	3-(2-methoxyphenyl)propan-1-ol	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0041584	3-Hydroxy-p-mentha-1,8-dien-7-al	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0135742	3-(4-methoxyphenyl)propan-1-ol	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0127496	1-ethyl-3,5-dimethoxybenzene	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0062603	2-(4-methoxyphenyl)propan-2-ol	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0004586	Perillic acid	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0037044	Rotundifolone	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0040176	4-Ethyl-1,2-dimethoxybenzene	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0032462	Pentyl 2-furyl ketone	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0032615	1,1-Dimethoxy-2-phenylethane	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0036878	1,4-Epidioxy-p-mentha-2,8-diene	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0032135	2-Methoxy-4-propylphenol	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0036042	Marmelolactone A	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0034922	alpha-Teresantallic acid	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0039382	(1xi,4xi,6xi)-Carvone oxide	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0041000	Karahana lactone	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0032062	2-tert-Butyl-1,4-benzenediol	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0037011	5-Hydroxy-p-mentha-6,8-dien-2-one	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0031085	6-Pentyl-2H-pyran-2-one	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0029691	Wine lactone	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0036084	Isomintlactone	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0035235	2,4,7-Decatrienoic acid	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0036879	1,2:3,4-Diepoxy-p-menth-8-ene	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0035063	Epinepetalactone	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0035328	Perilla ketone	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0037012	2-Hydroxy-p-mentha-1,8-dien-6-one	C10H14O2	M+FA-H	211.0976	1.5
	HMDB0179461	2-methyl-5-(propan-2-yl)benzene-1,4-diol	C10H14O2	M+FA-H	211.0976	1.5
211.1338	HMDB0033546	2,5-Undecadienal	C11H18O	M+FA-H	211.1340	-0.8
	HMDB0036190	2-Heptylfuran	C11H18O	M+FA-H	211.1340	-0.8
	HMDB0031359	2,4-Undecadienal	C11H18O	M+FA-H	211.1340	-0.8
	HMDB0036815	Norecasantalol	C11H18O	M+FA-H	211.1340	-0.8
	HMDB0032540	2,6,6-Trimethyl-1-cyclohexen-1-acetaldehyde	C11H18O	M+FA-H	211.1340	-0.8
	HMDB0031565	Dihydrojasnone	C11H18O	M+FA-H	211.1340	-0.8
	HMDB0030252	Limonene aldehyde	C11H18O	M+FA-H	211.1340	-0.8
	HMDB0030002	(-)-Nopol	C11H18O	M+FA-H	211.1340	-0.8
	HMDB0031728	2-Hexylidenecyclopentanone	C11H18O	M+FA-H	211.1340	-0.8
	HMDB0035085	Vulgarole	C12H20O3	M-H	211.1340	-0.8
	HMDB0033601	Dihydrojasmonic acid	C12H20O3	M-H	211.1340	-0.8
	HMDB0037326	Traumatin	C12H20O3	M-H	211.1340	-0.8
	HMDB0041572	3-Ethenyl-4-hydroxy-2,5-dimethylhex-5-en-2-yl acetate	C12H20O3	M-H	211.1340	-0.8
	HMDB0029388	Cucurbitic acid	C12H20O3	M-H	211.1340	-0.8
	HMDB0030143	Talaromycin A	C12H22O4	M-H2O-H	211.1334	1.8
	HMDB0000623	Dodecanedioic acid	C12H22O4	M-H2O-H	211.1334	1.8

	HMDB0041614	Dipropyl hexanedioate	C12H22O4	M-H2O-H	211.1334	1.8
	HMDB0041613	Bis(1-methylethyl) hexanedioate	C12H22O4	M-H2O-H	211.1334	1.8
211.1702	HMDB0032537	trans-2-trans-4-Nonadiene	C12H22	M+FA-H	211.1704	-0.7
	HMDB0061817	1,1'-Ethylidenebis-cyclopentane	C12H22	M+FA-H	211.1704	-0.7
	HMDB0061818	(E,Z)-2,4-Dodecadiene	C12H22	M+FA-H	211.1704	-0.7
	HMDB0031028	Methyl (E)-2-dodecenoate	C13H24O2	M-H	211.1704	-0.7
	HMDB0037907	2,6,-Tetramethyl-1-oxaspiro[4.5]decan-6-ol	C13H24O2	M-H	211.1704	-0.7
	HMDB0040451	Oxacyclotetradecan-2-one	C13H24O2	M-H	211.1704	-0.7
	HMDB0037226	Citronellyl propionate	C13H24O2	M-H	211.1704	-0.7
	HMDB0034286	Ethyl -undecenoate	C13H24O2	M-H	211.1704	-0.7
	HMDB0039805	4-(3-Hydroxybutyl)-3,3,5-trimethylcyclohexanone	C13H24O2	M-H	211.1704	-0.7
	HMDB0037187	Rhodinyl propionate	C13H24O2	M-H	211.1704	-0.7
	HMDB0031741	Coniferan	C13H24O2	M-H	211.1704	-0.7
	HMDB0031017	-Undecenyl acetate	C13H24O2	M-H	211.1704	-0.7
	HMDB0037626	1-Ethylhexyl tiglate	C13H24O2	M-H	211.1704	-0.7
	HMDB0032792	(E)-3-Methyl-4-decen-1-yl acetate	C13H24O2	M-H	211.1704	-0.7
	HMDB0038078	1,1-Diethoxy-2,6-nonadiene	C13H24O2	M-H	211.1704	-0.7
	HMDB0036133	3-[[5-Methyl-2-(1-methylethyl)cyclohexyl]oxy]-1,2-propanediol	C13H26O3	M-H2O-H	211.1698	1.9
	HMDB0061655	3-hydroxytridecanoic acid	C13H26O3	M-H2O-H	211.1698	1.9
211.2063	HMDB0172397	1,14-Tetradecanediol	C14H30O2	M-H2O-H	211.2062	0.5
	HMDB0172396	1,13-tetradecandiol	C14H30O2	M-H2O-H	211.2062	0.5
	HMDB0038678	1,1-Dihexyloxyethane	C14H30O2	M-H2O-H	211.2062	0.5
	HMDB0032246	Dodecanal dimethyl acetal	C14H30O2	M-H2O-H	211.2062	0.5
	HMDB0034283	Tetradecanal	C14H28O	M-H	211.2067	-2.1
	HMDB0032432	12-Methyltridecanal	C14H28O	M-H	211.2067	-2.1
	HMDB0061955	(E)-9-Tetradecen-1-ol	C14H28O	M-H	211.2067	-2.1
	HMDB0030924	2-Tetradecanone	C14H28O	M-H	211.2067	-2.1
213.0773	HMDB0170506	(2E,4E)-2-(hydroxymethyl)-7-methylocta-2,4-dienedioic acid	C10H14O5	M-H	213.0768	2.1
	HMDB0170505	(2E,4E)-7-hydroxy-2,7-dimethylocta-2,4-dienedioic acid	C10H14O5	M-H	213.0768	2.1
	HMDB0170508	3-[(1E)-4-carboxy-4-methylbut-1-en-1-yl]-2-methyloxirane-2-carboxylic acid	C10H14O5	M-H	213.0768	2.1
	HMDB0159583	Fareanol	C10H14O5	M-H	213.0768	2.1
	HMDB0170509	(2E)-3-[3-(2-carboxy-2-methylethyl)oxiran-2-yl]-2-methylprop-2-enoic acid	C10H14O5	M-H	213.0768	2.1
	HMDB0170507	(2E,4E)-6-hydroxy-2,7-dimethylocta-2,4-dienedioic acid	C10H14O5	M-H	213.0768	2.1
	HMDB0170510	(2E,4E)-7-(hydroxymethyl)-2-methylocta-2,4-dienedioic acid	C10H14O5	M-H	213.0768	2.1
	HMDB0131223	3,5-dimethoxy-2-methylphenol	C9H12O3	M+FA-H	213.0768	2.1
	HMDB0125531	5-ethyl-3-methoxybenzene-1,2-diol	C9H12O3	M+FA-H	213.0768	2.1
	HMDB0125541	4-ethyl-2-methoxybenzene-1,3-diol	C9H12O3	M+FA-H	213.0768	2.1
	HMDB0126600	5-methoxy-2,4-dimethylbenzene-1,3-diol	C9H12O3	M+FA-H	213.0768	2.1
	HMDB0151518	SCHEMBL1954	C9H12O3	M+FA-H	213.0768	2.1
	HMDB0125521	4-ethyl-6-methoxybenzene-1,3-diol	C9H12O3	M+FA-H	213.0768	2.1
	HMDB0168685	2-(4-(Hydroxymethyl)phenoxy)ethanol	C9H12O3	M+FA-H	213.0768	2.1
	HMDB0059963	1,3,5-Trimethoxybenzene	C9H12O3	M+FA-H	213.0768	2.1
	HMDB0032252	Epoxyoxophorone	C9H12O3	M+FA-H	213.0768	2.1
	HMDB0030473	1-Ipomeanol	C9H12O3	M+FA-H	213.0768	2.1
	HMDB0038925	(4-Hydroxy-3-methoxyphenyl)ethanol	C9H12O3	M+FA-H	213.0768	2.1
	HMDB0030472	4-Ipomeanol	C9H12O3	M+FA-H	213.0768	2.1
	HMDB0029680	2,6-Dimethoxy-4-methylphenol	C9H12O3	M+FA-H	213.0768	2.1
	HMDB0032921	Ethyl 2-furanpropionate	C9H12O3	M+FA-H	213.0768	2.1
	HMDB0037729	2-Furanylmethyl butanoate	C9H12O3	M+FA-H	213.0768	2.1
	HMDB0030985	alpha-Carboxy-delta-decalactone	C11H18O4	M-H	213.1132	0.3
	HMDB0030984	5-Hexyltetrahydro-2-oxo-3-furancarboxylic acid	C11H18O4	M-H	213.1132	0.3
	HMDB0030986	2-Carboxy-5,7-dimethyl-4-octanolide	C11H18O4	M-H	213.1132	0.3
	HMDB0169534	geranic acid	C10H16O2	M+FA-H	213.1132	0.3
	HMDB0176281	6-hydroxycamphor	C10H16O2	M+FA-H	213.1132	0.3
	HMDB0182617	25435-53-4	C10H16O2	M+FA-H	213.1132	0.3
	HMDB0181693	3-(hydroxymethyl)-2,3-dimethyltricyclo[2.2.1,heptan-1-ol	C10H16O2	M+FA-H	213.1132	0.3

HMDB0181692	7-(hydroxymethyl)-1,7-dimethyltricyclo[2.2.1,heptan-3-ol	C10H16O2	M+FA-H	213.1132	0.3
HMDB0181691	[7-(hydroxymethyl)-7-methyltricyclo[2.2.1,heptan-1-yl]methanol	C10H16O2	M+FA-H	213.1132	0.3
HMDB0181690	[3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptan-3-yl]methanol	C10H16O2	M+FA-H	213.1132	0.3
HMDB0181638	2-methyl-5-(propan-2-yl)bicyclo[3.1]hex-3-ene-2,6-	C10H16O2	M+FA-H	213.1132	0.3
HMDB0181639	5-(1-hydroxypropan-2-yl)-2-methylbicyclo[3.1]hex-3-en-2-ol	C10H16O2	M+FA-H	213.1132	0.3
HMDB0181635	5-(2-hydroxypropan-2-yl)-2-methylbicyclo[3.1]hex-3-en-2-ol	C10H16O2	M+FA-H	213.1132	0.3
HMDB0181634	2-(hydroxymethyl)-5-(propan-2-yl)bicyclo[3.1]hex-3-en-2-ol	C10H16O2	M+FA-H	213.1132	0.3
HMDB0181636	5-methyl-1-(propan-2-yl)-3-oxatricyclo[4.1,heptan-5-ol	C10H16O2	M+FA-H	213.1132	0.3
HMDB0181637	2-methyl-5-(propan-2-yl)bicyclo[3.1]hex-3-ene-1,2-	C10H16O2	M+FA-H	213.1132	0.3
HMDB0182618	2-hydroxy-2-(2,2,3-trimethylcyclopent-3-en-1-yl)acetaldehyde	C10H16O2	M+FA-H	213.1132	0.3
HMDB0182621	SCHEMBL14359771	C10H16O2	M+FA-H	213.1132	0.3
HMDB0182619	2-[2-(hydroxymethyl)-2,3-dimethylcyclopent-3-en-1-yl]acetaldehyde	C10H16O2	M+FA-H	213.1132	0.3
HMDB0240639	(1S,4R,6R)-1,3,3-Trimethyl-6-hydroxybicyclo[2.2.1]heptane-2-one	C10H16O2	M+FA-H	213.1132	0.3
HMDB0182798	(1S,4R,6S)-1,3,3-Trimethyl-6-hydroxybicyclo[2.2.1]heptane-2-one	C10H16O2	M+FA-H	213.1132	0.3
HMDB0182796	3-(hydroxymethyl)-1,3-dimethylbicyclo[2.2.1]heptan-2-one	C10H16O2	M+FA-H	213.1132	0.3
HMDB0182797	7-hydroxy-1,3,3-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O2	M+FA-H	213.1132	0.3
HMDB0182799	5-hydroxy-1,3,3-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O2	M+FA-H	213.1132	0.3
HMDB0182685	6-Hydroxycarvotanacetone	C10H16O2	M+FA-H	213.1132	0.3
HMDB0182684	SCHEMBL6689811	C10H16O2	M+FA-H	213.1132	0.3
HMDB0182680	2-(hydroxymethyl)-5-(propan-2-yl)cyclohex-2-en-1-	C10H16O2	M+FA-H	213.1132	0.3
HMDB0182683	1-methyl-4-(propan-2-yl)-7-oxabicyclo[4.1]heptan-2-one	C10H16O2	M+FA-H	213.1132	0.3
HMDB0182620	2-[3-(hydroxymethyl)-2,2-dimethylcyclopent-3-en-1-yl]acetaldehyde	C10H16O2	M+FA-H	213.1132	0.3
HMDB0179485	14-64-6	C10H16O2	M+FA-H	213.1132	0.3
HMDB0179394	2E,4Z-decadienoic acid	C10H16O2	M+FA-H	213.1132	0.3
HMDB0136694	6-hydroxy-3,7-dimethylocta-2,7-dienal	C10H16O2	M+FA-H	213.1132	0.3
HMDB0182795	ACMC-mnpl	C10H16O2	M+FA-H	213.1132	0.3
HMDB0163100	(7Z)-9-hydroxydeca-4,7-dienal	C10H16O2	M+FA-H	213.1132	0.3
HMDB0163102	(4Z)-6-(3-ethyloxiran-2-yl)hex-4-enal	C10H16O2	M+FA-H	213.1132	0.3
HMDB0178761	SCHEMBL7756279	C10H16O2	M+FA-H	213.1132	0.3
HMDB0163117	(z,z)-4,7-decadienoic acid	C10H16O2	M+FA-H	213.1132	0.3
HMDB0163110	(2E,4Z)-6-(3-ethyloxiran-2-yl)hexa-2,4-dien-1-ol	C10H16O2	M+FA-H	213.1132	0.3
HMDB0163108	{3-[(1Z,4Z)-hepta-1,4-dien-1-yl]oxiran-2-yl}methanol	C10H16O2	M+FA-H	213.1132	0.3
HMDB0163109	(2E)-3-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}prop-2-en-1-ol	C10H16O2	M+FA-H	213.1132	0.3
HMDB0163104	(4Z,7Z)-2-hydroxydeca-4,7-dienal	C10H16O2	M+FA-H	213.1132	0.3
HMDB0163106	(4Z,7Z)-deca-2,4,7-triene-1,-diol	C10H16O2	M+FA-H	213.1132	0.3
HMDB0163103	(4Z,7Z)--hydroxydeca-4,7-dienal	C10H16O2	M+FA-H	213.1132	0.3
HMDB0163105	(2E,7Z)-deca-2,4,7-triene-1,9-diol	C10H16O2	M+FA-H	213.1132	0.3
HMDB0163101	3-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}propanal	C10H16O2	M+FA-H	213.1132	0.3
HMDB0163099	(4Z,7Z)-3-hydroxydeca-4,7-dienal	C10H16O2	M+FA-H	213.1132	0.3
HMDB0182682	4-hydroxy-2-methyl-5-(propan-2-yl)cyclohex-2-en-1-one	C10H16O2	M+FA-H	213.1132	0.3
HMDB0182681	8-Hydroxycarvotanacetone	C10H16O2	M+FA-H	213.1132	0.3
HMDB0034452	5,6-Dihydro-6-pentyl-2H-pyran-2-one	C10H16O2	M+FA-H	213.1132	0.3
HMDB0033700	(-)-(Z)-Tetrahydro-6-(2-pentenyl)-2H-pyran-2-one	C10H16O2	M+FA-H	213.1132	0.3
HMDB0031273	Methyl octynecarboxylate	C10H16O2	M+FA-H	213.1132	0.3
HMDB0031156	Ethyl (4Z)-4,7-octadienoate	C10H16O2	M+FA-H	213.1132	0.3
HMDB0035714	Epoxycarvotanacetone	C10H16O2	M+FA-H	213.1132	0.3
HMDB0040639	(xi)-(Z)-5-(3-Hexenyl)dihydro-2(3H)-furanone	C10H16O2	M+FA-H	213.1132	0.3
HMDB0037175	4-Isopropyl-3-cyclohexene-1-carboxylic acid	C10H16O2	M+FA-H	213.1132	0.3
HMDB0036067	Epoxycampholenic aldehyde	C10H16O2	M+FA-H	213.1132	0.3
HMDB0037821	xi-1,8,8-Trimethyl-2-oxabicyclo[3.2.1]octan-3-one	C10H16O2	M+FA-H	213.1132	0.3

	HMDB0036103	Geranic acid	C10H16O2	M+FA-H	213.1132	0.3
	HMDB0035766	Ascaridole	C10H16O2	M+FA-H	213.1132	0.3
	HMDB0032313	2,4-Hexadienyl isobutyrate	C10H16O2	M+FA-H	213.1132	0.3
	HMDB0032312	2,4-Hexadienyl butyrate	C10H16O2	M+FA-H	213.1132	0.3
	HMDB0032219	(+/-)-Dihydromintlactone	C10H16O2	M+FA-H	213.1132	0.3
	HMDB0032319	cis-3-Hexenyl crotonate	C10H16O2	M+FA-H	213.1132	0.3
	HMDB0032434	(+/-)-2-(5-Methyl-5-vinyltetrahydrofuran-2-yl)propionaldehyde	C10H16O2	M+FA-H	213.1132	0.3
	HMDB0035829	Dihydronepetalactone	C10H16O2	M+FA-H	213.1132	0.3
	HMDB0034670	6-Hydroxy-2,6-dimethyl-2,7-octadien-4-one	C10H16O2	M+FA-H	213.1132	0.3
	HMDB0037014	gamma-Diosphenol	C10H16O2	M+FA-H	213.1132	0.3
	HMDB0013105	trans-4,5-epoxy-2(E)-decenal	C10H16O2	M+FA-H	213.1132	0.3
213.1495	HMDB0163220	(2E,5Z)-2,5-undecadien-1-ol	C11H20O	M+FA-H	213.1496	-0.5
	HMDB0032238	(+/-)-trans- and cis-4,8-Dimethyl-3,7-nonadien-2-ol	C11H20O	M+FA-H	213.1496	-0.5
	HMDB0037807	9-Undecenal	C11H20O	M+FA-H	213.1496	-0.5
	HMDB0031128	-Undecenal	C11H20O	M+FA-H	213.1496	-0.5
	HMDB0033577	-Undecen-2-one	C11H20O	M+FA-H	213.1496	-0.5
	HMDB0035417	(1R,2R)-1,2,7,7-Tetramethylbicyclo[2.2.1]heptan-2-ol	C11H20O	M+FA-H	213.1496	-0.5
	HMDB0040247	2-Undecenal	C11H20O	M+FA-H	213.1496	-0.5
	HMDB0163219	(Z)-5-Undecenal	C11H20O	M+FA-H	213.1496	-0.5
	HMDB0061995	2-Methyl-3-decen-5-one	C11H20O	M+FA-H	213.1496	-0.5
	HMDB0159931	(5Z)-7-hydroxydodec-5-enoic acid	C12H22O3	M-H	213.1496	-0.6
	HMDB0159932	(5Z)-4-hydroxydodec-5-enoic acid	C12H22O3	M-H	213.1496	-0.6
	HMDB0159934	4-(3-hexyloxiran-2-yl)butanoic acid	C12H22O3	M-H	213.1496	-0.6
	HMDB0159935	SCHEMBL14224944	C12H22O3	M-H	213.1496	-0.6
	HMDB0159933	(5Z)-11-hydroxydodec-5-enoic acid	C12H22O3	M-H	213.1496	-0.6
	HMDB0159936	(5Z)-2-hydroxydodec-5-enoic acid	C12H22O3	M-H	213.1496	-0.6
	HMDB0037398	4-Acetoxy-2-hexyltetrahydrofuran	C12H22O3	M-H	213.1496	-0.6
	HMDB0010727	3-Oxododecanoic acid	C12H22O3	M-H	213.1496	-0.6
	HMDB0158298	3,11-dihydroxydodecanoic acid	C12H24O4	M-H2O-H	213.1491	2.0
	HMDB0158300	2,3-dihydroxydodecanoic acid	C12H24O4	M-H2O-H	213.1491	2.0
	HMDB0158299	3,12-dihydroxydodecanoic acid	C12H24O4	M-H2O-H	213.1491	2.0
213.1858	HMDB0061819	(E)-2-Dodecene	C12H24	M+FA-H	213.1860	-0.9
	HMDB0062120	N-Hexyleyclohexadiene	C12H24	M+FA-H	213.1860	-0.9
	HMDB0061821	(E)-3-Dodecene	C12H24	M+FA-H	213.1860	-0.9
	HMDB0061820	(Z)-3-Dodecene	C12H24	M+FA-H	213.1860	-0.9
	HMDB0059874	1-Dodecene	C12H24	M+FA-H	213.1860	-0.9
	HMDB0032236	(+/-)-N,N-Dimethyl menthyl succinamide	C12H24	M+FA-H	213.1860	-0.9
	HMDB0062786	4,6,8-trimethyl-1-nonene	C12H24	M+FA-H	213.1860	-0.9
	HMDB0094667	(2Z)-3-methylundec-2-ene	C12H24	M+FA-H	213.1860	-0.9
	HMDB0094665	(3E)-2,2,4,4,6,6-pentamethylhept-3-ene	C12H24	M+FA-H	213.1860	-0.9
	HMDB0094666	nonylcyclopropane	C12H24	M+FA-H	213.1860	-0.9
	HMDB0171028	12-hydroxy-2-tridecanone	C13H26O2	M-H	213.1860	-1.0
	HMDB0171029	13-hydroxytridecan-2-one	C13H26O2	M-H	213.1860	-1.0
	HMDB0171031	SCHEMBL1782851	C13H26O2	M-H	213.1860	-1.0
	HMDB0171030	2-Tridecanone, 1-hydroxy-	C13H26O2	M-H	213.1860	-1.0
	HMDB0059900	Propyl decanoate	C13H26O2	M-H	213.1860	-1.0
	HMDB0032211	Decanal propyleneglycol acetal	C13H26O2	M-H	213.1860	-1.0
	HMDB0031018	Methyl dodecanoate	C13H26O2	M-H	213.1860	-1.0
	HMDB0037311	Decyl propionate	C13H26O2	M-H	213.1860	-1.0
	HMDB0034140	Octyl 3-methylbutanoate	C13H26O2	M-H	213.1860	-1.0
	HMDB0029552	Ethyl undecanoate	C13H26O2	M-H	213.1860	-1.0
	HMDB0038729	3-Methylbutyl octanoate	C13H26O2	M-H	213.1860	-1.0
	HMDB0036217	Pentyl octanoate	C13H26O2	M-H	213.1860	-1.0
	HMDB0061828	9-Methyldodecanoic acid	C13H26O2	M-H	213.1860	-1.0
	HMDB0036219	Octyl 2-methylbutyrate	C13H26O2	M-H	213.1860	-1.0
	HMDB0061829	Isopropyl dodecanoic acid	C13H26O2	M-H	213.1860	-1.0
	HMDB0000910	Tridecanoic acid	C13H26O2	M-H	213.1860	-1.0
	HMDB0059660	sn-glycero-3-Phosphoethanolamine	C5H14NO6P	M-H	214.0486	0.5
	HMDB0000114	Glycerylphosphorylethanolamine	C5H14NO6P	M-H	214.0486	0.5
	HMDB0060244	Phosphodimethylethanolamine	C4H12NO4P	M+FA-H	214.0486	0.5

214.0487	HMDB0162023	7-(hydroxymethyl)-5H,6H,7H-cyclopenta[c]pyridine-4-carboxylic acid	C10H11NO3	M+Na-2H	214.0486	0.7
	HMDB0162022	5-hydroxy-7-methyl-5H,6H,7H-cyclopenta[c]pyridine-4-carboxylic acid	C10H11NO3	M+Na-2H	214.0486	0.7
	HMDB0162020	7-hydroxy-7-methyl-5H,6H,7H-cyclopenta[c]pyridine-4-carboxylic acid	C10H11NO3	M+Na-2H	214.0486	0.7
	HMDB0000859	Methyl hippurate	C10H11NO3	M+Na-2H	214.0486	0.7
	HMDB0011723	2-Methylhippuric acid	C10H11NO3	M+Na-2H	214.0486	0.7
	HMDB0060366	3-Carbamoyl-2-phenylpropionaldehyde	C10H11NO3	M+Na-2H	214.0486	0.7
	HMDB0060389	4-Hydroxy-5-phenyltetrahydro-1,3-oxazin-2-one	C10H11NO3	M+Na-2H	214.0486	0.7
	HMDB0034250	Betamipron	C10H11NO3	M+Na-2H	214.0486	0.7
	HMDB0032388	Methyl n-acetylanthranilate	C10H11NO3	M+Na-2H	214.0486	0.7
	HMDB0013245	m-Methylhippuric acid	C10H11NO3	M+Na-2H	214.0486	0.7
	HMDB0013292	p-Methylhippuric acid	C10H11NO3	M+Na-2H	214.0486	0.7
	HMDB0060758	4-Anilino-4-oxobutanoic acid	C10H11NO3	M+Na-2H	214.0486	0.7
	HMDB0240317	N-formyl-L-phenylalanine	C10H11NO3	M+Na-2H	214.0486	0.7
	HMDB0000821	Phenylacetyl glycine	C10H11NO3	M+Na-2H	214.0486	0.7
214.0835	HMDB0000001	1-Methylhistidine	C7H11N3O2	M+FA-H	214.0833	0.8
	HMDB0000479	3-Methylhistidine	C7H11N3O2	M+FA-H	214.0833	0.8
	HMDB0155761	3-Methylhistidine	C7H11N3O2	M+FA-H	214.0833	0.8
215.0330	HMDB0146403	SCHEMBL2535852	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0146630	3-(2-methoxyphenyl)oxirane-2-carboxylic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0146628	ZINC2222827	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0146629	CTK4057	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0154365	3-(3-hydroxy-2-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0166608	3-(6-hydroxy-2H-1,3-benzodioxol-5-yl)propanal	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0166607	3-(2H-1,3-benzodioxol-5-yl)-3-hydroxypropanal	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0166611	3-(2H-1,3-benzodioxol-5-yl)-2-hydroxypropanal	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0166609	2815-95-4	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0166614	[3-(2H-1,3-benzodioxol-5-yl)oxiran-2-yl]methanol	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0166613	6-[(1Z)-3-hydroxyprop-1-en-1-yl]-2H-1,3-benzodioxol-5-ol	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0178262	(2Z)-3-(3-hydroxy-5-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0142175	2-benzylpropanedioic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0141265	3-(3-methoxyphenyl)-2-oxopropanoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0141263	(2Z)-2-hydroxy-3-(3-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0131173	3-(4-methoxyphenyl)oxirane-2-carboxylic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0125096	3-(4-hydroxy-3-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0125524	(2E)-3-(3-hydroxy-5-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0125588	3-(3-hydroxy-5-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0127500	3-(4-methoxyphenyl)-2-oxopropanoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0131137	3-(3-hydroxy-4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0131172	(2E)-3-(2-hydroxy-4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0131171	(2Z)-2-hydroxy-3-(4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0137510	3-(4-hydroxy-2-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0140957	(2E)-3-(3-hydroxy-2-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0000954	Ferulic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0135741	3-(2-hydroxy-4-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0000955	Isoferulic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0002120	Monoethyl phthalate	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0030765	(-)-trans-3,4-Dihydro-4,8-dihydroxy-3-methyl-1H-2-benzopyran-1-one	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0039606	Repandiol	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0032652	Meconine	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0037644	3-(2-Hydroxy-3-methoxyphenyl)-2-propenoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0029663	Vanillin acetate	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0032614	Piperonyl acetate	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0165533	Ferulic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0240705	Ferulic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0059721	mono-Benzyl malonate	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0061686	2,5-Dihydroxycinnamic acid methyl ester	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0134088	3-(2-hydroxy-3-methoxyphenyl)prop-2-enoic acid	C10H10O4	M+Na-2H	215.0326	2.0
	HMDB0132906	3,5-dimethoxybenzene-1,2-diol	C8H10O4	M+FA-H	215.0561	1.8
	HMDB0133971	3,4-dimethoxybenzene-1,2-diol	C8H10O4	M+FA-H	215.0561	1.8
	HMDB0133972	2,3-dimethoxybenzene-1,4-diol	C8H10O4	M+FA-H	215.0561	1.8

215.0565	HMDB0133982	4,5-dimethoxybenzene-1,3-diol	C8H10O4	M+FA-H	215.0561	1.8
	HMDB0153684	2-(hydroxymethyl)-5-methoxybenzene-1,3-diol	C8H10O4	M+FA-H	215.0561	1.8
	HMDB0173106	2,5-dimethoxycyclohex-2-ene-1,4-dione	C8H10O4	M+FA-H	215.0561	1.8
	HMDB0179996	SCHEMBL285344	C8H10O4	M+FA-H	215.0561	1.8
	HMDB0000318	3,4-Dihydroxyphenylglycol	C8H10O4	M+FA-H	215.0561	1.8
	HMDB0132907	2,6-dimethoxybenzene-1,4-diol	C8H10O4	M+FA-H	215.0561	1.8
	HMDB0059756	3,4-Methyleneadipic acid	C8H10O4	M+FA-H	215.0561	1.8
	HMDB0038760	Herierin III	C8H10O4	M+FA-H	215.0561	1.8
	HMDB0038761	Herierin IV	C8H10O4	M+FA-H	215.0561	1.8
	HMDB0032966	Furaneol acetate	C8H10O4	M+FA-H	215.0561	1.8
	HMDB0153685	6-methoxy-3-methylbenzene-1,2,4-triol	C8H10O4	M+FA-H	215.0561	1.8
215.0925	HMDB0182564	2-(1-carboxyethyl)-3-hydroxy-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0160551	(4Z)-2-hydroxydec-4-enedioic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0160549	(4Z)-3-hydroxydec-4-enedioic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0160547	(4Z)-8-hydroxydec-4-enedioic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0160548	(4Z)-6-hydroxydec-4-enedioic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0160550	5-[3-(2-carboxyethyl)oxiran-2-yl]pentanoic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0175344	1-Hydroxymethyl-2,2-dimethyl-cyclopentane-1,3-dicarboxylic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0160546	(4Z)-7-hydroxydec-4-enedioic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0160552	(4Z)-9-hydroxydec-4-enedioic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0182565	2-(1-carboxy-2-hydroxyethyl)-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0170511	(4E)-2-hydroxy-2,7-dimethyloct-4-enedioic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0182566	2-(1-carboxyethyl)-1-hydroxy-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0182562	2-(1-carboxy-1-hydroxyethyl)-5-methylcyclopentane-1-carboxylic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0182561	5-(1-carboxyethyl)-2-hydroxy-2-methylcyclopentane-1-carboxylic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0182563	5-(1-carboxyethyl)-3-hydroxy-2-methylcyclopentane-1-carboxylic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0182560	2-(1-carboxyethyl)-5-(hydroxymethyl)cyclopentane-1-carboxylic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0175348	SCHEMBL1335666	C10H16O5	M-H	215.0925	0.0
	HMDB0175346	5-hydroxy-1,2,2-trimethylcyclopentane-1,3-dicarboxylic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0175347	4-hydroxy-1,2,2-trimethylcyclopentane-1,3-dicarboxylic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0175345	2-(hydroxymethyl)-1,2-dimethylcyclopentane-1,3-dicarboxylic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0170513	3-[3-(2-carboxy-2-methylethyl)oxiran-2-yl]-2-methylpropanoic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0170514	(4E)-2-(hydroxymethyl)-7-methyloct-4-enedioic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0170512	(4E)-3-hydroxy-2,7-dimethyloct-4-enedioic acid	C10H16O5	M-H	215.0925	0.0
	HMDB0164924	7-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M+FA-H	215.0925	0.0
	HMDB0164923	3-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M+FA-H	215.0925	0.0
	HMDB0164925	6-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M+FA-H	215.0925	0.0
	HMDB0167051	(2E,6Z)-4-hydroxynona-2,6-dienoic acid	C9H14O3	M+FA-H	215.0925	0.0
	HMDB0167052	(2E,6Z)-8-hydroxynona-2,6-dienoic acid	C9H14O3	M+FA-H	215.0925	0.0
	HMDB0167053	(2E,6Z)-5-hydroxynona-2,6-dienoic acid	C9H14O3	M+FA-H	215.0925	0.0
	HMDB0167056	(2E,6Z)-9-hydroxynona-2,6-dienoic acid	C9H14O3	M+FA-H	215.0925	0.0
	HMDB0038276	cis-3-Hexenyl pyruvate	C9H14O3	M+FA-H	215.0925	0.0
	HMDB0167054	3-[(3Z)-hex-3-en-1-yl]oxirane-2-carboxylic acid	C9H14O3	M+FA-H	215.0925	0.0
	HMDB0030471	1,4-Ipomeadiol	C9H14O3	M+FA-H	215.0925	0.0
	HMDB0167055	(2E)-5-(3-ethyloxiran-2-yl)pent-2-enoic acid	C9H14O3	M+FA-H	215.0925	0.0
	HMDB0164926	5-hydroxy-1-(hydroxymethyl)-3-methylbicyclo[2.2.1]heptan-2-one	C9H14O3	M+FA-H	215.0925	0.0
	HMDB0164922	1,3-bis(hydroxymethyl)bicyclo[2.2.1]heptan-2-one	C9H14O3	M+FA-H	215.0925	0.0
	HMDB0169421	2-ethenyl-4,6-diethyl-1,3,5-trioxane	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0163469	(2Z)-4-hydroxy-2-methyloct-2-enoic acid	C9H16O3	M+FA-H	217.1081	-1.1

217.1079	HMDB0163470	2-methyl-3-pentylloxirane-2-carboxylic acid	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0163468	SCHEMBL7173369	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0163465	(2Z)-7-hydroxy-2-methyloct-2-enoic acid	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0163466	(2Z)-8-hydroxy-2-methyloct-2-enoic acid	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0094711	9-oxononanoic acid	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0179168	3-caproyl propionic acid	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0060287	4-Hydroperoxy-2-nonenal	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0036188	Tetrahydrofurfuryl butyrate	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0040203	2-Methylpropyl 3-hydroxy-2-methylidenebutanoate	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0040202	Butyl 3-hydroxy-2-methylidenebutanoate	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0059937	6-Pentyl-1,4-dioxan-2-one	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0059936	5-Pentyl-1,4-dioxan-2-one	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0062081	9-oxononanoate	C9H15O3	M+FA-H	217.1081	-1.1
	HMDB0036396	3-Methylbutyl 3-oxobutanoate	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0040165	Butyl levulinate	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0036213	cis-3-Hexenyl lactate	C9H16O3	M+FA-H	217.1081	-1.1
	HMDB0000350	3-Hydroxysebacic acid	C10H18O5	M-H	217.1081	-1.1
	HMDB0000424	2-Hydroxydecanedioic acid	C10H18O5	M-H	217.1081	-1.1
	HMDB0029189	5-Hydroxysebacate	C10H18O5	M-H	217.1081	-1.1
	HMDB0182057	5-{2,3-dimethyltricyclo[2.2.1,]heptan-3-yl}-2-methylpent-2-en-1-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0182061	3-(2-{2,3-dimethyltricyclo[2.2.1,]heptan-3-yl}ethyl)-2,2-dimethyloxirane	C15H24O	M-H	219.1754	-1.1
	HMDB0182873	[1-methylidene-7-(prop-1-en-2-yl)-decahydronaphthalen-4a-yl]methanol	C15H24O	M-H	219.1754	-1.1
	HMDB0182151	1-(6-methylhept-5-en-2-yl)-4-methylidenebicyclo[3.1]hexan-2-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0182152	2,2-dimethyl-3-(3-{4-methylidenebicyclo[3.1]hexan-1-yl}butyl)oxirane	C15H24O	M-H	219.1754	-1.1
	HMDB0182155	6-methyl-2-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-5-en-1-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0182153	5-(6-methylhept-5-en-2-yl)-2-methylidenebicyclo[3.1]hexan-1-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0182154	1-(6-methylhept-5-en-2-yl)-4-methylidenebicyclo[3.1]hexan-6-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0182874	4a-methyl-8-methylidene-2-(prop-1-en-2-yl)-decahydronaphthalen-2-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0182875	2-(4a-methyl-8-methylidene-decahydronaphthalen-2-yl)-2-methyloxirane	C15H24O	M-H	219.1754	-1.1
	HMDB0182149	2-methyl-6-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-2-en-1-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0182150	2-methyl-6-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-2-en-4-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0134152	2-benzyl-octan-1-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0182055	[2-methyl-3-(4-methylpent-3-en-1-yl)tricyclo[2.2.1,heptan-3-yl]methanol	C15H24O	M-H	219.1754	-1.1
	HMDB0182054	[7-methyl-7-(4-methylpent-3-en-1-yl)tricyclo[2.2.1,heptan-1-yl]methanol	C15H24O	M-H	219.1754	-1.1
	HMDB0182056	1-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-4-methylpent-3-en-1-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0182058	.alpha.-Santalol	C15H24O	M-H	219.1754	-1.1
	HMDB0182059	1-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-4-methylpent-3-en-2-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0182060	1,7-dimethyl-7-(4-methylpent-3-en-1-yl)tricyclo[2.2.1,heptan-3-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0182062	santal--en-2-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0182147	6-methyl-2-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-5-en-2-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0182148	1-(6-methylhept-5-en-2-yl)-4-methylidenebicyclo[3.1]hexan-3-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0036420	spathulenol	C15H24O	M-H	219.1754	-1.1
	HMDB0060356	2-trans,6-trans-Farnesal	C15H24O	M-H	219.1754	-1.1
	HMDB0037392	4(15)-Copaen-11-ol	C15H24O	M-H	219.1754	-1.1
	HMDB0038982	4-Nonylphenol	C15H24O	M-H	219.1754	-1.1
	HMDB0038119	Eremofukinone	C15H24O	M-H	219.1754	-1.1

HMDB0034718	Isospathulenol	C15H24O	M-H	219.1754	-1.1
HMDB0034661	alpha-Valerenol	C15H24O	M-H	219.1754	-1.1
HMDB0032220	Dihydronootkatone	C15H24O	M-H	219.1754	-1.1
HMDB0038210	Humulene epoxide II	C15H24O	M-H	219.1754	-1.1
HMDB0035391	Preisocalamendiol	C15H24O	M-H	219.1754	-1.1
HMDB0038512	Bisacurool	C15H24O	M-H	219.1754	-1.1
HMDB0038211	Humulenol I	C15H24O	M-H	219.1754	-1.1
HMDB0036192	Apritone	C15H24O	M-H	219.1754	-1.1
HMDB0035739	(R)-2,7(14),9-Bisabolatrien-11-ol	C15H24O	M-H	219.1754	-1.1
HMDB0038212	Humulenol II	C15H24O	M-H	219.1754	-1.1
HMDB0035793	Fukinone	C15H24O	M-H	219.1754	-1.1
HMDB0035026	alpha-Cyperol	C15H24O	M-H	219.1754	-1.1
HMDB0037069	Acoragermacrone	C15H24O	M-H	219.1754	-1.1
HMDB0035704	Acorenone	C15H24O	M-H	219.1754	-1.1
HMDB0038146	Calacone	C15H24O	M-H	219.1754	-1.1
HMDB0036402	alpha-Bergamotenol	C15H24O	M-H	219.1754	-1.1
HMDB0036798	8alpha-3-Copaen-8-ol	C15H24O	M-H	219.1754	-1.1
HMDB0036716	beta-Santalol	C15H24O	M-H	219.1754	-1.1
HMDB0060295	3,7,7,-tetramethyl-2-oxatetracyclo[7.3.7]dodecane	C15H24O	M-H	219.1754	-1.1
HMDB0059836	Cabreuva oxide D	C15H24O	M-H	219.1754	-1.1
HMDB0013688	Nootkatol	C15H24O	M-H	219.1754	-1.1
HMDB0037811	Vetiverol	C15H24O	M-H	219.1754	-1.1
HMDB0038160	7(14)-Isodaucen--one	C15H24O	M-H	219.1754	-1.1
HMDB0034940	Mammea E/BB	C15H24O	M-H	219.1754	-1.1
HMDB0036793	3,15-Epoxy-6-caryophyllene	C15H24O	M-H	219.1754	-1.1
HMDB0038134	Bisabolene oxide	C15H24O	M-H	219.1754	-1.1
HMDB0039532	(6Z,9Z,12Z)-6,9,12-Pentadecatrien-2-one	C15H24O	M-H	219.1754	-1.1
HMDB0035718	Isocyperol	C15H24O	M-H	219.1754	-1.1
HMDB0035306	Epishyobunone	C15H24O	M-H	219.1754	-1.1
HMDB0036118	(3S,6E)-6-Caryophyllen-15-al	C15H24O	M-H	219.1754	-1.1
HMDB0033826	2,6-Di-tert-butyl-4-methylphenol	C15H24O	M-H	219.1754	-1.1
HMDB0030232	(2R,6S,7S,Z)-beta-Santala-3(15),-dien-12-ol	C15H24O	M-H	219.1754	-1.1
HMDB0035097	beta-Costol	C15H24O	M-H	219.1754	-1.1
HMDB0036789	Caryophyllene alpha-oxide	C15H24O	M-H	219.1754	-1.1
HMDB0040763	Neoacrimarine E	C15H24O	M-H	219.1754	-1.1
HMDB0038123	1,5-Epoxy-4(14)-salvialene	C15H24O	M-H	219.1754	-1.1
HMDB0038193	Isoshyobunone	C15H24O	M-H	219.1754	-1.1
HMDB0037395	11-Copaen-4-ol	C15H24O	M-H	219.1754	-1.1
HMDB0035645	Epoxyguaiene	C15H24O	M-H	219.1754	-1.1
HMDB0035020	Acolamone	C15H24O	M-H	219.1754	-1.1
HMDB0036717	trans-beta-Santalol	C15H24O	M-H	219.1754	-1.1
HMDB0039711	Aromadendrene epoxide	C15H24O	M-H	219.1754	-1.1
HMDB0036788	beta-Betulenol	C15H24O	M-H	219.1754	-1.1
HMDB0035720	Isoacolamone	C15H24O	M-H	219.1754	-1.1
HMDB0038208	Humuladienone	C15H24O	M-H	219.1754	-1.1
HMDB0182219	7-(2-hydroxypropan-2-yl)-1,8a-dimethyl-1,2,3,5,6,7,8,8a-octahydronaphthalen-1-ol	C15H26O2	M-H20-H	219.1749	1.4
HMDB0182221	6-(2-hydroxypropan-2-yl)-4,4a-dimethyl-2,3,4,4a,5,6,7,8-octahydronaphthalen-2-ol	C15H26O2	M-H20-H	219.1749	1.4
HMDB0182217	2-[8a-(hydroxymethyl)-8-methyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl]propan-2-ol	C15H26O2	M-H20-H	219.1749	1.4
HMDB0182218	2-[8-(hydroxymethyl)-8a-methyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl]propan-2-ol	C15H26O2	M-H20-H	219.1749	1.4
HMDB0182220	3-(2-hydroxypropan-2-yl)-4a,5-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalen-1-ol	C15H26O2	M-H20-H	219.1749	1.4
HMDB0036032	3beta-7-Drimene-3,11-diol	C15H26O2	M-H20-H	219.1749	1.4
HMDB0031384	beta-Kessyl alcohol	C15H26O2	M-H20-H	219.1749	1.4
HMDB0182767	2-(1-hydroxypropan-2-yl)-4a-methyl-8-methylidene-decahydronaphthalen-1-ol	C15H26O2	M-H20-H	219.1749	1.4
HMDB0182764	4a-(hydroxymethyl)-8-methylidene-2-(propan-2-yl)-decahydronaphthalen-1-ol	C15H26O2	M-H20-H	219.1749	1.4
HMDB0035887	Germacrenone	C15H26O2	M-H20-H	219.1749	1.4
HMDB0039130	Methyl (Z,Z)-5,8-tetradecadienoate	C15H26O2	M-H20-H	219.1749	1.4
HMDB0038247	Bornyl valerate	C15H26O2	M-H20-H	219.1749	1.4
HMDB0062130	methyl tetradec-13-ynoate	C15H26O2	M-H20-H	219.1749	1.4

HMDB0041589	alpha-Kessyl alcohol	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0030428	Linalyl isovalerate	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0038138	alpha-Bisabolol oxide C	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0036730	Tricyclohumuladiol	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0038136	Curcumiadiol	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0038196	alpha-Bisabolol oxide A	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0040273	Terpenyl isovalerate	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0037195	2-Propenyl cyclohexanecarboxylate	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0040281	Geranyl valerate	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0029350	Geranyl 3-methylbutanoate	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0038197	alpha-Bisabolol oxide B	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0032054	alpha-Terpinyl pentanoate	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0038248	Bornyl isovalerate	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0037284	5(1->)-Abeo-1,12-patchoulanediol	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0032343	Isobornyl 2-methylbutyrate	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0031383	(3S,4S,6R,7S)-1,8-Bisaboladiene-3,4-diol	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0038250	Isobornyl isovalerate	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0033228	Guaidiol	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0032209	Citronellyl trans-2-methyl-2-butenate	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0034673	Calamendiol	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0035287	Daucol	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0036880	1,6,9-Farnesatriene-3,11-diol	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0179265	2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0032291	Geranyl 2-methylbutyrate	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0037279	2,8-Bisaboladiene-1,4-diol	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0182765	2-(2-hydroxypropan-2-yl)-4a-methyl-8-methylidene-decahydronaphthalen-1-ol	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0182766	4a-methyl-8-methylidene-2-(propan-2-yl)-decahydronaphthalene-1,7-diol	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0182222	2-(8,8a-dimethyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl)propane-1,2-diol	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0039745	(2E,6E,9xi)-Farnesol	C15H26O2	M-H2O-H	219.1749	1.4
HMDB0126379	2,2-dimethyl-2H-chromen-5-ol	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0126467	2-[(1E)-3-methylbuta-1,3-dien-1-yl]benzene-1,3-diol	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0132973	(1E)-1-(4-hydroxyphenyl)pent-1-en-3-one	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0133466	4-(3-methoxyphenyl)but-3-en-2-one	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0133679	4-(3-hydroxyphenyl)-3-methylbut-3-en-2-one	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0133678	3-(hydroxymethyl)-4-phenylbut-3-en-2-one	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0133677	1-hydroxy-3-methyl-4-phenylbut-3-en-2-one	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0132267	5-benzylloxolan-2-one	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0133681	1-(2-methyl-3-phenyloxiran-2-yl)ethan-1-one	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0036905	2-Propenyl phenylacetate	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0037145	3-(4-Methoxyphenyl)-2-methyl-2-propenal	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0029699	Cinnamyl acetate	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0163608	alpha-Isopropenylbenzeneacetic acid	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0033834	Ethyl cinnamate	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0037142	2-(Phenylethenyl)-1,3-dioxolane	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0133680	4-(4-hydroxyphenyl)-3-methylbut-3-en-2-one	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0151237	119711-59	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0151231	2-(4-methoxybenzyl)acrylaldehyde	C11H12O2	M+FA-H	221.0819	-1.0
HMDB0164058	4-(1-hydroxy-3-oxobutyl)phenyl acetate	C12H14O4	M-H	221.0819	-1.1
HMDB0170979	2-methoxy-4-[(1Z)-prop-1-en-1-yl]phenyl 2-hydroxyacetate	C12H14O4	M-H	221.0819	-1.1
HMDB0135904	3-[(3,3-dimethyloxiran-2-yl)methyl]-4-hydroxybenzoic acid	C12H14O4	M-H	221.0819	-1.1
HMDB0135906	3,4-dihydroxy-5-(3-methylbut-2-en-1-yl)benzoic acid	C12H14O4	M-H	221.0819	-1.1
HMDB0170977	5-hydroxy-2-methoxy-4-[(1Z)-prop-1-en-1-yl]phenyl acetate	C12H14O4	M-H	221.0819	-1.1
HMDB0170978	1-acetoxy-2-methoxy-4-(3-methyl-oxiranyl)-benzene	C12H14O4	M-H	221.0819	-1.1
HMDB0164055	4-(3-oxobutyl)phenyl 2-hydroxyacetate	C12H14O4	M-H	221.0819	-1.1
HMDB0127824	5-[(3-hydroxy-4-methoxyphenyl)methyl]oxolan-2-one	C12H14O4	M-H	221.0819	-1.1
HMDB0131281	2-Hydroxy-3-(4-methoxyphenyl)propenoic acid ethyl ester	C12H14O4	M-H	221.0819	-1.1

221.0817

HMDB0131283	ethyl (2E)-3-(2-hydroxy-4-methoxyphenyl)prop-2-enoate	C12H14O4	M-H	221.0819	-1.1
HMDB0131285	2-hydroxyethyl (2E)-3-(4-methoxyphenyl)prop-2-enoate	C12H14O4	M-H	221.0819	-1.1
HMDB0131284	ethyl 3-(4-methoxyphenyl)oxirane-2-carboxylate	C12H14O4	M-H	221.0819	-1.1
HMDB0135902	4-hydroxy-3-(4-hydroxy-3-methylbut-2-en-1-yl)benzoic acid	C12H14O4	M-H	221.0819	-1.1
HMDB0164056	4-(2-hydroxy-3-oxobutyl)phenyl acetate	C12H14O4	M-H	221.0819	-1.1
HMDB0170976	3-hydroxy-2-methoxy-4-[(1Z)-prop-1-en-1-yl]phenyl acetate	C12H14O4	M-H	221.0819	-1.1
HMDB0170974	4-[(1Z)-3-hydroxyprop-1-en-1-yl]-2-methoxyphenyl acetate	C12H14O4	M-H	221.0819	-1.1
HMDB0135689	4-(4-hydroxy-3,5-dimethoxyphenyl)but-3-en-2-one	C12H14O4	M-H	221.0819	-1.1
HMDB0170845	2-methoxy-4-[(oxiran-2-yl)methyl]phenyl acetate	C12H14O4	M-H	221.0819	-1.1
HMDB0170846	2-methoxy-4-(prop-2-en-1-yl)phenyl 2-hydroxyacetate	C12H14O4	M-H	221.0819	-1.1
HMDB0164057	4-(4-hydroxy-3-oxobutyl)phenyl acetate	C12H14O4	M-H	221.0819	-1.1
HMDB0135900	4-hydroxy-3-(4-hydroxy-3-methylbut-2-en-1-yl)benzoic acid	C12H14O4	M-H	221.0819	-1.1
HMDB0002056	Monoisobutyl phthalic acid	C12H14O4	M-H	221.0819	-1.1
HMDB0030725	Dillapiol	C12H14O4	M-H	221.0819	-1.1
HMDB0037130	Piperonyl isobutyrate	C12H14O4	M-H	221.0819	-1.1
HMDB0029470	Isodillapiole	C12H14O4	M-H	221.0819	-1.1
HMDB0037681	Vanillin isobutyrate	C12H14O4	M-H	221.0819	-1.1
HMDB0034056	5-(3,4-Methylenedioxyphenyl)pentanoic acid	C12H14O4	M-H	221.0819	-1.1
HMDB0031668	Dihydrodeoxy-8-epiaustdiol	C12H14O4	M-H	221.0819	-1.1
HMDB0033776	Apiole	C12H14O4	M-H	221.0819	-1.1
HMDB0041379	2,3-Dihydro-3-hydroxy-6-methoxy-2,2-dimethyl-4H-1-benzopyran-4-one	C12H14O4	M-H	221.0819	-1.1
HMDB0029226	5'-(3'-Methoxy-4'-hydroxyphenyl)-gamma-valerolactone	C12H14O4	M-H	221.0819	-1.1
HMDB0094660	Diethyl phthalic acid	C12H14O4	M-H	221.0819	-1.1
HMDB0038563	(Z)-3-(2,4,5-Trimethoxyphenyl)-2-propenal	C12H14O4	M-H	221.0819	-1.1
HMDB0013247	Monobutylphthalate	C12H14O4	M-H	221.0819	-1.1
HMDB0137288	3-(4,7-Dimethoxy-1,3-benzodioxol-5-yl)-1-propanol	C12H16O5	M-H2O-H	221.0814	1.4
HMDB0142074	3-(2,3,4-trimethoxyphenyl)propanoic acid	C12H16O5	M-H2O-H	221.0814	1.4
HMDB0061112	3-Carboxy-4-methyl-5-propyl-2-furanpropionic acid	C12H16O5	M-H2O-H	221.0814	1.4
HMDB0062776	3-Carboxy-4-methyl-5-propyl-2-furanpropionic acid	C12H16O5	M-H2O-H	221.0814	1.4
HMDB0038627	Ethyl 3,4,5-trimethoxybenzoate	C12H16O5	M-H2O-H	221.0814	1.4
HMDB0030254	3-(3,4,5-Trimethoxyphenyl)propanoic acid	C12H16O5	M-H2O-H	221.0814	1.4
HMDB0041756	Isopropyl 3-(3,4-dihydroxyphenyl)-2-hydroxypropanoate	C12H16O5	M-H2O-H	221.0814	1.4
HMDB0125802	7-methoxy-2,2-dimethyl-3,4-dihydro-2H-1-benzopyran-4,5,6-triol	C12H16O5	M-H2O-H	221.0814	1.4
HMDB0125804	2-(hydroxymethyl)-7-methoxy-2-methyl-3,4-dihydro-2H-1-benzopyran-4,5-diol	C12H16O5	M-H2O-H	221.0814	1.4
HMDB0128705	3-(4-hydroxy-2,3,5-trimethoxyphenyl)propanal	C12H16O5	M-H2O-H	221.0814	1.4
HMDB0128721	4-(3-hydroxyprop-1-en-1-yl)-2,3,6-trimethoxyphenol	C12H16O5	M-H2O-H	221.0814	1.4
HMDB0128672	3-(6,7-dimethoxy-2H-1,3-benzodioxol-5-yl)propan-1-ol	C12H16O5	M-H2O-H	221.0814	1.4
HMDB0127826	4-hydroxy-5-(3-hydroxy-4-methoxyphenyl)pentanoic acid	C12H16O5	M-H2O-H	221.0814	1.4
HMDB0127748	4-hydroxy-5-(4-hydroxy-3-methoxyphenyl)pentanoic acid	C12H16O5	M-H2O-H	221.0814	1.4
HMDB0094661	1-phenylhexan-2-one	C12H16O	M+FA-H	221.1183	-0.5
HMDB0036171	3-(4-Isopropylphenyl)propanal	C12H16O	M+FA-H	221.1183	-0.5
HMDB0031569	4-Methyl-1-phenyl-2-pentanone	C12H16O	M+FA-H	221.1183	-0.5
HMDB0036021	Rhubafuran	C12H16O	M+FA-H	221.1183	-0.5
HMDB0034177	(S)-4-(4-Methylphenyl)-2-pentanone	C12H16O	M+FA-H	221.1183	-0.5
HMDB0140967	3-hydroxy-2-[4-(2-methylpropyl)phenyl]propanoic acid	C13H18O3	M-H	221.1183	-0.5
HMDB0132941	1-hydroxy-1-(4-methoxyphenyl)-4-methylpentan-3-one	C13H18O3	M-H	221.1183	-0.5
HMDB0140966	2-hydroxy-2-[4-(2-methylpropyl)phenyl]propanoic acid	C13H18O3	M-H	221.1183	-0.5
HMDB0132943	1-hydroxy-5-(4-methoxyphenyl)-2-methylpentan-3-one	C13H18O3	M-H	221.1183	-0.5
HMDB0132946	2-hydroxy-1-(4-methoxyphenyl)-4-methylpentan-3-one	C13H18O3	M-H	221.1183	-0.5
HMDB0132945	4-hydroxy-1-(4-methoxyphenyl)-4-methylpentan-3-one	C13H18O3	M-H	221.1183	-0.5
HMDB0183005	3-methylbutyl 2-(4-hydroxyphenyl)acetate	C13H18O3	M-H	221.1183	-0.5
HMDB0176251	4-(2-hydroxyphenyl)-2-methylbutan-2-yl acetate	C13H18O3	M-H	221.1183	-0.5

221.1182	HMDB0183008	3-methylbutyl 2-(3-hydroxyphenyl)acetate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175270	2-(2-hydroxyphenyl)propyl 2-methylpropanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0183006	4-hydroxy-3-methylbutyl 2-phenylacetate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175233	2-(2-hydroxyphenyl)propyl butanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175234	2-hydroxy-2-phenylpropyl butanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175305	3-(2-hydroxyphenyl)propyl 2-methylpropanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175306	3-hydroxy-3-phenylpropyl 2-methylpropanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175307	3-phenylpropyl 2-hydroxy-2-methylpropanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0183003	3-methylbutyl 2-(2-hydroxyphenyl)acetate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175309	3-phenylpropyl 3-hydroxy-2-methylpropanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175308	3-(4-hydroxyphenyl)propyl 2-methylpropanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0176247	4-(3-hydroxyphenyl)-2-methylbutan-2-yl acetate	C13H18O3	M-H	221.1183	-0.5
	HMDB0176250	2-methyl-4-phenylbutan-2-yl 2-hydroxyacetate	C13H18O3	M-H	221.1183	-0.5
	HMDB0176248	4-(4-hydroxyphenyl)-2-methylbutan-2-yl acetate	C13H18O3	M-H	221.1183	-0.5
	HMDB0176249	1-hydroxy-2-methyl-4-phenylbutan-2-yl acetate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175276	2-(3-hydroxyphenyl)propyl 2-methylpropanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175275	2-phenylpropyl 3-hydroxy-2-methylpropanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0183004	3-hydroxy-3-methylbutyl 2-phenylacetate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175235	2-(4-hydroxyphenyl)propyl butanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175237	3-hydroxy-2-phenylpropyl butanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175236	2-phenylpropyl 3-hydroxybutanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175238	2-phenylpropyl 4-hydroxybutanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175239	2-phenylpropyl 2-hydroxybutanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0183007	Isoamyl mandelate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175271	2-hydroxy-2-phenylpropyl 2-methylpropanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175274	3-hydroxy-2-phenylpropyl 2-methylpropanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175272	2-phenylpropyl 2-hydroxy-2-methylpropanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0175273	2-(4-hydroxyphenyl)propyl 2-methylpropanoate	C13H18O3	M-H	221.1183	-0.5
	HMDB0176246	4-hydroxy-2-methyl-4-phenylbutan-2-yl acetate	C13H18O3	M-H	221.1183	-0.5
	HMDB0038894	Isoamyl p-anisate	C13H18O3	M-H	221.1183	-0.5
	HMDB0032121	Annuionone B	C13H18O3	M-H	221.1183	-0.5
	HMDB0060565	1-Hydroxyibuprofen	C13H18O3	M-H	221.1183	-0.5
	HMDB0060920	2-Hydroxyibuprofen	C13H18O3	M-H	221.1183	-0.5
	HMDB0036819	Dehydrovomifoliol	C13H18O3	M-H	221.1183	-0.5
	HMDB0060921	3-Hydroxyibuprofen	C13H18O3	M-H	221.1183	-0.5
	HMDB0061943	Hexyl salicylic acid	C13H18O3	M-H	221.1183	-0.5
	HMDB0176442	(9E,11E)-2-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M-H2O-H	221.1178	1.9
	HMDB0176436	(9E,11E)-5-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M-H2O-H	221.1178	1.9
	HMDB0176435	(9E,11E)-6-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M-H2O-H	221.1178	1.9
	HMDB0176434	(9E,11E)-7-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M-H2O-H	221.1178	1.9
	HMDB0176440	(9E)--(3-formyloxiran-2-yl)dec-9-enoic acid	C13H20O4	M-H2O-H	221.1178	1.9
	HMDB0176439	(9E,11E)-8-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M-H2O-H	221.1178	1.9
	HMDB0176441	8-{3-[(1E)-3-oxoprop-1-en-1-yl]oxiran-2-yl}octanoic acid	C13H20O4	M-H2O-H	221.1178	1.9
	HMDB0176437	(9E,11E)-4-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M-H2O-H	221.1178	1.9
	HMDB0176438	(9E,11E)-3-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M-H2O-H	221.1178	1.9
	HMDB0176432	SCHEMBL2554147	C13H20O4	M-H2O-H	221.1178	1.9
221.1539	HMDB0032369	L-Menthyl acetoacetate	C14H24O3	M-H2O-H	221.1542	-1.2
	HMDB0160289	(5Z,8Z)-4-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M-H2O-H	221.1542	-1.2
	HMDB0160290	(8Z)--hydroxytetradeca-5,8-dienoic acid	C14H24O3	M-H2O-H	221.1542	-1.2
	HMDB0160292	4-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}butanoic acid	C14H24O3	M-H2O-H	221.1542	-1.2
	HMDB0160291	SCHEMBL8918721	C14H24O3	M-H2O-H	221.1542	-1.2
	HMDB0160294	(5Z,8Z)-14-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M-H2O-H	221.1542	-1.2
	HMDB0160296	(5Z,8Z)-7-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M-H2O-H	221.1542	-1.2
	HMDB0160293	(5Z)-7-(3-pentyloxiran-2-yl)hept-5-enoic acid	C14H24O3	M-H2O-H	221.1542	-1.2
	HMDB0160295	(5Z,8Z)-2-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M-H2O-H	221.1542	-1.2
	HMDB0160298	(8Z)-5-hydroxytetradeca-6,8-dienoic acid	C14H24O3	M-H2O-H	221.1542	-1.2
	HMDB0160297	(5Z,7E)-9-hydroxytetradeca-5,7-dienoic acid	C14H24O3	M-H2O-H	221.1542	-1.2
	HMDB0031162	3,3'-Thiobispropanoic acid	C6H10O4S	M+FA-H	223.0282	-0.4
	HMDB0179354	[(2Z,4E)-hexa-2,4-dien-1-yloxy]sulfonic acid	C6H10O4S	M+FA-H	223.0282	-0.4
	HMDB0240388	2,3-Dihydroxy-5-methylthio-4-pentenoic acid	C6H10O4S	M+FA-H	223.0282	-0.4
	HMDB0165618	{[(2Z)-2-methylpenta-2,4-dien-1-yl]oxy} sulfonic acid	C6H10O4S	M+FA-H	223.0282	-0.4
	HMDB0166508	(4Z)-3-(sulfooxy)hept-4-enoic acid	C7H12O6S	M-H	223.0282	-0.4
	HMDB0180352	{[(2E)-3-[3-(2-hydroxyethyl)oxiran-2-yl]prop-2-en-1-yl]oxy} sulfonic acid	C7H12O6S	M-H	223.0282	-0.4

223.0281	HMDB0180351	(2-{3-[(1E)-3-hydroxyprop-1-en-1-yl]oxiran-2-yl}ethoxy)sulfonic acid	C7H12O6S	M-H	223.0282	-0.4
	HMDB0180345	{[(2E)-3-[3-(1-hydroxyethyl)oxiran-2-yl]prop-2-en-1-yl]oxy}sulfonic acid	C7H12O6S	M-H	223.0282	-0.4
	HMDB0180346	(1-{3-[(1E)-3-hydroxyprop-1-en-1-yl]oxiran-2-yl}ethoxy)sulfonic acid	C7H12O6S	M-H	223.0282	-0.4
	HMDB0166790	(2E)-7-(sulfooxy)hept-2-enoic acid	C7H12O6S	M-H	223.0282	-0.4
	HMDB0166784	(2E)-6-(sulfooxy)hept-2-enoic acid	C7H12O6S	M-H	223.0282	-0.4
	HMDB0166781	(2E)-4-(sulfooxy)hept-2-enoic acid	C7H12O6S	M-H	223.0282	-0.4
	HMDB0166517	(4Z)-2-(sulfooxy)hept-4-enoic acid	C7H12O6S	M-H	223.0282	-0.4
	HMDB0166514	(4Z)-7-(sulfooxy)hept-4-enoic acid	C7H12O6S	M-H	223.0282	-0.4
	HMDB0164746	(5-hydroxy-5-methyl-2-oxocyclohexyl)oxidanesulfonic acid	C7H12O6S	M-H	223.0282	-0.4
	HMDB0166505	(4Z)-6-(sulfooxy)hept-4-enoic acid	C7H12O6S	M-H	223.0282	-0.4
	HMDB0165789	(5-ethyl-2-methyl-4-oxooxolan-3-yl)oxidanesulfonic acid	C7H12O6S	M-H	223.0282	-0.4
	HMDB0163411	(5-ethyl-4-methyl-2-oxooxolan-3-yl)oxidanesulfonic acid	C7H12O6S	M-H	223.0282	-0.4
	HMDB0164743	[(1-hydroxy-4-oxocyclohexyl)methoxy]sulfonic acid	C7H12O6S	M-H	223.0282	-0.4
223.0760	HMDB0168443	2-hydroxy-2-phenylethyl benzoate	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0151857	1-(2,4-dihydroxyphenyl)-3-phenylpropan-1-one	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0135408	1,3-bis(3-hydroxyphenyl)propan-1-one	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0135409	1-(3-hydroxyphenyl)-3-(4-hydroxyphenyl)propan-1-	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0135593	3-hydroxy-3-(4-hydroxyphenyl)-1-phenylpropan-1-one	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0135594	1,3-bis(4-hydroxyphenyl)propan-1-one	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0135596	1-(2-hydroxyphenyl)-3-(4-hydroxyphenyl)propan-1-	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0135595	3-(3,4-dihydroxyphenyl)-1-phenylpropan-1-one	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0135601	3-(2,4-dihydroxyphenyl)-1-phenylpropan-1-one	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0148520	336268-3	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0168442	2-(2-hydroxyphenyl)ethyl benzoate	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0168444	PHENETHYL 3-HYDROXYBENZOATE	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0168446	Phenethyl 4-hydroxybenzoate	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0168445	2-(3-hydroxyphenyl)ethyl benzoate	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0168447	Benzoic acid 4-hydroxyphenethyl ester	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0135406	1-(3,5-dihydroxyphenyl)-3-phenylpropan-1-one	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0135407	3-hydroxy-1-(3-hydroxyphenyl)-3-phenylpropan-1-one	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0135405	3-(2-hydroxyphenyl)-1-(3-hydroxyphenyl)propan-1-	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0130496	3-phenyl-3,4-dihydro-2H-1-benzopyran-4,7-diol	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0130497	1-(2,4-dihydroxyphenyl)-2-phenylpropan-1-one	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0135355	1-(2,5-dihydroxyphenyl)-3-phenylpropan-1-one	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0135397	1-(3,4-dihydroxyphenyl)-3-phenylpropan-1-one	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0182848	(4-hydroxyphenyl)methyl 2-phenylacetate	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0014713	Fenoprofen	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0130495	3-(4-hydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-7-ol	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0002209	Equol	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0036347	2,3-Dihydroxy-1,3-diphenyl-1-propanone	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0029302	1-Phenyl-6,7-dihydroxy-isochroman	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0035019	Phenethyl salicylate	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0037679	Guaicyl phenylacetate	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0039146	Citribuntin	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0061303	2-(benzhydryloxy)acetic acid	C15H14O3	M-H20-H	223.0759	0.4
	HMDB0162572	(2-amino-2-carboxyethyl)(2-aminoethyl)methylsulfonium	C6H15N2O2S	M+FA-H	223.0758	0.9
	HMDB0033187	2,12-Tetradecadiene-4,6,8,-tetrayne	C14H10	M+FA-H	223.0765	-2.0
	HMDB0141386	(2E)-3-(4-hydroxyphenyl)-1-phenylprop-2-en-1-one	C15H12O2	M-H	223.0765	-2.0
	HMDB0141385	(2E)-3-(3-hydroxyphenyl)-1-phenylprop-2-en-1-one	C15H12O2	M-H	223.0765	-2.0
	HMDB0141387	2-benzoyl-3-phenyloxirane	C15H12O2	M-H	223.0765	-2.0
	HMDB0135607	(2E)-1-(4-hydroxyphenyl)-3-phenylprop-2-en-1-one	C15H12O2	M-H	223.0765	-2.0
	HMDB0135602	3-(4-hydroxyphenyl)-1-phenylprop-2-en-1-one	C15H12O2	M-H	223.0765	-2.0
	HMDB0135603	1-(4-hydroxyphenyl)-3-phenylprop-2-en-1-one	C15H12O2	M-H	223.0765	-2.0
	HMDB0135599	1-(2-hydroxyphenyl)-3-phenylprop-2-en-1-one	C15H12O2	M-H	223.0765	-2.0
	HMDB0135404	(2E)-1-(3-hydroxyphenyl)-3-phenylprop-2-en-1-one	C15H12O2	M-H	223.0765	-2.0
	HMDB0032584	4-Hydroxychalcone	C15H12O2	M-H	223.0765	-2.0
	HMDB0135604	1-(3-hydroxyphenyl)-3-phenylprop-2-en-1-one	C15H12O2	M-H	223.0765	-2.0

223.1340	HMDB0135600	3-(3-hydroxyphenyl)-1-phenylprop-2-en-1-one	C15H12O2	M-H	223.0765	-2.0
	HMDB0163216	(2E,4E)-6-(3-pentylloxiran-2-yl)hexa-2,4-dienoic acid	C13H20O3	M-H	223.1340	0.1
	HMDB0112084	3-(3-methyl-5-pentylfuran-2-yl)propanoic acid	C13H20O3	M-H	223.1340	0.1
	HMDB0163210	(2E,4E,7Z)-12-hydroxytrideca-2,4,7-trienoic acid	C13H20O3	M-H	223.1340	0.1
	HMDB0036583	Methyl jasmonate	C13H20O3	M-H	223.1340	0.1
	HMDB0032679	Annuionone A	C13H20O3	M-H	223.1340	0.1
	HMDB0163213	(2E,4E,7Z)-9-hydroxytrideca-2,4,7-trienoic acid	C13H20O3	M-H	223.1340	0.1
	HMDB0163211	(2E,4E,7Z)-13-hydroxytrideca-2,4,7-trienoic acid	C13H20O3	M-H	223.1340	0.1
	HMDB0037736	3-Methylbutyl 2-furanbutanoate	C13H20O3	M-H	223.1340	0.1
	HMDB0163214	3-[(1E,4Z)-deca-1,4-dien-1-yl]oxirane-2-carboxylic acid	C13H20O3	M-H	223.1340	0.1
	HMDB0163215	(2E)-3-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}prop-2-enoic acid	C13H20O3	M-H	223.1340	0.1
	HMDB0032689	Annuionone C	C13H20O3	M-H	223.1340	0.1
	HMDB0029670	Epoxyeremopetasinorol	C13H20O3	M-H	223.1340	0.1
	HMDB0037244	(8alpha,beta,11beta)-3-Hydroxy-4,15-dinor-1(5)-xanthen-12,8-olide	C13H20O3	M-H	223.1340	0.1
	HMDB0037726	Octyl 2-furoate	C13H20O3	M-H	223.1340	0.1
	HMDB0034564	13-Oxo-9,11-tridecadienoic acid	C13H20O3	M-H	223.1340	0.1
	HMDB0037730	Furfuryl octanoate	C13H20O3	M-H	223.1340	0.1
	HMDB0014956	Propofol	C12H18O	M+FA-H	223.1340	0.2
	HMDB0031194	Tricycloekasantal	C12H18O	M+FA-H	223.1340	0.2
	HMDB0038194	Geijerone	C12H18O	M+FA-H	223.1340	0.2
	HMDB0032579	2,5-Diisopropylphenol	C12H18O	M+FA-H	223.1340	0.2
	HMDB0037272	2-Ethoxy-1-methyl-4-(1-methylethyl)benzene	C12H18O	M+FA-H	223.1340	0.2
	HMDB0038107	Quinceoxepine	C12H18O	M+FA-H	223.1340	0.2
	HMDB0031731	3-Methyl-1-phenyl-3-pentanol	C12H18O	M+FA-H	223.1340	0.2
	HMDB0035055	Photocitral A	C12H18O	M+FA-H	223.1340	0.2
	HMDB0036681	7-Isopropyl-5-methylbicyclo[2.2.2]oct-5-en-2-one	C12H18O	M+FA-H	223.1340	0.2
	HMDB0031568	4-Methyl-1-phenyl-2-pentanol	C12H18O	M+FA-H	223.1340	0.2
	HMDB0176459	(9E)-[3-(hydroxymethyl)oxiran-2-yl]dec-9-enoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176451	(9E)-12-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176461	(9E,11E)-2,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176448	(9E)-8-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176447	(9E)-3-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176446	(9E)-4-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176444	(9E)-6-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176450	8-[3-(3-oxopropyl)oxiran-2-yl]octanoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176449	(9E)-11-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176457	(9E,11E)-3,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176456	(9E,11E)-4,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176460	8-{3-[(1E)-3-hydroxyprop-1-en-1-yl]oxiran-2-yl}octanoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176454	(9E,11E)-6,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176455	(9E,11E)-5,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176453	(9E,11E)-7,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176458	(9E,11E)-8,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176452	(9E)-2-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176445	(9E)-5-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0176443	(9E)-7-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0030987	2-Carboxy-4-dodecanolide	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0038736	(3S,5R,6R,7E)-3,5,6-Trihydroxy-7-megastigmen-9-one	C13H22O4	M-H2O-H	223.1334	2.6
	HMDB0038259	Neryl butyrate	C14H24O2	M-H	223.1704	-0.7
	HMDB0031015	Ethyl (2E,6Z)-dodecadienoate	C14H24O2	M-H	223.1704	-0.7
	HMDB0032342	Isobornyl isobutyrate	C14H24O2	M-H	223.1704	-0.7
	HMDB0030427	Linalyl butyrate	C14H24O2	M-H	223.1704	-0.7
	HMDB0038260	Geranyl 2-methylpropanoate	C14H24O2	M-H	223.1704	-0.7
	HMDB0038246	Bornyl butyrate	C14H24O2	M-H	223.1704	-0.7
	HMDB0037814	2-Propenyl cyclohexanepentanoate	C14H24O2	M-H	223.1704	-0.7
	HMDB0032053	alpha-Terpineol butanoate	C14H24O2	M-H	223.1704	-0.7
	HMDB0030426	Linalyl isobutyrate	C14H24O2	M-H	223.1704	-0.7
	HMDB0036424	Allyl undecylenate	C14H24O2	M-H	223.1704	-0.7
	HMDB0032524	Terpinyl isobutyrate	C14H24O2	M-H	223.1704	-0.7
	HMDB0000560	Goshuyic acid	C14H24O2	M-H	223.1704	-0.7
	HMDB0039129	Goshuyic acid	C14H24O2	M-H	223.1704	-0.7

223.1702	HMDB0159613	(5E)-14-hydroxytetradec-5-enoic acid	C14H26O3	M-H2O-H	223.1698	1.8
	HMDB0159614	(5E)-2-hydroxytetradec-5-enoic acid	C14H26O3	M-H2O-H	223.1698	1.8
	HMDB0159799	(5Z)-7-hydroxytetradec-5-enoic acid	C14H26O3	M-H2O-H	223.1698	1.8
	HMDB0159800	(5Z)-4-hydroxytetradec-5-enoic acid	C14H26O3	M-H2O-H	223.1698	1.8
	HMDB0159801	SCHEMBL157578	C14H26O3	M-H2O-H	223.1698	1.8
	HMDB0159802	14-hydroxy-5Z-tetradecenoic acid	C14H26O3	M-H2O-H	223.1698	1.8
	HMDB0159803	(5Z)-2-hydroxytetradec-5-enoic acid	C14H26O3	M-H2O-H	223.1698	1.8
	HMDB0176319	13-hydroxy-3-oxotetradecanal	C14H26O3	M-H2O-H	223.1698	1.8
	HMDB0176320	14-hydroxy-3-oxotetradecanal	C14H26O3	M-H2O-H	223.1698	1.8
	HMDB0159612	4-(3-octyloxiran-2-yl)butanoic acid	C14H26O3	M-H2O-H	223.1698	1.8
	HMDB0159611	(5E)-13-hydroxytetradec-5-enoic acid	C14H26O3	M-H2O-H	223.1698	1.8
	HMDB0159610	(5E)-4-hydroxytetradec-5-enoic acid	C14H26O3	M-H2O-H	223.1698	1.8
	HMDB0159609	(5E)-7-hydroxytetradec-5-enoic acid	C14H26O3	M-H2O-H	223.1698	1.8
	HMDB0032370	L-Menthyl (R,S)-3-hydroxybutyrate	C14H26O3	M-H2O-H	223.1698	1.8
	HMDB0030982	6-Ketomyristic acid	C14H26O3	M-H2O-H	223.1698	1.8
	HMDB0010730	3-Oxotetradecanoic acid	C14H26O3	M-H2O-H	223.1698	1.8
225.0075	HMDB0161131	4-methyl-2-oxo-5-(sulfooxy)pentanoic acid	C6H10O7S	M-H	225.0074	0.2
	HMDB0159492	3-methyl-2-oxo-5-(sulfooxy)pentanoic acid	C6H10O7S	M-H	225.0074	0.2
	HMDB0159489	2-oxo-3-[(sulfooxy)methyl]pentanoic acid	C6H10O7S	M-H	225.0074	0.2
	HMDB0159486	3-methyl-2-oxo-4-(sulfooxy)pentanoic acid	C6H10O7S	M-H	225.0074	0.2
	HMDB0158760	2-methyl-3-oxo-5-(sulfooxy)pentanoic acid	C6H10O7S	M-H	225.0074	0.2
	HMDB0158757	3-oxo-2-[(sulfooxy)methyl]pentanoic acid	C6H10O7S	M-H	225.0074	0.2
	HMDB0158754	2-methyl-3-oxo-4-(sulfooxy)pentanoic acid	C6H10O7S	M-H	225.0074	0.2
	HMDB0161134	4-methyl-2-oxo-3-(sulfooxy)pentanoic acid	C6H10O7S	M-H	225.0074	0.2
	HMDB0149285	[(3-methyl-1-oxobut-3-en-2-yl)oxy]sulfonic acid	C5H8O5S	M+FA-H	225.0074	0.2
	HMDB0163745	SCHEMBL438962	C5H8O5S	M+FA-H	225.0074	0.2
	HMDB0163747	(2-methylidene-3-oxobutoxy)sulfonic acid	C5H8O5S	M+FA-H	225.0074	0.2
	HMDB0180202	{[(2E)-2-methyl-4-oxobut-2-en-1-yl]oxy}sulfonic acid	C5H8O5S	M+FA-H	225.0074	0.2
	HMDB0184837	SCHEMBL18653399	C6H12O8S	M-H2O-H	225.0069	2.7
	HMDB0184835	[(3,4,5-trihydroxyoxan-2-yl)methoxy]sulfonic acid	C6H12O8S	M-H2O-H	225.0069	2.7
	HMDB0184836	[4,5-dihydroxy-2-(hydroxymethyl)oxan-3-yl]oxidanesulfonic acid	C6H12O8S	M-H2O-H	225.0069	2.7
	HMDB0184838	[4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxidanesulfonic acid	C6H12O8S	M-H2O-H	225.0069	2.7
	HMDB0166674	[5-hydroxy-2-(hydroxymethyl)-4-methoxyoxolan-3-yl]oxidanesulfonic acid	C6H12O8S	M-H2O-H	225.0069	2.7
	HMDB0166673	[(3,5-dihydroxy-4-methoxyoxolan-2-yl)methoxy]sulfonic acid	C6H12O8S	M-H2O-H	225.0069	2.7
225.1493	HMDB0002327	1,11-Undecanedicarboxylic acid	C13H24O4	M-H2O-H	225.1491	1.0
	HMDB0037184	1,4-Nonanediol diacetate	C13H24O4	M-H2O-H	225.1491	1.0
	HMDB0036141	Menthyl ethylene glycol carbonate	C13H24O4	M-H2O-H	225.1491	1.0
	HMDB0038108	cis-Quinceoxepane	C12H20O	M+FA-H	225.1496	-1.4
	HMDB0039590	(2E,4E)-2,4-Dodecadienal	C12H20O	M+FA-H	225.1496	-1.4
	HMDB0039339	Tricycloekasantalol	C12H20O	M+FA-H	225.1496	-1.4
	HMDB0031181	Homodihydrojasnone	C12H20O	M+FA-H	225.1496	-1.4
	HMDB0032531	2-trans-6-cis-Dodecadienal	C12H20O	M+FA-H	225.1496	-1.4
	HMDB0037562	Riesling acetal	C13H22O3	M-H	225.1496	-1.4
	HMDB0176430	(9E)-13-oxotridec-9-enoic acid	C13H22O3	M-H	225.1496	-1.4
	HMDB0176431	(9E,11E)-13-hydroxytrideca-9,11-dienoic acid	C13H22O3	M-H	225.1496	-1.4
	HMDB0031740	Methyl dihydrojasmonate	C13H22O3	M-H	225.1496	-1.4
	HMDB0040615	4,5-Dihydrovomifolliol	C13H22O3	M-H	225.1496	-1.4
	HMDB0010731	(R)-3-Hydroxy-tetradecanoic acid	C14H28O3	M-H2O-H	225.1855	1.1
	HMDB0171057	14-hydroxymyristic acid	C14H28O3	M-H2O-H	225.1855	1.1
	HMDB0032417	3-(L-Menthoxo)-2-methylpropane-1,2-diol	C14H28O3	M-H2O-H	225.1855	1.1
	HMDB0094672	3-hydroxytetradecanoic acid	C14H28O3	M-H2O-H	225.1855	1.1
	HMDB0059850	Ethyl 3-hydroxydodecanoate	C14H28O3	M-H2O-H	225.1855	1.1
	HMDB0171056	13-hydroxytetradecanoic acid	C14H28O3	M-H2O-H	225.1855	1.1
	HMDB0061656	(S)-3-hydroxytetradecanoic acid	C14H28O3	M-H2O-H	225.1855	1.1
	HMDB0002261	2-Hydroxymyristic acid	C14H28O3	M-H2O-H	225.1855	1.1
	HMDB0176324	1,4-dihydroxytetradecan-3-one	C14H28O3	M-H2O-H	225.1855	1.1
	HMDB0176322	1,14-dihydroxytetradecan-3-one	C14H28O3	M-H2O-H	225.1855	1.1
	HMDB0176323	1,2-dihydroxytetradecan-3-one	C14H28O3	M-H2O-H	225.1855	1.1
	HMDB0176321	1,13-dihydroxytetradecan-3-one	C14H28O3	M-H2O-H	225.1855	1.1
	HMDB0041081	(Z)-1,5-Tridecadiene	C13H24	M+FA-H	225.1860	-1.3
	HMDB0062248	(9E)-tetradecenoic acid	C14H26O2	M-H	225.1860	-1.3

225.1857	HMDB0094671	cyclohexyl octanoate	C14H26O2	M-H	225.1860	-1.3
	HMDB0062243	cis-tetradec-7-enoic acid	C14H26O2	M-H	225.1860	-1.3
	HMDB0037369	Butyl 2-decenoate	C14H26O2	M-H	225.1860	-1.3
	HMDB0037228	Citronellyl isobutyrate	C14H26O2	M-H	225.1860	-1.3
	HMDB0037227	Citronellyl butyrate	C14H26O2	M-H	225.1860	-1.3
	HMDB0037189	Rhodinyl isobutyrate	C14H26O2	M-H	225.1860	-1.3
	HMDB0037188	Rhodinyl butyrate	C14H26O2	M-H	225.1860	-1.3
	HMDB0031073	12-Methyl-13-tridecanolide	C14H26O2	M-H	225.1860	-1.3
	HMDB0034561	Houttuynin	C14H26O2	M-H	225.1860	-1.3
	HMDB0038056	delta-Tetradecalactone	C14H26O2	M-H	225.1860	-1.3
	HMDB0031029	Ethyl (E)-2-dodecenoate	C14H26O2	M-H	225.1860	-1.3
	HMDB0037633	xi-Tetrahydro-3-nonyl-2H-pyran-2-one	C14H26O2	M-H	225.1860	-1.3
	HMDB0010732	trans-Tetra-dec-2-enoic acid	C14H26O2	M-H	225.1860	-1.3
	HMDB0005051	Tsuzuic acid	C14H26O2	M-H	225.1860	-1.3
	HMDB0002000	Myristoleic acid	C14H26O2	M-H	225.1860	-1.3
	HMDB0000521	5Z-Tetradecenoic acid	C14H26O2	M-H	225.1860	-1.3
	HMDB0040228	1,1-Diethoxy-3,7-dimethyl-2,6-octadiene	C14H26O2	M-H	225.1860	-1.3
	HMDB0032321	2-Hexenyl octanoate	C14H26O2	M-H	225.1860	-1.3
	HMDB0030921	(R)-14-Methyloxacyclotetradecan-2-one	C14H26O2	M-H	225.1860	-1.3
	HMDB0061991	Menthyl butyrate	C14H26O2	M-H	225.1860	-1.3
	HMDB0032152	Acetaldehyde di-cis-3-hexenyl acetal	C14H26O2	M-H	225.1860	-1.3
	HMDB0000499	5-Tetradecenoic acid	C14H26O2	M-H	225.1860	-1.3
225.2221	HMDB0031078	Pentadecanal	C15H30O	M-H	225.2224	-1.3
	HMDB0061956	Z--Pentadecen-1-ol	C15H30O	M-H	225.2224	-1.3
	HMDB0059813	Heptyl ketone	C15H30O	M-H	225.2224	-1.3
	HMDB0031081	2-Pentadecanone	C15H30O	M-H	225.2224	-1.3
226.0837	HMDB0000014	Deoxycytidine	C9H13N3O4	M-H	226.0833	1.6
227.0922	HMDB0142086	4-ethyl-2,3-dimethoxyphenol	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179469	2-(2-hydroxypropan-2-yl)-5-methylcyclohex-2-ene-1,4-dione	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0145930	SCHEMBL83728	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179475	1-methyl-4-(propan-2-yl)-7-oxabicyclo[4.1]heptane-2,5-dione	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179477	6-hydroxy-2-methyl-5-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179483	2-(1-hydroxypropan-2-yl)-5-methylbenzene-1,4-diol	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179482	6-methyl-3-(propan-2-yl)benzene-1,2,4-triol	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179480	2,5-dihydroxy-4-isopropylbenzyl alcohol	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179479	CTK8G51	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0181694	3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0181695	2-(hydroxymethyl)-3-methyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0181696	5-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0181697	1-hydroxy-2,3-dimethyltricyclo[2.2.1,heptane-3-carboxylic acid	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179478	2-hydroxy-2-isopropyl-5-methylcyclohex-5-ene-1,4-dione	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179476	5-(1-hydroxypropan-2-yl)-2-methylcyclohex-2-ene-1,4-dione	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179471	2-(1-hydroxypropan-2-yl)-5-methylcyclohex-2-ene-1,4-dione	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0163112	3-[(1Z,4Z)-hepta-1,4-dien-1-yl]oxirane-2-carboxylic acid	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0163114	(2E,4Z)-6-(3-ethyloxiran-2-yl)hexa-2,4-dienoic acid	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0163113	(2E)-3-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}prop-2-enoic acid	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0163111	(2E,7Z)-9-hydroxydeca-2,4,7-trienoic acid	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0163115	(2E,4Z,7Z)--hydroxydeca-2,4,7-trienoic acid	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179470	4-methyl-1-(propan-2-yl)-7-oxabicyclo[4.1]heptane-2,5-dione	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179468	5-hydroxy-5-methyl-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M+FA-H	227.0925	-1.3

	HMDB0179467	5-(hydroxymethyl)-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179473	2-(hydroxymethyl)-5-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179472	6-hydroxy-5-methyl-2-(propan-2-yl)cyclohex-2-ene-1,4-dione	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179474	5-(2-hydroxypropan-2-yl)-2-methylcyclohex-2-ene-1,4-dione	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0036522	Verimol J	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0033394	4-Ethyl-2,6-dimethoxyphenol	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0037641	4-(Ethoxymethyl)-2-methoxyphenol	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0037727	Furfuryl pentanoate	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0038354	2-Ethoxy-4-(methoxymethyl)phenol	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0032607	threo-Anethole glycol	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0038181	Peperinic acid	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0029456	Amyl 2-furoate	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0039874	Furfuryl isovalerate	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0059891	Isoamyl 2-furoate	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0179481	4427-54-7	C10H14O3	M+FA-H	227.0925	-1.3
	HMDB0153819	2-(1,3-dihydroxy-3-methylbutyl)benzene-1,3,5-triol	C11H16O5	M-H	227.0925	-1.3
	HMDB0032496	Propyl propane thiosulfonate	C11H16O5	M-H	227.0925	-1.3
	HMDB0153812	2-(3,4-dihydroxy-3-methylbutyl)benzene-1,3,5-triol	C11H16O5	M-H	227.0925	-1.3
227.1287	HMDB0163222	(2E,5Z)-7-hydroxyundeca-2,5-dienal	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0163224	3-[(2Z)-oct-2-en-1-yl]oxirane-2-carbaldehyde	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0163225	(2E)-4-(3-pentylloxiran-2-yl)but-2-enal	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0163223	(2E,5Z)--hydroxyundeca-2,5-dienal	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0163226	(2E,5Z)-11-hydroxyundeca-2,5-dienal	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0038068	(3E,6Z)-Nonadien-1-yl acetate	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0034708	Methyl 4,8-decadienoate	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0030006	2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]non-3-ene	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0163221	(2E,5Z)-undeca-2,5-dienoic acid	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0038079	(2E,6Z)-2,6-Nonadien-1-Yl acetate	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0030424	Linalyl formate	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0037388	Tsibulin 2	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0034730	Methyl (2E,4Z)-decadienoate	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0040595	Allyl cyclohexylacetate	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0037829	6-(3-Hexenyl)tetrahydro-2H-pyran-2-one	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0036191	4-Hydroxy-4-methyl-7-decenoic acid gamma-lactone	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0035156	Neryl formate	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0038005	xi-2-Hexyl-5-methyl-3(2H)-furanone	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0036215	Ethyl octynecarboxylate	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0038245	Bornyl formate	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0038279	cis-3-Hexenyl tiglate	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0059816	Methyl geranate	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0032463	5-Pentyl-3h-furan-2-one	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0032050	alpha-Terpineol formate	C11H18O2	M+FA-H	227.1289	-0.8
	HMDB0164283	2-hydroxy-2-(3-oxo-2-pentylcyclopentyl)acetic acid	C12H20O4	M-H	227.1289	-0.8
	HMDB0164282	2-(4-hydroxy-3-oxo-2-pentylcyclopentyl)acetic acid	C12H20O4	M-H	227.1289	-0.8
	HMDB0164280	2-(5-hydroxy-3-oxo-2-pentylcyclopentyl)acetic acid	C12H20O4	M-H	227.1289	-0.8
	HMDB0164284	2-(2-hydroxy-3-oxo-2-pentylcyclopentyl)acetic acid	C12H20O4	M-H	227.1289	-0.8
	HMDB0000933	Traumatic acid	C12H20O4	M-H	227.1289	-0.8
	HMDB0164281	2-[2-(5-hydroxypentyl)-3-oxocyclopentyl]acetic acid	C12H20O4	M-H	227.1289	-0.8
	HMDB0030994	5-Heptyltetrahydro-2-oxo-3-furancarboxylic acid	C12H20O4	M-H	227.1289	-0.8
	HMDB0164279	2-[2-(4-hydroxypentyl)-3-oxocyclopentyl]acetic acid	C12H20O4	M-H	227.1289	-0.8
	HMDB0031696	Dibutyl malate	C12H22O5	M-H2O-H	227.1283	1.6
	HMDB0000413	3-Hydroxydodecanedioic acid	C12H22O5	M-H2O-H	227.1283	1.6
	HMDB0160679	5-hydroxydodecanedioic acid	C12H22O5	M-H2O-H	227.1283	1.6
	HMDB0160678	4-hydroxydodecanedioic acid	C12H22O5	M-H2O-H	227.1283	1.6
	HMDB0160680	6-Hydroxydodecanedioic acid	C12H22O5	M-H2O-H	227.1283	1.6
	HMDB0160681	2-Hydroxydodecanedioic acid	C12H22O5	M-H2O-H	227.1283	1.6
	HMDB0031020	2-Dodecenal	C12H22O	M+FA-H	227.1653	-1.2
	HMDB0036461	Geosmin	C12H22O	M+FA-H	227.1653	-1.2
	HMDB0031102	(Z,Z)-3,6-Dodecadien-1-ol	C12H22O	M+FA-H	227.1653	-1.2
	HMDB0038972	(E)-2-Butyl-2-octenal	C12H22O	M+FA-H	227.1653	-1.2
	HMDB0031341	Cyclododecanone	C12H22O	M+FA-H	227.1653	-1.2

227.1650	HMDB0032279	2-Ethyl-1,3,3-trimethyl-2-norbornanol	C12H22O	M+FA-H	227.1653	-1.2
	HMDB0032542	trans- and cis-2,4,8-Trimethyl-3,7-nona-dien-2-ol	C12H22O	M+FA-H	227.1653	-1.2
	HMDB0037212	Menthyl lactate	C13H24O3	M-H	227.1653	-1.2
	HMDB0036139	Menthone 1,2-glyceryl ketal	C13H24O3	M-H	227.1653	-1.2
	HMDB0035881	11-Hydroxy-9-tridecenoic acid	C13H24O3	M-H	227.1653	-1.2
	HMDB0040004	Menthone 1,3-glyceryl ketal	C13H24O3	M-H	227.1653	-1.2
	HMDB0072874	MG/)	C13H26O4	M-H2O-H	227.1647	1.2
227.2014	HMDB0072866	MG()	C13H26O4	M-H2O-H	227.1647	1.2
	HMDB0030930	1-Tridecene	C13H26	M+FA-H	227.2017	-1.1
	HMDB0061827	6-Tridecene	C13H26	M+FA-H	227.2017	-1.1
	HMDB0176318	1-hydroxytetradecan-3-one	C14H28O2	M-H	227.2017	-1.1
	HMDB0172395	2-hydroxy-tetradecaldehyde	C14H28O2	M-H	227.2017	-1.1
	HMDB0172394	SCHEMBL1959824	C14H28O2	M-H	227.2017	-1.1
	HMDB0172393	SCHEMBL4937612	C14H28O2	M-H	227.2017	-1.1
	HMDB0031072	12-Methyltridecanoic acid	C14H28O2	M-H	227.2017	-1.1
	HMDB0038969	Dodecyl acetate	C14H28O2	M-H	227.2017	-1.1
	HMDB0033788	Ethyl dodecanoate	C14H28O2	M-H	227.2017	-1.1
	HMDB0034461	Heptyl heptanoate	C14H28O2	M-H	227.2017	-1.1
	HMDB0037495	3-Methylbutyl nonanoate	C14H28O2	M-H	227.2017	-1.1
	HMDB0038034	Nonyl isovalerate	C14H28O2	M-H	227.2017	-1.1
	HMDB0037312	Decyl butanoate	C14H28O2	M-H	227.2017	-1.1
	HMDB0036216	Hexyl octanoate	C14H28O2	M-H	227.2017	-1.1
	HMDB0002221	2,6,-Trimethylundecanoic acid	C14H28O2	M-H	227.2017	-1.1
	HMDB0032318	Hexanal octane-1,3-diol acetal	C14H28O2	M-H	227.2017	-1.1
	HMDB0032548	Undecanal propyleneglycol acetal	C14H28O2	M-H	227.2017	-1.1
	HMDB0061781	-Methyltridecanoic acid	C14H28O2	M-H	227.2017	-1.1
	HMDB0059865	Isobutyl decanoate	C14H28O2	M-H	227.2017	-1.1
228.0991	HMDB0000806	Myristic acid	C14H28O2	M-H	227.2017	-1.1
	HMDB0034557	8,8-Diethoxy-2,6-dimethyl-2-octanol	C14H30O3	M-H2O-H	227.2011	1.3
	HMDB0028739	Asparaginy-Proline	C9H15N3O4	M-H	228.0990	0.5
	HMDB0029012	Prolyl-Asparagine	C9H15N3O4	M-H	228.0990	0.5
	HMDB0029059	Thr-Gln	C9H17N3O5	M-H2O-H	228.0984	2.9
	HMDB0028807	Glutaminythreonine	C9H17N3O5	M-H2O-H	228.0984	2.9
	HMDB0029075	Threoniny-Gamma-glutamate	C9H17N3O5	M-H2O-H	228.0984	2.9
	HMDB0163857	SCHEMBL11481214	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163859	3-hydroxyundec--en-2-one	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163858	9-(oxiran-2-yl)nonan-2-one	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163853	7-hydroxyundec--en-2-one	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163854	6-hydroxyundec--en-2-one	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0180763	4-Hydroxy-2-undecenal	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0180765	3-octyloxirane-2-carbaldehyde	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0180764	(2E)--hydroxyundec-2-enal	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0180766	(2E)-11-hydroxyundec-2-enal	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0175165	SCHEMBL15641446	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163860	1-hydroxyundec--en-2-one	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163856	4-hydroxyundec--en-2-one	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163855	5-hydroxyundec--en-2-one	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163235	{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}methanol	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163228	(5Z)-4-hydroxyundec-5-enal	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163229	(5Z)--hydroxyundec-5-enal	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163230	4-(3-pentyloxiran-2-yl)butanal	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163227	(5Z)-7-hydroxyundec-5-enal	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163232	(5Z)-2-hydroxyundec-5-enal	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163231	(5Z)-11-hydroxyundec-5-enal	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163234	(2E,5Z)-undeca-2,5-diene-1,1-diol	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163233	(2E,5Z)-undeca-2,5-diene-1,7-diol	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163236	(2E)-4-(3-pentyloxiran-2-yl)but-2-en-1-ol	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163852	8-hydroxyundec--en-2-one	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163245	5Z-undecenoic acid	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0163237	(2E,5Z)-undeca-2,5-diene-1,11-diol	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0038311	xi-gamma-Undecalactone	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0038273	2-Hexenyl valerate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0038278	cis-3-Hexenyl 3-methylbutanoate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0032308	(E)-3-Heptenyl 2-methylpropanoate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0036784	6-Hexyltetrahydro-2H-pyran-2-one	C11H20O2	M+FA-H	229.1445	-1.4

229.1442	HMDB0034428	Cyclohexyl 3-methylbutanoate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0034429	Cyclohexyl pentanoate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0037225	Methyl citronellate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0033724	Undecylenic acid	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0038277	cis-3-Hexenyl 2-methylbutanoate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0040593	2-Propenyl octanoate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0037185	Rhodinyl formate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0032396	Methyl 2-decenoate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0038274	2-Hexenyl isovalerate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0031843	2,3-Undecanedione	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0031062	(Z)-3-Methyl-3-decenoic acid	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0031272	Ethyl (E)-2-nonenoate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0031063	(Z)-3-Methyl-4-decenoic acid	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0031087	trans-2-Hexyl-1-cyclopropanecetic acid	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0033371	Citronellyl formate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0037106	(x)-1-Nonen-3-yl acetate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0036140	5-Hexyldihydro-5-methyl-2(3H)-furanone	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0031691	cis-3-Hexenyl pentanoate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0031406	Ethyl 3-cyclohexylpropionate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0038906	5-Octenyl propanoate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0037309	5-Hexyldihydro-4-methyl-2(3H)-furanone	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0032453	cis-3-Octenyl propionate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0032320	3-Hexenyl 2-methylbutyrate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0032489	Prenyl caproate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0032404	6-Methyl-5-hepten-2-one propyleneglycol acetal	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0062090	butyl cyclohexanecarboxylate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0032534	trans-2-Hexenyl 2-methylbutyrate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0032461	Pent-2-enyl hexanoate	C11H20O2	M+FA-H	229.1445	-1.4
	HMDB0030143	Talaromycin A	C12H22O4	M-H	229.1445	-1.5
	HMDB0041613	Bis(1-methylethyl) hexanedioate	C12H22O4	M-H	229.1445	-1.5
	HMDB0041614	Dipropyl hexanedioate	C12H22O4	M-H	229.1445	-1.5
	HMDB0000623	Dodecanedioic acid	C12H22O4	M-H	229.1445	-1.5
230.1520	HMDB0036031	Labienoxime	C13H23NO	M+Na-2H	230.1526	-2.7
231.0877	HMDB0031640	Glycerol 1-propanoate diacetate	C10H16O6	M-H	231.0874	1.2
	HMDB0030992	5-Butyltetrahydro-2-oxo-3-furancarboxylic acid	C9H14O4	M+FA-H	231.0874	1.3
	HMDB0030988	5-(2-Methylpropyl)tetrahydro-2-oxo-3-furancarboxylic acid	C9H14O4	M+FA-H	231.0874	1.3
231.1751	HMDB0240361	(7Z,Z,13Z)-hexadecatrienoate	C16H25O2	M-H2O-H	231.1749	0.9
	HMDB0159344	(7Z,Z)-hexadeca-7,,15-trienoic acid	C16H26O2	M-H2O-H	231.1749	0.9
	HMDB0061952	AC1LBPUV	C16H26O2	M-H2O-H	231.1749	0.9
	HMDB0035293	Norambreinolide	C16H26O2	M-H2O-H	231.1749	0.9
	HMDB0037631	3-Methyl-alpha-ionyl acetate	C16H26O2	M-H2O-H	231.1749	0.9
	HMDB0037712	[2,2-Bis(2-methylpropoxy)ethyl]benzene	C16H26O2	M-H2O-H	231.1749	0.9
	HMDB0029704	1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1,6-heptadien-3-one	C16H24O	M-H	231.1754	-1.5
	HMDB0179144	1,7-dimethyl-4-(propan-2-yl)-11-oxabicyclo[8.1]undecane-3,6-dione	C15H24O3	M-H2O-H	233.1542	1.1
	HMDB0182320	7-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H2O-H	233.1542	1.1
	HMDB0182321	7-hydroxy--(hydroxymethyl)-6-methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H2O-H	233.1542	1.1
	HMDB0182317	2-hydroxy-6-(hydroxymethyl)--methyl-3-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H2O-H	233.1542	1.1
	HMDB0037969	Urodienone	C15H24O3	M-H2O-H	233.1542	1.1
	HMDB0182316	1-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H2O-H	233.1542	1.1
	HMDB0182318	1-hydroxy-6-(hydroxymethyl)--methyl-3-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H2O-H	233.1542	1.1
	HMDB0182319	6-(hydroxymethyl)--methyl-2-(2-methyloxiran-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H2O-H	233.1542	1.1
	HMDB0032122	3(4->5)-Abeo-4,11:4,12-diepoxy-3-eudesmanol	C15H24O3	M-H2O-H	233.1542	1.1
	HMDB0112086	5-(3-methyl-5-pentylfuran-2-yl)-pentanoic acid	C15H24O3	M-H2O-H	233.1542	1.1
	HMDB0112094	3-Methyl-5-propyl-2-furanheptanoic acid	C15H24O3	M-H2O-H	233.1542	1.1
	HMDB0184273	(4aS)-4a-(hydroxymethyl)-4-methyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M-H2O-H	233.1542	1.1

HMDB0184275	(4aR)-4,4a-dimethyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3,7-triol	C15H24O3	M-H20-H	233.1542	1.1
HMDB0037063	Toxin FS2	C15H24O3	M-H20-H	233.1542	1.1
HMDB0183496	(8aS)-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalene-1,2,4-triol	C15H24O3	M-H20-H	233.1542	1.1
HMDB0183500	(4aR)-4,4a-dimethyl-6-(2-methyloxiran-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M-H20-H	233.1542	1.1
HMDB0183498	(4aR)-6-(3-hydroxyprop-1-en-2-yl)-4,4a-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M-H20-H	233.1542	1.1
HMDB0183495	(4aR)-4-(hydroxymethyl)-4a-methyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M-H20-H	233.1542	1.1
HMDB0182313	6-hydroxy--(hydroxymethyl)-6-methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H20-H	233.1542	1.1
HMDB0182314	2-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H20-H	233.1542	1.1
HMDB0030918	1-Hydroxyepiacorone	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179140	(6Z)--(hydroxymethyl)-6-methyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M-H20-H	233.1542	1.1
HMDB0035597	alpha-Carissanol	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179142	(6Z)-3-(2-hydroxypropan-2-yl)-6,-dimethylcyclodec-6-ene-1,4-dione	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179143	(6Z)-8-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179269	1-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179141	(6Z)--hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179145	(6Z)-3-(1-hydroxypropan-2-yl)-6,-dimethylcyclodec-6-ene-1,4-dione	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179147	(6Z)-2-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179148	(6Z)-3-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179266	6-[4-hydroxy-4-(hydroxymethyl)cyclohex-2-en-1-yl]-2-methylhept-2-en-4-one	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179146	(6Z)-5-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179257	1,8a-dihydroxy-1,4-dimethyl-7-(propan-2-ylidene)-decahydroazulen-6-one	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179258	3,3a-dihydroxy-3,8-dimethyl-5-(propan-2-yl)-1,2,3,3a,4,5,6,8a-octahydroazulen-6-one	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179139	(6E)-6-(hydroxymethyl)--methyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179267	6-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M-H20-H	233.1542	1.1
HMDB0182312	6,-bis(hydroxymethyl)-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H20-H	233.1542	1.1
HMDB0182315	6-(hydroxymethyl)-2-(3-hydroxyprop-1-en-2-yl)--methylspiro[4.5]decan-8-one	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179270	1-(3,3-dimethyloxiran-2-yl)-3-(4-hydroxy-4-methylcyclohex-2-en-1-yl)butan-1-one	C15H24O3	M-H20-H	233.1542	1.1
HMDB0035729	Dihydromyoporone	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179271	6-{5-hydroxy-5-methyl-7-oxabicyclo[4.1]heptan-2-yl}-2-methylhept-2-en-4-one	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179273	5-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M-H20-H	233.1542	1.1
HMDB0168751	(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trienal	C15H24O3	M-H20-H	233.1542	1.1
HMDB0177221	(4aR,7aS,7bR)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4-diol	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179272	7-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M-H20-H	233.1542	1.1
HMDB0179268	6-(1,4-dihydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M-H20-H	233.1542	1.1

HMDB0033149	(4R,5S,7R,11R)-11,12-Dihydroxy-1(-)-spirovetiven-2-one	C15H24O3	M-H20-H	233.1542	1.1
HMDB0038502	Bisacurone B	C15H24O3	M-H20-H	233.1542	1.1
HMDB0035309	6alpha-Carissanol	C15H24O3	M-H20-H	233.1542	1.1
HMDB0035767	Piperlol	C15H24O3	M-H20-H	233.1542	1.1
HMDB0030919	Acorusdiol	C15H24O3	M-H20-H	233.1542	1.1
HMDB0040685	2,3-Dihydroabscisic alcohol	C15H24O3	M-H20-H	233.1542	1.1
HMDB0034574	Apotrichodiol	C15H24O3	M-H20-H	233.1542	1.1
HMDB0036663	Hydroxypelenolide	C15H24O3	M-H20-H	233.1542	1.1
HMDB0035613	Epioxylubimin	C15H24O3	M-H20-H	233.1542	1.1
HMDB0036448	Zedoarondiol	C15H24O3	M-H20-H	233.1542	1.1
HMDB0183493	(8aR)-4-hydroxy-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O2	M-H	233.1547	-1.3
HMDB0240643	3,5-di-tert-butyl-4-hydroxybenzaldehyde	C15H22O2	M-H	233.1547	-1.3
HMDB0134142	(2-hexyl-3-phenyloxiran-2-yl)methanol	C15H22O2	M-H	233.1547	-1.3
HMDB0134141	(2Z)-2-(phenylmethylidene)octane-1,7-diol	C15H22O2	M-H	233.1547	-1.3
HMDB0134138	2-(phenylmethylidene)octane-1,3-diol	C15H22O2	M-H	233.1547	-1.3
HMDB0134140	4-[(1Z)-2-hexyl-3-hydroxyprop-1-en-1-yl]phenol	C15H22O2	M-H	233.1547	-1.3
HMDB0134143	(2Z)-2-(phenylmethylidene)octane-1,8-diol	C15H22O2	M-H	233.1547	-1.3
HMDB0177700	(1E)-1-ethylidene-5-hydroxy-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O2	M-H	233.1547	-1.3
HMDB0177624	(1Z)-1-ethylidene-5-hydroxy-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O2	M-H	233.1547	-1.3
HMDB0150675	2,5,5,8a-tetramethyl-6-oxo-1,4,4a,5,6,7,8,8a-octahydronaphthalene-1-carbaldehyde	C15H22O2	M-H	233.1547	-1.3
HMDB0134153	2-benzyl-octanoic acid	C15H22O2	M-H	233.1547	-1.3
HMDB0134136	2-benzyl-2-hydroxyoctanal	C15H22O2	M-H	233.1547	-1.3
HMDB0134131	2-[hydroxy(phenyl)methyl]octanal	C15H22O2	M-H	233.1547	-1.3
HMDB0134132	2-[(3-hydroxyphenyl)methyl]octanal	C15H22O2	M-H	233.1547	-1.3
HMDB0134137	2-[(2-hydroxyphenyl)methyl]octanal	C15H22O2	M-H	233.1547	-1.3
HMDB0134139	3-[(1Z)-2-hexyl-3-hydroxyprop-1-en-1-yl]phenol	C15H22O2	M-H	233.1547	-1.3
HMDB0134135	2-benzyl-8-hydroxyoctanal	C15H22O2	M-H	233.1547	-1.3
HMDB0134134	2-benzyl-7-hydroxyoctanal	C15H22O2	M-H	233.1547	-1.3
HMDB0134133	2-[(4-hydroxyphenyl)methyl]octanal	C15H22O2	M-H	233.1547	-1.3
HMDB0035408	1,-Epoxygermacrone	C15H22O2	M-H	233.1547	-1.3
HMDB0037710	4-Methylphenyl octanoate	C15H22O2	M-H	233.1547	-1.3
HMDB0035639	Petasalbin	C15H22O2	M-H	233.1547	-1.3
HMDB0037391	p-Hydroxynonanophenone	C15H22O2	M-H	233.1547	-1.3
HMDB0038190	Rishitinol	C15H22O2	M-H	233.1547	-1.3
HMDB0038795	7,9-Illudadiene-3,14-diol	C15H22O2	M-H	233.1547	-1.3
HMDB0036390	3-Phenylpropyl hexanoate	C15H22O2	M-H	233.1547	-1.3
HMDB0041036	Sugeonol	C15H22O2	M-H	233.1547	-1.3
HMDB0038796	2,7(14)-Illudadiene-1,15-diol	C15H22O2	M-H	233.1547	-1.3
HMDB0034742	Saussurea lactone	C15H22O2	M-H	233.1547	-1.3
HMDB0033253	Curcumenone	C15H22O2	M-H	233.1547	-1.3
HMDB0030016	Valerenic acid	C15H22O2	M-H	233.1547	-1.3
HMDB0038698	xi-2-Hydroxy-1,3,5-bisabolatrien-9-one	C15H22O2	M-H	233.1547	-1.3
HMDB0036647	Isocurcumenol	C15H22O2	M-H	233.1547	-1.3
HMDB0039621	beta-Santalal acid	C15H22O2	M-H	233.1547	-1.3
HMDB0034562	9-Pentadecene-12,14-diyne-1,11-diol	C15H22O2	M-H	233.1547	-1.3
HMDB0036449	(1alpha,4beta,5beta)-4-Hydroxy-7(11),(14)-guaiadien-8-one	C15H22O2	M-H	233.1547	-1.3
HMDB0033960	Curcumenol	C15H22O2	M-H	233.1547	-1.3
HMDB0035935	Dihydroisoalantolactone	C15H22O2	M-H	233.1547	-1.3
HMDB0031349	Epiacoronene	C15H22O2	M-H	233.1547	-1.3
HMDB0035413	(4alpha,5alpha)-11-Eremophilene-2,9-dione	C15H22O2	M-H	233.1547	-1.3
HMDB0036392	(Z)-alpha-Bergamotenoic acid	C15H22O2	M-H	233.1547	-1.3
HMDB0034956	Oxysolavetivone	C15H22O2	M-H	233.1547	-1.3
HMDB0035869	alpha-Rotunol	C15H22O2	M-H	233.1547	-1.3
HMDB0038914	4,6-Decadiyn-1-ol isovalerate	C15H22O2	M-H	233.1547	-1.3
HMDB0033252	Curcumanolide A	C15H22O2	M-H	233.1547	-1.3
HMDB0036466	Zerumbone oxide	C15H22O2	M-H	233.1547	-1.3
HMDB0037640	2-Methyl-4-phenyl-2-butyl 2-methylpropanoate	C15H22O2	M-H	233.1547	-1.3
HMDB0035202	7-Hydroxycostal	C15H22O2	M-H	233.1547	-1.3
HMDB0038198	3,7-Bisaboladiene-2,8-dione	C15H22O2	M-H	233.1547	-1.3

	HMDB0037038	Cyclodehydroisolubimin	C15H22O2	M-H	233.1547	-1.3
	HMDB0035407	Dehydrocurdione	C15H22O2	M-H	233.1547	-1.3
	HMDB0032081	4,-Longipinanedione	C15H22O2	M-H	233.1547	-1.3
	HMDB0036035	Acutissimin A	C15H22O2	M-H	233.1547	-1.3
	HMDB0035889	Germacrone 4,5-epoxide	C15H22O2	M-H	233.1547	-1.3
	HMDB0037739	7-(1,3-Cyclohexadienyl)-5-hydroxy-2,6-dimethyl-2-hepten-4-one	C15H22O2	M-H	233.1547	-1.3
	HMDB0036427	Procurecumenol	C15H22O2	M-H	233.1547	-1.3
234.1614	HMDB0035794	beta-Costic acid	C15H22O2	M-H	233.1547	-1.3
	HMDB0015169	Procainamide	C13H21N3O	M-H	234.1612	0.9
235.1337	HMDB0037763	xi-3-(4-Isopropylphenyl)-2-methylpropanal	C13H18O	M+FA-H	235.1340	-1.1
	HMDB0151806	2-benzylhex-5-en-1-ol	C13H18O	M+FA-H	235.1340	-1.1
	HMDB0151770	2-Benzylidene-1-hexanol	C13H18O	M+FA-H	235.1340	-1.1
	HMDB0151769	2-benzylhexanal	C13H18O	M+FA-H	235.1340	-1.1
	HMDB0059906	Megastigmatrienone	C13H18O	M+FA-H	235.1340	-1.1
	HMDB0036178	2-(3-Phenylpropyl)tetrahydrofuran	C13H18O	M+FA-H	235.1340	-1.1
	HMDB0036685	2,2,6,7-Tetramethylbicyclo[4.3]nona-1(9),4-dien-8-one	C13H18O	M+FA-H	235.1340	-1.1
	HMDB0059904	dehydro-beta-Ionone	C13H18O	M+FA-H	235.1340	-1.1
	HMDB0013804	beta-Damascenone	C13H18O	M+FA-H	235.1340	-1.1
	HMDB0036572	beta-Damascenone	C13H18O	M+FA-H	235.1340	-1.1
	HMDB0034462	Heptyl 4-hydroxybenzoate	C14H20O3	M-H	235.1340	-1.1
	HMDB0040778	Eremopetasidione	C14H20O3	M-H	235.1340	-1.1
	HMDB0040276	5-Acetoxydihydrotheaespirane	C15H26O3	M-H2O-H	235.1698	0.8
	HMDB0179277	2-(1,4-dihydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M-H2O-H	235.1698	0.8
	HMDB0179279	1-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylheptan-4-one	C15H26O3	M-H2O-H	235.1698	0.8
	HMDB0179278	2-{5-hydroxy-5-methyl-7-oxabicyclo[4.1]heptan-2-yl}-6-methylheptan-4-one	C15H26O3	M-H2O-H	235.1698	0.8
	HMDB0179281	3-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylheptan-4-one	C15H26O3	M-H2O-H	235.1698	0.8
	HMDB0029604	Lubiminol	C15H26O3	M-H2O-H	235.1698	0.8
	HMDB0179280	1-hydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M-H2O-H	235.1698	0.8
	HMDB0179282	3-hydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M-H2O-H	235.1698	0.8
	HMDB0036866	7-Drimene-11,12,14-triol	C15H26O3	M-H2O-H	235.1698	0.8
	HMDB0179274	2-[4-hydroxy-4-(hydroxymethyl)cyclohex-2-en-1-yl]-6-methylheptan-4-one	C15H26O3	M-H2O-H	235.1698	0.8
	HMDB0035780	8-Hydroxy-4(6)-lactarene-5,14-diol	C15H26O3	M-H2O-H	235.1698	0.8
	HMDB0179276	2-hydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M-H2O-H	235.1698	0.8
	HMDB0037197	Kessyl glycol	C15H26O3	M-H2O-H	235.1698	0.8
	HMDB0179275	2-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylheptan-4-one	C15H26O3	M-H2O-H	235.1698	0.8
	HMDB0036053	(3beta,9beta)-7-Drimene-3,11,12-triol	C15H26O3	M-H2O-H	235.1698	0.8
	HMDB0094670	1,4-Di-tert-butylbenzene	C14H22	M+FA-H	235.1704	-1.5
	HMDB0061923	1,3-Di-tert-butylbenzene	C14H22	M+FA-H	235.1704	-1.5
	HMDB0059739	1-Ethyl-3,5-diisopropyl-benzene	C14H22	M+FA-H	235.1704	-1.5
	HMDB0013820	2-Methyl-2-phenyl-undecane	C14H22	M+FA-H	235.1704	-1.5
	HMDB0177920	[3-(3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl)-2-methyloxiran-2-yl]methanol	C15H24O2	M-H	235.1704	-1.5
	HMDB0179226	5-(hydroxymethyl)-1,1,2-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-ol	C15H24O2	M-H	235.1704	-1.5
	HMDB0177914	(2E)-3-[3-(hydroxymethyl)-7-methyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl]-2-methylprop-2-en-1-ol	C15H24O2	M-H	235.1704	-1.5
	HMDB0177915	(2E)-3-[7-(hydroxymethyl)-3-methyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl]-2-methylprop-2-en-1-ol	C15H24O2	M-H	235.1704	-1.5
	HMDB0179225	2-(hydroxymethyl)-1,1,5-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-ol	C15H24O2	M-H	235.1704	-1.5
	HMDB0179228	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,6-diol	C15H24O2	M-H	235.1704	-1.5

235.1700

HMDB0179224	1-(hydroxymethyl)-1,2,5-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-ol	C15H24O2	M-H	235.1704	-1.5
HMDB0177917	2-[(3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl)methylidene]propane-1,3-diol	C15H24O2	M-H	235.1704	-1.5
HMDB0177916	4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-7-ol	C15H24O2	M-H	235.1704	-1.5
HMDB0177919	4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-1-ol	C15H24O2	M-H	235.1704	-1.5
HMDB0177918	4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-2-ol	C15H24O2	M-H	235.1704	-1.5
HMDB0179229	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,3-diol	C15H24O2	M-H	235.1704	-1.5
HMDB0182081	(2Z)-5-[3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-en-1-ol	C15H24O2	M-H	235.1704	-1.5
HMDB0182082	(2Z)-5-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-ene-1,5-diol	C15H24O2	M-H	235.1704	-1.5
HMDB0182086	[3-(2-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]ethyl)-2-methyloxiran-2-yl]methanol	C15H24O2	M-H	235.1704	-1.5
HMDB0182084	(2Z)-5-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-ene-1,4-diol	C15H24O2	M-H	235.1704	-1.5
HMDB0182085	7-[(3Z)-5-hydroxy-4-methylpent-3-en-1-yl]-1,7-dimethyltricyclo[2.2.1,heptan-3-ol	C15H24O2	M-H	235.1704	-1.5
HMDB0182080	(2Z)-5-[2-(hydroxymethyl)-3-methyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-en-1-ol	C15H24O2	M-H	235.1704	-1.5
HMDB0179227	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,4-diol	C15H24O2	M-H	235.1704	-1.5
HMDB0179231	1,1,4,7-tetramethyl-1H,1aH,2H,3H,5H,6H,7H,7aH,7bH-cyclopropa[e]azulene-7,7b-diol	C15H24O2	M-H	235.1704	-1.5
HMDB0179230	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,7a-diol	C15H24O2	M-H	235.1704	-1.5
HMDB0182087	3-[(3Z)-5-hydroxy-4-methylpent-3-en-1-yl]-2,3-dimethyltricyclo[2.2.1,heptan-1-ol	C15H24O2	M-H	235.1704	-1.5
HMDB0166723	396--2	C15H24O2	M-H	235.1704	-1.5
HMDB0182083	2-(3-{2,3-dimethyltricyclo[2.2.1,]heptan-3-yl}propylidene)propane-1,3-diol	C15H24O2	M-H	235.1704	-1.5
HMDB0166722	UNII-7B7Y8CEM7E	C15H24O2	M-H	235.1704	-1.5
HMDB0166721	2,4-di-tert-butyl-6-methylbenzene-1,3-diol	C15H24O2	M-H	235.1704	-1.5
HMDB0163044	(2Z)-5-(5-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl)-3-methylpent-2-enal	C15H24O2	M-H	235.1704	-1.5
HMDB0150688	5-(hydroxymethyl)-1,1,4a,6-tetramethyl-1,2,3,4,4a,5,8,8a-octahydronaphthalen-2-one	C15H24O2	M-H	235.1704	-1.5
HMDB0137903	6-hydroxy-5,5,8a-trimethyl-2-methylidene-decahydronaphthalene-1-carbaldehyde	C15H24O2	M-H	235.1704	-1.5
HMDB0002352	Capsidiol	C15H24O2	M-H	235.1704	-1.5
HMDB0035301	4alpha,5alpha-Epoxy-11-eudesmen-3a-ol	C15H24O2	M-H	235.1704	-1.5
HMDB0030916	2-Hydroxyacorenone	C15H24O2	M-H	235.1704	-1.5
HMDB0032048	2,6-Di-tert-butyl-4-hydroxymethylphenol	C15H24O2	M-H	235.1704	-1.5
HMDB0036680	Cyperolone	C15H24O2	M-H	235.1704	-1.5
HMDB0035032	Epilubimin	C15H24O2	M-H	235.1704	-1.5
HMDB0036687	Tanavulgarol	C15H24O2	M-H	235.1704	-1.5
HMDB0038144	Petasitolone	C15H24O2	M-H	235.1704	-1.5
HMDB0034722	3-Hydroxy-1,-bisaboladien-9-one	C15H24O2	M-H	235.1704	-1.5
HMDB0038178	Davanone	C15H24O2	M-H	235.1704	-1.5
HMDB0037393	(3xi,7(11)Z)-7(11)-Copaene-4,12-diol	C15H24O2	M-H	235.1704	-1.5
HMDB0035040	7-Hydroxycostol	C15H24O2	M-H	235.1704	-1.5
HMDB0035827	Aubergenone	C15H24O2	M-H	235.1704	-1.5
HMDB0036446	(4alpha,alpha)-1(5),6-Guaiadiene	C15H24O2	M-H	235.1704	-1.5
HMDB0032681	alpha-4,5-Seco-11-eudesmene-4,5-dione	C15H24O2	M-H	235.1704	-1.5

	HMDB0031348	Epiacorone	C15H24O2	M-H	235.1704	-1.5
	HMDB0030891	(2E,6E)-1-Hydroxy-2,6,-farnesatrien-9-one	C15H24O2	M-H	235.1704	-1.5
	HMDB0039688	Tuberone	C15H24O2	M-H	235.1704	-1.5
	HMDB0035147	Rishitinone	C15H24O2	M-H	235.1704	-1.5
	HMDB0030920	Acorusnol	C15H24O2	M-H	235.1704	-1.5
	HMDB0039525	Isomelitic acid A	C15H24O2	M-H	235.1704	-1.5
	HMDB0036668	Humulene-8-hydroperoxide	C15H24O2	M-H	235.1704	-1.5
	HMDB0035648	Isolubimin	C15H24O2	M-H	235.1704	-1.5
	HMDB0035127	(-)-Myrtenyl isovalerate	C15H24O2	M-H	235.1704	-1.5
	HMDB0036549	Apotrichothecene	C15H24O2	M-H	235.1704	-1.5
	HMDB0037906	Hernandulcin	C15H24O2	M-H	235.1704	-1.5
	HMDB0034714	Curdione	C15H24O2	M-H	235.1704	-1.5
	HMDB0033104	Calamensesquiterpinenol	C15H24O2	M-H	235.1704	-1.5
	HMDB0033083	(4S)-Dihydrocurcumenone	C15H24O2	M-H	235.1704	-1.5
	HMDB0040712	Humulene diepoxide A	C15H24O2	M-H	235.1704	-1.5
	HMDB0038027	beta-Ionyl acetate	C15H24O2	M-H	235.1704	-1.5
	HMDB0038122	5-Methyl-5-hexen-2-one	C15H24O2	M-H	235.1704	-1.5
	HMDB0032292	Geranyl tiglate	C15H24O2	M-H	235.1704	-1.5
236.1417	HMDB0015508	Fencamfamine	C15H21N	M+Na-2H	236.1421	-1.5
237.0765	HMDB0141330	2-hydroxy-3-(3,4,5-trimethoxyphenyl)propanoic acid	C12H16O6	M-H2O-H	237.0763	0.9
	HMDB0141333	3-(2-hydroxy-3,4,5-trimethoxyphenyl)propanoic acid	C12H16O6	M-H2O-H	237.0763	0.9
	HMDB0141328	3-hydroxy-3-(3,4,5-trimethoxyphenyl)propanoic acid	C12H16O6	M-H2O-H	237.0763	0.9
	HMDB0142082	2-hydroxy-3-(2,3,4-trimethoxyphenyl)propanoic acid	C12H16O6	M-H2O-H	237.0763	0.9
	HMDB0142088	3-(6-hydroxy-2,3,4-trimethoxyphenyl)propanoic acid	C12H16O6	M-H2O-H	237.0763	0.9
	HMDB0142079	3-hydroxy-3-(2,3,4-trimethoxyphenyl)propanoic acid	C12H16O6	M-H2O-H	237.0763	0.9
	HMDB0146436	SCHEMBL7293162	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0146409	3-(3-methoxyphenyl)-2-methylprop-2-enoic acid	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0137170	2-[(1E)-3-methylbuta-1,3-dien-1-yl]benzene-1,3,5-triol	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0133534	1-hydroxy-4-(3-methoxyphenyl)but-3-en-2-one	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0133510	4-(3-hydroxy-5-methoxyphenyl)but-3-en-2-one	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0126381	2,2-dimethyl-2H-chromene-5,6-diol	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0151223	AC1L67O8	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0126382	5,5-dimethyl-3,6-dioxatricyclo[5.4.undeca-1(11),7,9-trien-11-ol	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0133482	1-(3-methoxyphenyl)butane-2,3-dione	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0133477	(3Z)-3-hydroxy-4-(3-methoxyphenyl)but-3-en-2-one	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0129370	1-(4-methoxy-1-benzofuran-5-yl)ethan-1-ol	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0126383	2-(hydroxymethyl)-2-methyl-2H-chromen-5-ol	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0126380	2,2-dimethyl-2H-chromene-5,7-diol	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0146664	2-hydroxyethyl 3-phenylprop-2-enoate	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0062067	5-[(4-hydroxyphenyl)methyl]oxolan-2-one	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0131282	ethyl (2E)-3-(4-hydroxyphenyl)prop-2-enoate	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0062066	5-[(3-hydroxyphenyl)methyl]oxolan-2-one	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0182825	4-methoxybenzyl acrylate	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0170975	2-hydroxy-4-[(1Z)-prop-1-en-1-yl]phenyl acetate	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0133439	4-(4-hydroxy-3-methoxyphenyl)but-3-en-2-one	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0170844	2-hydroxy-4-(prop-2-en-1-yl)phenyl acetate	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0031623	Ethyl phenylglycidate	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0032591	Dehydrozingerone	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0035873	Myristicin	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0030580	(R)-Shinanolone	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0035894	(Z)-4-Methoxy-6-(1-propenyl)-1,3-benzodioxole	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0041007	1'-Hydroxychavicol acetate	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0040446	Benzyl acetoacetate	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0030752	Methyl trans-p-methoxycinnamate	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0035275	Isomyristicin	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0041481	4-(3,4-Methylenedioxyphenyl)-2-butanone	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0040268	Ethyl 3-oxo-3-phenylpropanoate	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0037277	Isoeugenol formate	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0031610	Allyl phenoxyacetate	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0037877	Eugenyl formate	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0151227	3-(4-methoxyphenyl)-2-methyloxirane-2-carbaldehyde	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0151224	2-(hydroxymethyl)-3-(4-methoxyphenyl)prop-2-enal	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0151226	3-(2-hydroxy-4-methoxyphenyl)-2-methylprop-2-enal	C11H12O3	M+FA-H	237.0768	-1.5
	HMDB0146665	3-(3-hydroxy-phenyl)-acrylic acid ethyl ester	C11H12O3	M+FA-H	237.0768	-1.5

	HMDB0169591	5-(6-hydroxy-2H-1,3-benzodioxol-5-yl)pentanoic acid	C12H14O5	M-H	237.0768	-1.5
	HMDB0169590	AKO2231	C12H14O5	M-H	237.0768	-1.5
	HMDB0169592	AKO222717	C12H14O5	M-H	237.0768	-1.5
	HMDB0169593	5-(2H-1,3-benzodioxol-5-yl)-2-hydroxypentanoic acid	C12H14O5	M-H	237.0768	-1.5
	HMDB0128658	3-(6,7-dimethoxy-2H-1,3-benzodioxol-5-yl)propanal	C12H14O5	M-H	237.0768	-1.5
	HMDB0137272	3-(4,7-dimethoxy-2H-1,3-benzodioxol-5-yl)propanal	C12H14O5	M-H	237.0768	-1.5
	HMDB0169153	4,7-dihydroxy-2,2-dimethyl-3,4-dihydro-2H-1-benzopyran-6-carboxylic acid	C12H14O5	M-H	237.0768	-1.5
	HMDB0166244	4,7-dimethoxy-5-[(oxiran-2-yl)methyl]-2H-1,3-benzodioxole	C12H14O5	M-H	237.0768	-1.5
	HMDB0166241	4,7-dimethoxy-6-(prop-2-en-1-yl)-2H-1,3-benzodioxol-5-ol	C12H14O5	M-H	237.0768	-1.5
	HMDB0169589	5-(2H-1,3-benzodioxol-5-yl)-4-hydroxypentanoic acid	C12H14O5	M-H	237.0768	-1.5
	HMDB0128697	3-(4-hydroxy-2,3,5-trimethoxyphenyl)prop-2-enal	C12H14O5	M-H	237.0768	-1.5
	HMDB0137273	3-(4,7-dimethoxy-2H-1,3-benzodioxol-5-yl)prop-2-en-1-ol	C12H14O5	M-H	237.0768	-1.5
	HMDB0011721	Trans-2, 3, 4-Trimethoxycinnamate	C12H14O5	M-H	237.0768	-1.5
	HMDB0031771	1-(2,4,5-Trimethoxyphenyl)-1,2-propanedione	C12H14O5	M-H	237.0768	-1.5
	HMDB0002511	3,4,5-Trimethoxycinnamic acid	C12H14O5	M-H	237.0768	-1.5
	HMDB0128659	3-(6,7-dimethoxy-2H-1,3-benzodioxol-5-yl)prop-2-en-1-ol	C12H14O5	M-H	237.0768	-1.5
	HMDB0124869	3-(3,4,5-trimethoxyphenyl)prop-2-enoic acid	C12H14O5	M-H	237.0768	-1.5
237.1493	HMDB0036143	Monomenthyl succinate	C14H24O4	M-H20-H	237.1491	1.0
	HMDB0062364	(6S,8Z)-6-Hydroxy-3-oxotetradecenoic acid	C14H24O4	M-H20-H	237.1491	1.0
	HMDB0062363	(6R,8Z)-6-Hydroxy-3-oxotetradecenoic acid	C14H24O4	M-H20-H	237.1491	1.0
	HMDB0030993	5-Nonyltetrahydro-2-oxo-3-furancarboxylic acid	C14H24O4	M-H20-H	237.1491	1.0
	HMDB0151804	2-benzylhexan-1-ol	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0035682	delta-Damascone	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0041615	Phenethyl isoamyl ether	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0029825	2,3-Diisopropyl-5-methylphenol	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0035753	(R)-(E)-4,7-Megastigmadien-9-one	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0036022	Isospirene	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0034959	Edulan I	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0031733	4-(4-Methyl-3-pentenyl)-3-cyclohexene-1-carboxaldehyde	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0036818	Vitispirane	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0034671	(E)-5,8-Megastigmadien-4-one	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0029823	2,4-Diisopropyl-5-methylphenol	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0036027	alpha-Damascone	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0059883	alpha-Ionone	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0036684	2,4,5,7alpha-Tetrahydro-1,4,4,7a-tetramethyl-1H-inden-2-ol	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0033545	(2E,4Z,7Z)-2,4,7-Tridecatrienal	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0036565	beta-Ionone	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0036144	Cycloionone	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0034979	gamma-Ionone	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0029822	2,5-Diisopropyl-3-methylphenol	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0029824	2,4-Diisopropyl-3-methylphenol	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0029820	2,6-Diisopropyl-3-methylphenol	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0032498	Pseudoionone	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0032541	4-(2,6,6-Trimethylcyclohex-1-enyl)but-2-en-4-one	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0037139	4-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-butanone	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0029821	2,5-Diisopropyl-4-methylphenol	C13H20O	M+FA-H	237.1496	-1.3
	HMDB0038256	Geranyl acetoacetate	C14H22O3	M-H	237.1496	-1.3
	HMDB0112083	3-(3,4-dimethyl-5-pentylfuran-2-yl)-propanoic acid	C14H22O3	M-H	237.1496	-1.3
	HMDB0061832	1-Acetyl-2-methylcyclopentene	C14H24	M+FA-H	237.1860	-0.9
	HMDB0061847	1-Acetyl-2-methylcyclopentene	C14H24	M+FA-H	237.1860	-0.9
	HMDB0182764	4a-(hydroxymethyl)-8-methylidene-2-(propan-2-yl)-decahydronaphthalen-1-ol	C15H26O2	M-H	237.1860	-0.9
	HMDB0182767	2-(1-hydroxypropan-2-yl)-4a-methyl-8-methylidene-decahydronaphthalen-1-ol	C15H26O2	M-H	237.1860	-0.9
	HMDB0182220	3-(2-hydroxypropan-2-yl)-4a,5-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalen-1-ol	C15H26O2	M-H	237.1860	-0.9
	HMDB0182219	7-(2-hydroxypropan-2-yl)-1,8a-dimethyl-1,2,3,5,6,7,8,8a-octahydronaphthalen-1-ol	C15H26O2	M-H	237.1860	-0.9

237.1858	HMDB0182221	6-(2-hydroxypropan-2-yl)-4,4a-dimethyl-2,3,4,4a,5,6,7,8-octahydronaphthalen-2-ol	C15H26O2	M-H	237.1860	-0.9
	HMDB0182217	2-[8a-(hydroxymethyl)-8-methyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl]propan-2-ol	C15H26O2	M-H	237.1860	-0.9
	HMDB0182218	2-[8-(hydroxymethyl)-8a-methyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl]propan-2-ol	C15H26O2	M-H	237.1860	-0.9
	HMDB0179265	2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O2	M-H	237.1860	-0.9
	HMDB0041589	alpha-Kessyl alcohol	C15H26O2	M-H	237.1860	-0.9
	HMDB0038247	Bornyl valerate	C15H26O2	M-H	237.1860	-0.9
	HMDB0036730	Tricyclohumuladiol	C15H26O2	M-H	237.1860	-0.9
	HMDB0038196	alpha-Bisabolol oxide A	C15H26O2	M-H	237.1860	-0.9
	HMDB0037284	5(1->)-Abeo-1,12-patchoulanediol	C15H26O2	M-H	237.1860	-0.9
	HMDB0036880	1,6,9-Farnesatriene-3,11-diol	C15H26O2	M-H	237.1860	-0.9
	HMDB0037279	2,-Bisaboladiene-1,4-diol	C15H26O2	M-H	237.1860	-0.9
	HMDB0034673	Calamendiol	C15H26O2	M-H	237.1860	-0.9
	HMDB0031383	(3S,4S,6R,7S)-1,-Bisaboladiene-3,4-diol	C15H26O2	M-H	237.1860	-0.9
	HMDB0038250	Isobornyl isovalerate	C15H26O2	M-H	237.1860	-0.9
	HMDB0033228	Guadiol	C15H26O2	M-H	237.1860	-0.9
	HMDB0036032	3beta-7-Drimene-3,11-diol	C15H26O2	M-H	237.1860	-0.9
	HMDB0031384	beta-Kessyl alcohol	C15H26O2	M-H	237.1860	-0.9
	HMDB0035887	Germacrene	C15H26O2	M-H	237.1860	-0.9
	HMDB0039130	Methyl (Z,Z)-5,8-tetradecadienoate	C15H26O2	M-H	237.1860	-0.9
	HMDB0039745	(2E,6E,9xi)-Farnesol	C15H26O2	M-H	237.1860	-0.9
	HMDB0040273	Terpenyl isovalerate	C15H26O2	M-H	237.1860	-0.9
	HMDB0032054	alpha-Terpinyl pentanoate	C15H26O2	M-H	237.1860	-0.9
	HMDB0038248	Bornyl isovalerate	C15H26O2	M-H	237.1860	-0.9
	HMDB0062130	methyl tetradec-13-ynoate	C15H26O2	M-H	237.1860	-0.9
	HMDB0032343	Isobornyl 2-methylbutyrate	C15H26O2	M-H	237.1860	-0.9
	HMDB0032209	Citronellyl trans-2-methyl-2-butenate	C15H26O2	M-H	237.1860	-0.9
	HMDB0032291	Geranyl 2-methylbutyrate	C15H26O2	M-H	237.1860	-0.9
	HMDB0035287	Daucol	C15H26O2	M-H	237.1860	-0.9
	HMDB0038136	Curcumadiol	C15H26O2	M-H	237.1860	-0.9
	HMDB0038138	alpha-Bisabolol oxide C	C15H26O2	M-H	237.1860	-0.9
	HMDB0038197	alpha-Bisabolol oxide B	C15H26O2	M-H	237.1860	-0.9
	HMDB0030428	Linalyl isovalerate	C15H26O2	M-H	237.1860	-0.9
	HMDB0037195	2-Propenyl cyclohexanhexanoate	C15H26O2	M-H	237.1860	-0.9
	HMDB0040281	Geranyl valerate	C15H26O2	M-H	237.1860	-0.9
	HMDB0029350	Geranyl 3-methylbutanoate	C15H26O2	M-H	237.1860	-0.9
	HMDB0182222	2-(8,8a-dimethyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl)propane-1,2-diol	C15H26O2	M-H	237.1860	-0.9
	HMDB0182766	4a-methyl-8-methylidene-2-(propan-2-yl)-decahydronaphthalene-1,7-diol	C15H26O2	M-H	237.1860	-0.9
	HMDB0182765	2-(2-hydroxypropan-2-yl)-4a-methyl-8-methylidene-decahydronaphthalen-1-ol	C15H26O2	M-H	237.1860	-0.9
	HMDB0040904	Ipomeatetrahydrofuran	C15H28O3	M-H2O-H	237.1855	1.5
239.0595	HMDB0164652	[(6-hydroxy-8-oxooctan-2-yl)oxy]sulfonic acid	C8H16O6S	M-H	239.0595	0.1
	HMDB0161161	2-(sulfooxy)octanoic acid	C8H16O6S	M-H	239.0595	0.1
	HMDB0159453	82542-98-1	C8H16O6S	M-H	239.0595	0.1
	HMDB0172047	[(5-ethoxy-3-methyl-5-oxopentan-2-yl)oxy]sulfonic acid	C8H16O6S	M-H	239.0595	0.1
	HMDB0172049	[(5-ethoxy-3-methyl-5-oxopentyl)oxy]sulfonic acid	C8H16O6S	M-H	239.0595	0.1
	HMDB0172051	(4-ethoxy-2-ethyl-4-oxobutoxy)sulfonic acid	C8H16O6S	M-H	239.0595	0.1
	HMDB0172055	[(1-ethoxy-3-methyl-1-oxopentan-2-yl)oxy]sulfonic acid	C8H16O6S	M-H	239.0595	0.1
	HMDB0172053	{2-[(3-methylpentanoyl)oxy]ethoxy}sulfonic acid	C8H16O6S	M-H	239.0595	0.1
	HMDB0164651	[(7-hydroxy-1-oxooctan-3-yl)oxy]sulfonic acid	C8H16O6S	M-H	239.0595	0.1
	HMDB0166750	[(2E)-hept-2-en-1-yloxy]sulfonic acid	C7H14O4S	M+FA-H	239.0595	0.1
	HMDB0175186	(hept-6-en-1-yloxy)sulfonic acid	C7H14O4S	M+FA-H	239.0595	0.1
	HMDB0041610	(2,2-Diethoxyethyl)benzene	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0132986	1-(4-methoxyphenyl)pentan-3-ol	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0039685	8-Ocimenyl acetate	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0014018	4-Hydroxypropofol	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0035126	Myrtenyl acetate	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0035376	Ethyl (2E,4Z,7Z)-Decatrienoate	C12H18O2	M+FA-H	239.1289	-1.2

239.1286	HMDB0031840	(S,Z)-Lyralol acetate	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0037389	(R)-2-Acetoxy-p-mentha-1,8-diene	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0038292	Menthadienyl acetate	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0040439	1-(2-Furanyl)-1-octanone	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0038046	Carvyl acetate	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0037231	Perillyl acetate	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0034450	Neocnidilide	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0041497	(S)-Neolyratyl acetate	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0032567	Hexylresorcinol	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0035375	Ethyl (2E,4E,7Z)-Decatrienoate	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0037018	(S)-p-Mentha-1,8-dien--yl acetate	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0035801	(2S,4R)-p-Mentha-1(7),5-dien-2-ol acetate	C12H18O2	M+FA-H	239.1289	-1.2
	HMDB0176441	8-{3-[(1E)-3-oxoprop-1-en-1-yl]oxiran-2-yl} octanoic acid	C13H20O4	M-H	239.1289	-1.2
	HMDB0176442	(9E,11E)-2-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M-H	239.1289	-1.2
	HMDB0176438	(9E,11E)-3-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M-H	239.1289	-1.2
	HMDB0176437	(9E,11E)-4-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M-H	239.1289	-1.2
	HMDB0176439	(9E,11E)-8-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M-H	239.1289	-1.2
	HMDB0176432	SCHEMBL2554147	C13H20O4	M-H	239.1289	-1.2
	HMDB0176436	(9E,11E)-5-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M-H	239.1289	-1.2
	HMDB0176440	(9E)--(3-formyloxiran-2-yl)dec-9-enoic acid	C13H20O4	M-H	239.1289	-1.2
	HMDB0176435	(9E,11E)-6-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M-H	239.1289	-1.2
	HMDB0176434	(9E,11E)-7-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M-H	239.1289	-1.2
239.1649	HMDB0000872	Tetradecanedioic acid	C14H26O4	M-H2O-H	239.1647	0.8
	HMDB0059947	1-Hydroxypropan-2-yl 2-isopropyl-5-methylcyclohexyl carbonate	C14H26O4	M-H2O-H	239.1647	0.8
	HMDB0059946	2-Hydroxypropyl 2-isopropyl-5-methylcyclohexyl carbonate	C14H26O4	M-H2O-H	239.1647	0.8
	HMDB0041618	Diisobutyl adipate	C14H26O4	M-H2O-H	239.1647	0.8
	HMDB0176328	4-hydroxy-3-oxotetradecanoic acid	C14H26O4	M-H2O-H	239.1647	0.8
	HMDB0176326	14-hydroxy-3-oxotetradecanoic acid	C14H26O4	M-H2O-H	239.1647	0.8
	HMDB0176325	13-hydroxy-3-oxotetradecanoic acid	C14H26O4	M-H2O-H	239.1647	0.8
	HMDB0176327	SCHEMBL886	C14H26O4	M-H2O-H	239.1647	0.8
	HMDB0040429	Diethyl decanedioate	C14H26O4	M-H2O-H	239.1647	0.8
	HMDB0163189	(2E,4E,7Z)-trideca-2,4,7-trien-1-ol	C13H22O	M+FA-H	239.1653	-1.5
	HMDB0182746	4-(2,2-Dimethyl-6-methylenecyclohexyl)butan-2-one	C13H22O	M+FA-H	239.1653	-1.5
	HMDB0178134	3-[(2Z)-but-2-en-1-yl]-2,4,4-trimethylcyclohexan-1-one	C13H22O	M+FA-H	239.1653	-1.5
	HMDB0163188	SCHEMBL15656566	C13H22O	M+FA-H	239.1653	-1.5
	HMDB0036820	beta-Ionol	C13H22O	M+FA-H	239.1653	-1.5
	HMDB0031846	Geranylacetone	C13H22O	M+FA-H	239.1653	-1.5
	HMDB0032355	(+/-)-[R-(E)]-5-Isopropyl-8-methylnona-6,8-dien-2-one	C13H22O	M+FA-H	239.1653	-1.5
	HMDB0036184	7,8-Dehydro-3,4-dihydro-beta-ionol	C13H22O	M+FA-H	239.1653	-1.5
	HMDB0036823	Theaspirane	C13H22O	M+FA-H	239.1653	-1.5
	HMDB0036026	Octahydro-6-isopropyl-2(1H)-naphthalenone	C13H22O	M+FA-H	239.1653	-1.5
	HMDB0038897	(E)-2-(2-Octenyl)cyclopentanone	C13H22O	M+FA-H	239.1653	-1.5
	HMDB0038731	4,7-Megastigmadien-9-ol	C13H22O	M+FA-H	239.1653	-1.5
	HMDB0038026	Dihydro-alpha-ionone	C13H22O	M+FA-H	239.1653	-1.5
	HMDB0038216	5-Isopropyl-2-(2-methylpropyl)-2-cyclohexen-1-one	C13H22O	M+FA-H	239.1653	-1.5
	HMDB0032913	4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-butanone	C13H22O	M+FA-H	239.1653	-1.5
	HMDB0160290	(8Z)--hydroxytetradeca-5,8-dienoic acid	C14H24O3	M-H	239.1653	-1.5
	HMDB0160289	(5Z,8Z)-4-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M-H	239.1653	-1.5
	HMDB0160292	4-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}butanoic acid	C14H24O3	M-H	239.1653	-1.5
	HMDB0160291	SCHEMBL8918721	C14H24O3	M-H	239.1653	-1.5
	HMDB0160294	(5Z,8Z)-14-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M-H	239.1653	-1.5
	HMDB0160296	(5Z,8Z)-7-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M-H	239.1653	-1.5
	HMDB0160293	(5Z)-7-(3-pentyloxiran-2-yl)hept-5-enoic acid	C14H24O3	M-H	239.1653	-1.5
	HMDB0160297	(5Z,7E)-9-hydroxytetradeca-5,7-dienoic acid	C14H24O3	M-H	239.1653	-1.5
	HMDB0160295	(5Z,8Z)-2-hydroxytetradeca-5,8-dienoic acid	C14H24O3	M-H	239.1653	-1.5
	HMDB0160298	(8Z)-5-hydroxytetradeca-6,8-dienoic acid	C14H24O3	M-H	239.1653	-1.5
	HMDB0032369	L-Menthyl acetoacetate	C14H24O3	M-H	239.1653	-1.5
	HMDB0032347	Isobutyl-undecenoate	C15H28O2	M-H	239.2017	-1.1
	HMDB0037190	Rhodinyl isovalerate	C15H28O2	M-H	239.2017	-1.1
	HMDB0039715	Auberganol	C15H28O2	M-H	239.2017	-1.1
	HMDB0037229	Citronellyl pentanoate	C15H28O2	M-H	239.2017	-1.1
	HMDB0034455	Exaltolide	C15H28O2	M-H	239.2017	-1.1

239.2014	HMDB0036426	Butyl undecylenate	C15H28O2	M-H	239.2017	-1.1
	HMDB0038954	Citronellyl isovalerate	C15H28O2	M-H	239.2017	-1.1
	HMDB0037211	Menthyl isovalerate	C15H28O2	M-H	239.2017	-1.1
	HMDB0040997	15,5-Farnesanolide	C15H28O2	M-H	239.2017	-1.1
	HMDB0029765	9-Pentadecenoic acid	C15H28O2	M-H	239.2017	-1.1
	HMDB0031061	-Hydroxymyristic acid methyl ester	C15H30O3	M-H2O-H	239.2011	1.2
	HMDB0061657	3-hydroxypentadecanoic acid	C15H30O3	M-H2O-H	239.2011	1.2
241.1080	HMDB0059866	Ethyl 3-hydroxytridecanoate	C15H30O3	M-H2O-H	239.2011	1.2
	HMDB0179541	3-methoxy-2-methyl-5-(propan-2-yl)benzene-1,4-diol	C11H16O3	M+FA-H	241.1081	-0.6
	HMDB0135672	4-(3-hydroxybutyl)-2-methoxyphenol	C11H16O3	M+FA-H	241.1081	-0.6
	HMDB0179545	3-methoxy-5-methyl-2-(propan-2-yl)benzene-1,4-diol	C11H16O3	M+FA-H	241.1081	-0.6
	HMDB0037725	Hexyl 2-furoate	C11H16O3	M+FA-H	241.1081	-0.6
	HMDB0037734	Isobutyl 2-furanpropionate	C11H16O3	M+FA-H	241.1081	-0.6
	HMDB0036226	2,6-Dimethoxy-4-propylphenol	C11H16O3	M+FA-H	241.1081	-0.6
241.1442	HMDB0032857	Glycerol tripropanoate	C12H20O6	M-H2O-H	241.1076	1.7
	HMDB0183241	6-hydroxytridecanedioic acid	C13H24O5	M-H2O-H	241.1440	0.9
	HMDB0183240	4-hydroxytridecanedioic acid	C13H24O5	M-H2O-H	241.1440	0.9
	HMDB0183243	SCHEMBL1091	C13H24O5	M-H2O-H	241.1440	0.9
	HMDB0184194	2-hydroxytridecanedioic acid	C13H24O5	M-H2O-H	241.1440	0.9
	HMDB0032901	Yuzu lactone	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0039522	Linalyl acetate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0040725	Fenchyl acetate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0036048	Artemisia alcohol acetate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0040397	(-)-Bornyl acetate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0032051	alpha-Terpineol acetate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0041494	(S)-Santolina acetate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0040227	Isopulegol acetate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0037301	p-Menth-1-en-9-ol acetate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0040206	Allyl 3-cyclohexylpropionate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0030945	Methyl 2-undecynoate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0031692	cis-3-Hexenyl trans-4-hexenoate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0031030	6-Heptyl-5,6-dihydro-2H-pyran-2-one	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0036599	Ethyl 2Z,4E-decadienoic acid	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0034903	(3R,3aR,7aS)-3-Butylhexahydro-1(3H)-isobenzofuranone	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0038280	cis-3-Hexenyl trans-2-hexenoate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0041469	Dihydrocarveol acetate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0032193	alpha-Campholene acetate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0030867	Dihydro-5-(2-octenyl)-2(3H)-furanone	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0038270	cis-3-Hexenyl cis-3-hexenoate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0032331	(Z)-4-Hydroxy-6-dodecenoic acid lactone	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0061816	3,7-Dimethyl-2,6-octadien-1-ylacetate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0035157	geranyl acetate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0062144	p-Menth-1-en-4-yl acetate	C12H20O2	M+FA-H	241.1445	-1.4
	HMDB0176456	(9E,11E)-4,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176455	(9E,11E)-5,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176453	(9E,11E)-7,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176452	(9E)-2-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176451	(9E)-12-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176449	(9E)-11-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176450	8-[3-(3-oxopropyl)oxiran-2-yl]octanoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176457	(9E,11E)-3,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0030987	2-Carboxy-4-dodecanolide	C13H22O4	M-H	241.1445	-1.4
	HMDB0038736	(3S,5R,6R,7E)-3,5,6-Trihydroxy-7-megastigmen-9-one	C13H22O4	M-H	241.1445	-1.4
	HMDB0176461	(9E,11E)-2,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176458	(9E,11E)-8,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176454	(9E,11E)-6,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176460	8-{3-[(1E)-3-hydroxyprop-1-en-1-yl]oxiran-2-yl}octanoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176459	(9E)-[3-(hydroxymethyl)oxiran-2-yl]dec-9-enoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176448	(9E)-8-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176445	(9E)-5-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176447	(9E)-3-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176446	(9E)-4-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H	241.1445	-1.4
	HMDB0176444	(9E)-6-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H	241.1445	-1.4

	HMDB0176443	(9E)-7-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M-H	241.1445	-1.4
241.1808	HMDB0041404	2-Methylcyclododecanone	C13H24O	M+FA-H	241.1809	-0.5
	HMDB0163217	57981-61	C13H24O	M+FA-H	241.1809	-0.5
	HMDB0032247	(Z)-4-Dodecenal	C13H24O	M+FA-H	241.1809	-0.5
	HMDB0041490	Dihydrogeranylacetone	C13H24O	M+FA-H	241.1809	-0.5
	HMDB0037275	2-Tridecenal	C13H24O	M+FA-H	241.1809	-0.5
	HMDB0036172	4-(2,6,6-Trimethyl-1-cyclohexenyl)-2-butanol	C13H24O	M+FA-H	241.1809	-0.5
	HMDB0159610	(5E)-4-hydroxytetradec-5-enoic acid	C14H26O3	M-H	241.1809	-0.5
	HMDB0159611	(5E)-13-hydroxytetradec-5-enoic acid	C14H26O3	M-H	241.1809	-0.5
	HMDB0159613	(5E)-14-hydroxytetradec-5-enoic acid	C14H26O3	M-H	241.1809	-0.5
	HMDB0159612	4-(3-octyloxiran-2-yl)butanoic acid	C14H26O3	M-H	241.1809	-0.5
	HMDB0159614	(5E)-2-hydroxytetradec-5-enoic acid	C14H26O3	M-H	241.1809	-0.5
	HMDB0159799	(5Z)-7-hydroxytetradec-5-enoic acid	C14H26O3	M-H	241.1809	-0.5
	HMDB0159800	(5Z)-4-hydroxytetradec-5-enoic acid	C14H26O3	M-H	241.1809	-0.5
	HMDB0159801	SCHEMBL157578	C14H26O3	M-H	241.1809	-0.5
	HMDB0159802	14-hydroxy-5Z-tetradecenoic acid	C14H26O3	M-H	241.1809	-0.5
	HMDB0159803	(5Z)-2-hydroxytetradec-5-enoic acid	C14H26O3	M-H	241.1809	-0.5
	HMDB0176319	13-hydroxy-3-oxotetradecanal	C14H26O3	M-H	241.1809	-0.5
	HMDB0176320	14-hydroxy-3-oxotetradecanal	C14H26O3	M-H	241.1809	-0.5
	HMDB0159609	(5E)-7-hydroxytetradec-5-enoic acid	C14H26O3	M-H	241.1809	-0.5
	HMDB0030982	6-Ketomyristic acid	C14H26O3	M-H	241.1809	-0.5
	HMDB0010730	3-Oxotetradecanoic acid	C14H26O3	M-H	241.1809	-0.5
	HMDB0032370	L-Menthyl (R,S)-3-hydroxybutyrate	C14H26O3	M-H	241.1809	-0.5
241.2170	HMDB0061833	(E)-7-Tetradecene	C14H28	M+FA-H	241.2173	-1.3
	HMDB0061834	1-Tetradecene	C14H28	M+FA-H	241.2173	-1.3
	HMDB0033567	Cyclotetradecane	C14H28	M+FA-H	241.2173	-1.3
	HMDB0041588	2,6,-Trimethyldodecanoic acid	C15H30O2	M-H	241.2173	-1.3
	HMDB0059833	Ethyl tridecanoate	C15H30O2	M-H	241.2173	-1.3
	HMDB0032250	Dodecyl propionate	C15H30O2	M-H	241.2173	-1.3
	HMDB0032328	Hexyl nonanoate	C15H30O2	M-H	241.2173	-1.3
	HMDB0040998	7(14)-Farnesene-9,12-diol	C15H30O2	M-H	241.2173	-1.3
	HMDB0036218	Heptyl octanoate	C15H30O2	M-H	241.2173	-1.3
	HMDB0038907	3-Methylbutyl decanoate	C15H30O2	M-H	241.2173	-1.3
	HMDB0036220	Octyl heptanoate	C15H30O2	M-H	241.2173	-1.3
	HMDB0030469	Methyl tetradecanoate	C15H30O2	M-H	241.2173	-1.3
	HMDB0037306	Pentyl decanoate	C15H30O2	M-H	241.2173	-1.3
	HMDB0059820	Isopropyl laurate	C15H30O2	M-H	241.2173	-1.3
	HMDB0061707	13-Methylmyristic acid	C15H30O2	M-H	241.2173	-1.3
	HMDB0062084	12-methyltetradecanoic acid	C15H30O2	M-H	241.2173	-1.3
	HMDB0000826	Pentadecanoic acid	C15H30O2	M-H	241.2173	-1.3
242.0438	HMDB0062185	1-Alkyl-2-acylglycerophosphoethanolamine	C6H14NO7P	M-H	242.0435	1.2
	HMDB0180981	2-hydroxy-3-(7-hydroxy-1H-indol-3-yl)propanoic acid	C11H11NO4	M+Na-2H	242.0435	1.3
	HMDB0180979	2-hydroxy-3-(5-hydroxy-1H-indol-3-yl)propanoic acid	C11H11NO4	M+Na-2H	242.0435	1.3
	HMDB0180980	6-hydroxyindolelactic acid	C11H11NO4	M+Na-2H	242.0435	1.3
	HMDB0180982	2-hydroxy-3-(4-hydroxy-1H-indol-3-yl)propanoic acid	C11H11NO4	M+Na-2H	242.0435	1.3
	HMDB0038990	Methyl 5-hydroxyoxindole-3-acetate	C11H11NO4	M+Na-2H	242.0435	1.3
	HMDB0038991	Methyl dioxindole-3-acetate	C11H11NO4	M+Na-2H	242.0435	1.3
242.0782	HMDB0032055	N-acetyl-L-histidine	C8H11N3O3	M+FA-H	242.0782	-0.2
	HMDB0015122	Cytarabine	C9H13N3O5	M-H	242.0782	-0.2
	HMDB0155273	Cytarabine	C9H13N3O5	M-H	242.0782	-0.2
	HMDB0060478	gamma-Glutamyl-beta-cyanoalanine	C9H13N3O5	M-H	242.0782	-0.2
	HMDB0000089	Cytidine	C9H13N3O5	M-H	242.0782	-0.2
	HMDB0028730	Asparaginyglutamic acid	C9H15N3O6	M-H2O-H	242.0777	2.1
	HMDB0028814	Glutamylasparagine	C9H15N3O6	M-H2O-H	242.0777	2.1
	HMDB0029144	gamma-Glutamylasparagine	C9H15N3O6	M-H2O-H	242.0777	2.1
	HMDB0028793	Glutaminylaspartic acid	C9H15N3O6	M-H2O-H	242.0777	2.1
	HMDB0028751	Aspartyl-Glutamine	C9H15N3O6	M-H2O-H	242.0777	2.1
	HMDB0028767	Aspartyl-Gamma-glutamate	C9H15N3O6	M-H2O-H	242.0777	2.1
	HMDB0032297	Glyceryl 5-hydroxydecanoate	C13H26O5	M-H2O-H	243.1596	0.3
	HMDB0000529	5Z-Dodecenoic acid	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0029763	Allyl nonanoate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0040158	Hexyl 2-methyl-3-pentenoate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0033378	cis-3-Hexenyl hexanoate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0037498	1-Ethenylhexyl butanoate	C12H22O2	M+FA-H	243.1602	-2.0

243.1597	HMDB0039220	Ethyl 4-decenoate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0029585	Methyl -undecenoate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0037186	Rhodinyl acetate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0034844	Citronellyl acetate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0037329	Ethyl 2-decenoate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0041449	[(3,7-Dimethyl-6-octenyl)oxy]acetaldehyde	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0038081	2-Octenyl butyrate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0040361	1,1-Dimethoxy-3,7-dimethyl-2,6-octadiene	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0010729	trans-Dodec-2-enoic acid	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0037742	xi-5-Dodecanolide	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0031683	xi-Dihydro-5-octyl-2(3H)-furanone	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0037305	Methyl 9-undecenoate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0041264	Menthyl acetate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0037813	3-Heptyldihydro-5-methyl-2(3H)-furanone	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0038269	Hexyl 2E-hexenoate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0038895	7-Hexyl-2-oxepanone	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0036182	5,5-Dibutyl-4,5-dihydro-2(3H)furanone	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0040163	Hexyl 2-methyl-4-pentenoate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0038924	2-Hexenyl hexanoate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0032235	2,6-Dimethyl-5-heptenal propyleneglycol acetal	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0034160	Citronellyl acetate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0032214	cis-4-Decenyl acetate	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0032248	11-Dodecenoic acid	C12H22O2	M+FA-H	243.1602	-2.0
	HMDB0002327	1,11-Undecanedicarboxylic acid	C13H24O4	M-H	243.1602	-2.0
	HMDB0036141	Menthyl ethylene glycol carbonate	C13H24O4	M-H	243.1602	-2.0
	HMDB0037184	1,4-Nonanediol diacetate	C13H24O4	M-H	243.1602	-2.0
243.1965	HMDB0034148	2-Tridecanone	C13H26O	M+FA-H	243.1966	-0.3
	HMDB0030928	Tridecanal	C13H26O	M+FA-H	243.1966	-0.3
	HMDB0062117	6,-Dimethylundecan-2-one	C13H26O	M+FA-H	243.1966	-0.3
	HMDB0176324	1,4-dihydroxytetradecan-3-one	C14H28O3	M-H	243.1966	-0.3
	HMDB0171056	13-hydroxytetradecanoic acid	C14H28O3	M-H	243.1966	-0.3
	HMDB0176322	1,14-dihydroxytetradecan-3-one	C14H28O3	M-H	243.1966	-0.3
	HMDB0176323	1,2-dihydroxytetradecan-3-one	C14H28O3	M-H	243.1966	-0.3
	HMDB0061656	(S)-3-hydroxytetradecanoic acid	C14H28O3	M-H	243.1966	-0.3
	HMDB0176321	1,13-dihydroxytetradecan-3-one	C14H28O3	M-H	243.1966	-0.3
	HMDB0002261	2-Hydroxymyristic acid	C14H28O3	M-H	243.1966	-0.3
	HMDB0032417	3-(L-Menthox)-2-methylpropane-1,2-diol	C14H28O3	M-H	243.1966	-0.3
	HMDB0094672	3-hydroxytetradecanoic acid	C14H28O3	M-H	243.1966	-0.3
	HMDB0059850	Ethyl 3-hydroxydodecanoate	C14H28O3	M-H	243.1966	-0.3
	HMDB0171057	14-hydroxymyristic acid	C14H28O3	M-H	243.1966	-0.3
	HMDB0010731	(R)-3-Hydroxy-tetradecanoic acid	C14H28O3	M-H	243.1966	-0.3
247.1700	HMDB0060055	Tetranor 12-HETE	C16H26O3	M-H2O-H	247.1698	0.8
	HMDB0112089	7-(3,4-dimethyl-5-propylfuran-2-yl)heptanoic acid	C16H26O3	M-H2O-H	247.1698	0.8
	HMDB0112085	5-(3,4-dimethyl-5-pentylfuran-2-yl)-pentanoic acid	C16H26O3	M-H2O-H	247.1698	0.8
	HMDB0112088	6-(5-hexylfuran-2-yl)hexanoic acid	C16H26O3	M-H2O-H	247.1698	0.8
	HMDB0112097	5-Butyl-2-furanoctanoic acid	C16H26O3	M-H2O-H	247.1698	0.8
	HMDB0033917	4-Hydroxy-3-methoxy-2,-bisaboladien-9-one	C16H26O3	M-H2O-H	247.1698	0.8
	HMDB0112092	5-Pentyl-2-furanheptanoic acid	C16H26O3	M-H2O-H	247.1698	0.8
	HMDB0061838	(-)-alpha-Curcumene	C15H22	M+FA-H	247.1704	-1.4
	HMDB0059910	(E)-Calamene	C15H22	M+FA-H	247.1704	-1.4
	HMDB0061837	Calamenene	C15H22	M+FA-H	247.1704	-1.4
	HMDB0059676	beta-Vatirenene	C15H22	M+FA-H	247.1704	-1.4
	HMDB0059857	beta-Vetivenene	C15H22	M+FA-H	247.1704	-1.4
	HMDB0059878	alpha-Curcumene	C15H22	M+FA-H	247.1704	-1.4
	HMDB0036796	(1alpha,6alpha,7alphaH)-2,4(15)-Copadiene	C15H22	M+FA-H	247.1704	-1.4
	HMDB0035707	(6alpha,7alpha,alpha)-1(5),3-Aromadendradiene	C15H22	M+FA-H	247.1704	-1.4
	HMDB0036416	beta-Spathulene	C15H22	M+FA-H	247.1704	-1.4
	HMDB0038125	1,4,9-Cadinatriene	C15H22	M+FA-H	247.1704	-1.4
	HMDB0036640	Furanofukinin	C16H24O2	M-H	247.1704	-1.4
	HMDB0037713	Octyl phenylacetate	C16H24O2	M-H	247.1704	-1.4
	HMDB0037719	2-Phenylethyl octanoate	C16H24O2	M-H	247.1704	-1.4
	HMDB0032228	Dimethylbenzyl carbiny hexanoate	C16H24O2	M-H	247.1704	-1.4
	HMDB0036221	[2-(Dimethoxymethyl)-1-heptenyl]benzene	C16H24O2	M-H	247.1704	-1.4
	HMDB0038154	3,11,12-Trihydroxy-1()-spirovetiven-2-one	C15H24O4	M-H2O-H	249.1491	0.9
	HMDB0038165	Acoric acid	C15H24O4	M-H2O-H	249.1491	0.9

HMDB0038153	1-(3-Furanyl)-6,7-dihydroxy-4,8-dimethyl-1-nonanone	C15H24O4	M-H2O-H	249.1491	0.9
HMDB0036150	4,11,13,15-Tetrahydroridentin B	C15H24O4	M-H2O-H	249.1491	0.9
HMDB0038503	Bisacurone epoxide	C15H24O4	M-H2O-H	249.1491	0.9
HMDB0177237	(7bR)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4,4a-triol	C15H24O4	M-H2O-H	249.1491	0.9
HMDB0177235	(7bR)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4,5-triol	C15H24O4	M-H2O-H	249.1491	0.9
HMDB0177236	(7bS)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4,7a-triol	C15H24O4	M-H2O-H	249.1491	0.9
HMDB0177233	(7bR)-3,6-bis(hydroxymethyl)-6,7b-dimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4-diol	C15H24O4	M-H2O-H	249.1491	0.9
HMDB0177232	(7bS)-3,7b-bis(hydroxymethyl)-6,6-dimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4-diol	C15H24O4	M-H2O-H	249.1491	0.9
HMDB0177234	(7bR)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4,7-triol	C15H24O4	M-H2O-H	249.1491	0.9
HMDB0060570	Deoxydihydro-artemisinin	C15H24O4	M-H2O-H	249.1491	0.9
HMDB0240213	Prostaglandin lactone-diol	C15H24O4	M-H2O-H	249.1491	0.9
HMDB0041482	3-Benzyl-4-heptanone	C14H20O	M+FA-H	249.1496	-1.3
HMDB0036170	2-Benzylidene-1-heptanol	C14H20O	M+FA-H	249.1496	-1.3
HMDB0133154	2-benzylheptanal	C14H20O	M+FA-H	249.1496	-1.3
HMDB0031776	(6R,7S)-6,7-Epoxy-1,3-tetradecadiyne	C14H20O	M+FA-H	249.1496	-1.3
HMDB0177704	(1E)-1-ethylidene-3,5-dihydroxy-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O3	M-H	249.1496	-1.3
HMDB0177702	(1E)-5-hydroxy-1-(2-hydroxyethylidene)-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O3	M-H	249.1496	-1.3
HMDB0177701	(1E)-1-ethylidene-5-hydroxy-7-(2-hydroxypropan-2-yl)-4-methylidene-octahydro-1H-inden-2-one	C15H22O3	M-H	249.1496	-1.3
HMDB0182302	6,-bis(hydroxymethyl)-2-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M-H	249.1496	-1.3
HMDB0182303	-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M-H	249.1496	-1.3
HMDB0182306	1-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M-H	249.1496	-1.3
HMDB0182304	2-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M-H	249.1496	-1.3
HMDB0182307	2-hydroxy-6-(hydroxymethyl)--methyl-3-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M-H	249.1496	-1.3
HMDB0182309	6-(hydroxymethyl)--methyl-2-(2-methyloxiran-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M-H	249.1496	-1.3
HMDB0177636	(1Z)-1-ethylidene-3,5-dihydroxy-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O3	M-H	249.1496	-1.3
HMDB0150689	2,5,5,8a-tetramethyl-6-oxo-1,4,4a,5,6,7,8,8a-octahydronaphthalene-1-carboxylic acid	C15H22O3	M-H	249.1496	-1.3
HMDB0177634	(1Z)-5-hydroxy-1-(2-hydroxyethylidene)-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O3	M-H	249.1496	-1.3
HMDB0177633	(1Z)-1-ethylidene-5-hydroxy-7-(2-hydroxypropan-2-yl)-4-methylidene-octahydro-1H-inden-2-one	C15H22O3	M-H	249.1496	-1.3
HMDB0177635	(1Z)-1-ethylidene-5-hydroxy-7-(1-hydroxypropan-2-yl)-4-methylidene-octahydro-1H-inden-2-one	C15H22O3	M-H	249.1496	-1.3
HMDB0182310	1-(hydroxymethyl)-3-methyl-3'-(prop-1-en-2-yl)-7-oxaspiro[bicyclo[4.1]heptane-2,1'-cyclopentane]-5-one	C15H22O3	M-H	249.1496	-1.3
HMDB0184279	(8aR)-3,4-dihydroxy-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M-H	249.1496	-1.3
HMDB0184276	(8aS)-4-hydroxy-8a-(hydroxymethyl)-1-methyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M-H	249.1496	-1.3

	HMDB0183506	(8aR)-4-hydroxy-1,8a-dimethyl-7-(2-methyloxiran-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M-H	249.1496	-1.3
	HMDB0183503	(8aR)-4,7-dihydroxy-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M-H	249.1496	-1.3
	HMDB0182900	2,2a-dihydroxy-6,6,7b-trimethyl-1H,2H,2aH,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-3-carbaldehyde	C15H22O3	M-H	249.1496	-1.3
	HMDB0182311	9-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M-H	249.1496	-1.3
	HMDB0182308	1-hydroxy-6-(hydroxymethyl)--methyl-3-(prop-1-en-2-yl)spiro[4.5]dec-6-en-8-one	C15H22O3	M-H	249.1496	-1.3
	HMDB0182305	6-(hydroxymethyl)-2-(3-hydroxyprop-1-en-2-yl)--methylspiro[4.5]dec-6-en-8-one	C15H22O3	M-H	249.1496	-1.3
	HMDB0183502	(8aS)-1,4-dihydroxy-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M-H	249.1496	-1.3
	HMDB0183504	(8aR)-4-hydroxy-7-(3-hydroxyprop-1-en-2-yl)-1,8a-dimethyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O3	M-H	249.1496	-1.3
	HMDB0240642	3,5-di-tert-butyl-4-hydroxybenzoic acid	C15H22O3	M-H	249.1496	-1.3
	HMDB0177703	(1E)-1-ethylidene-5-hydroxy-7-(1-hydroxypropan-2-yl)-4-methylidene-octahydro-1H-inden-2-one	C15H22O3	M-H	249.1496	-1.3
	HMDB0015371	Gemfibrozil	C15H22O3	M-H	249.1496	-1.3
	HMDB0035798	Piperdial	C15H22O3	M-H	249.1496	-1.3
	HMDB0036563	Valerenolic acid	C15H22O3	M-H	249.1496	-1.3
	HMDB0039644	Heliannuol A	C15H22O3	M-H	249.1496	-1.3
	HMDB0036036	6,6-Dimethoxy-2,5,5-trimethyl-2-hexene	C15H22O3	M-H	249.1496	-1.3
	HMDB0035760	3-Hydroxytrichothecene	C15H22O3	M-H	249.1496	-1.3
	HMDB0039635	Abscisic alcohol	C15H22O3	M-H	249.1496	-1.3
	HMDB0037529	Lactaronecatorin A	C15H22O3	M-H	249.1496	-1.3
	HMDB0035148	(6beta,8alpha)-6-Hydroxy-7(11)-eremophilen-12,8-olide	C15H22O3	M-H	249.1496	-1.3
	HMDB0030917	1-Hydroxyacorenone	C15H22O3	M-H	249.1496	-1.3
	HMDB0061839	Ethylhexyl salicylate	C15H22O3	M-H	249.1496	-1.3
	HMDB0035117	(3beta,6beta)-Furanoeremophilane-3,6-diol	C15H22O3	M-H	249.1496	-1.3
	HMDB0035137	Heliannuol D	C15H22O3	M-H	249.1496	-1.3
	HMDB0035358	Ketosantallic acid	C15H22O3	M-H	249.1496	-1.3
	HMDB0037064	FS4 toxin	C15H22O3	M-H	249.1496	-1.3
	HMDB0036037	13-Hydroxymarasmene	C15H22O3	M-H	249.1496	-1.3
	HMDB0034721	Procumadiol	C15H22O3	M-H	249.1496	-1.3
	HMDB0036664	Ketopelenolide a	C15H22O3	M-H	249.1496	-1.3
	HMDB0037559	Cadabicolone	C15H22O3	M-H	249.1496	-1.3
	HMDB0031901	Blennin A	C15H22O3	M-H	249.1496	-1.3
	HMDB0036550	3-Ketopotrichothecene	C15H22O3	M-H	249.1496	-1.3
	HMDB0040754	(3beta,8beta)-3-Hydroxy-7(11)-eremophilen-12,8-olide	C15H22O3	M-H	249.1496	-1.3
	HMDB0039156	3beta-Hydroxycinnamolide	C15H22O3	M-H	249.1496	-1.3
	HMDB0177902	3-hydroxy-7,7a-dimethyl-4'-methylidene-octahydrospiro[indene-2,3'-oxolane]-2'-one	C15H22O3	M-H	249.1496	-1.3
250.1446	HMDB0015072	Diethylpropion	C13H19NO	M+FA-H	250.1449	-1.1
	HMDB0060843	N-Desthiensylethyl-rotigotine	C13H19NO	M+FA-H	250.1449	-1.1
	HMDB0151790	4-[(1Z)-2-butyl-3-hydroxyprop-1-en-1-yl]phenol	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0151786	2-[(4-hydroxyphenyl)methyl]hexanal	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0151788	2-(phenylmethylidene)hexane-1,3-diol	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0151787	2-[(2-hydroxyphenyl)methyl]hexanal	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0151792	(2Z)-2-(phenylmethylidene)hexane-1,5-diol	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0151791	3-[(1Z)-2-butyl-3-hydroxyprop-1-en-1-yl]phenol	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0151789	2-[(1Z)-2-butyl-3-hydroxyprop-1-en-1-yl]phenol	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0151793	(2-butyl-3-phenyloxiran-2-yl)methanol	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0151794	(2Z)-2-(phenylmethylidene)hexane-1,6-diol	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0151805	2-benzylhexanoic acid	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0163212	(2E,4E,7Z)-trideca-2,4,7,12-tetraenoic acid	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0151785	2-[(3-hydroxyphenyl)methyl]hexanal	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0151783	2-benzyl-2-hydroxyhexanal	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0132932	1-(4-methoxyphenyl)-4-methylpentan-3-one	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0132940	1-(4-methoxyphenyl)-4-methylpent-1-en-3-ol	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0151780	2-benzyl-5-hydroxyhexanal	C13H18O2	M+FA-H	251.1289	-1.5
	HMDB0151784	2-[hydroxy(phenyl)methyl]hexanal	C13H18O2	M+FA-H	251.1289	-1.5

251.1285

HMDB0151781	2-benzyl-6-hydroxyhexanal	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0001925	Ibuprofen	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0040431	Hexyl benzoate	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0036391	alpha-Methylphenethyl butyrate	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0036025	2,4,6-Trimethyl-4-phenyl-1,3-dioxane	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0037194	Ethyl 2-ethyl-3-phenylpropanoate	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0034469	2-Phenylpropyl butyrate	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0037623	1-Methyl-1-phenylethyl isobutyrate	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0035017	2-Phenylethyl 3-methylbutanoate	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0037720	2-Phenylethyl 2-methylbutanoate	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0036240	Methyl 4-tert-butylphenylacetate	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0032176	Benzyl hexanoate	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0038605	Amyl phenylacetate	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0034470	2-Phenylpropyl isobutyrate	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0033196	(E)-6-Methyl-6-(5-methyl-2-furanyl)-3-hepten-2-one	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0037604	beta-12,13-Dinor-8-oxo-6-eremophilene-11-al	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0029669	Eremopetasinorone A	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0035181	xi-8,9-Dehydrotheaspirone	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0039101	Etrogol	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0034556	3-Acetoxy-3-methyl-1-phenylbutane	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0035016	2-Phenylethyl pentanoate	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0036386	1-Phenylpropyl butyrate	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0035008	3-Methylbutyl phenylacetate	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0034472	3-Phenylpropyl 2-methylpropanoate	C13H18O2	M+FA-H	251.1289	-1.5
HMDB0033197	2,2,4,4-Tetramethyl-6-(1-oxobutyl)-1,3,5-cyclohexanetrione	C14H20O4	M-H	251.1289	-1.5
HMDB0175188	7-hydroxyheptyl 4-hydroxybenzoate	C14H20O4	M-H	251.1289	-1.5
HMDB0175189	CHEMBL128785	C14H20O4	M-H	251.1289	-1.5
HMDB0175187	6-hydroxyheptyl 4-hydroxybenzoate	C14H20O4	M-H	251.1289	-1.5
HMDB0162484	2-[(3-hydroxy-5-methoxyphenyl)methyl]-6-methyloxan-4-ol	C14H20O4	M-H	251.1289	-1.5
HMDB0059661	QH(2)	C14H20O4	M-H	251.1289	-1.5
HMDB0036047	3alpha-Hydroxyoreadone	C14H20O4	M-H	251.1289	-1.5
HMDB0040459	Ethylene brassylate	C15H26O4	M-H2O-H	251.1647	0.7
HMDB0133179	2-benzylheptan-1-ol	C14H22O	M+FA-H	251.1653	-1.5
HMDB0013816	2,4-di-tert-Butylphenol	C14H22O	M+FA-H	251.1653	-1.5
HMDB0061831	(Z)-alpha-Irone	C14H22O	M+FA-H	251.1653	-1.5
HMDB0036023	Etaspiroene	C14H22O	M+FA-H	251.1653	-1.5
HMDB0031738	3-Methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	C14H22O	M+FA-H	251.1653	-1.5
HMDB0038130	1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one	C14H22O	M+FA-H	251.1653	-1.5
HMDB0031737	delta-Methylionone	C14H22O	M+FA-H	251.1653	-1.5
HMDB0035631	alpha-Irone	C14H22O	M+FA-H	251.1653	-1.5
HMDB0035245	1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1-penten-3-one	C14H22O	M+FA-H	251.1653	-1.5
HMDB0013825	4-(1,1,3,3-Tetramethylbutyl)-phenol	C14H22O	M+FA-H	251.1653	-1.5
HMDB0032528	4-(1,1,3,3-Tetramethylbutyl)-phenol	C14H22O	M+FA-H	251.1653	-1.5
HMDB0032397	Methyl-delta-ionone	C14H22O	M+FA-H	251.1653	-1.5
HMDB0036024	-Isopropyl-2,7-dimethyl-1-oxaspiro[4.5]deca-3,6-diene	C14H22O	M+FA-H	251.1653	-1.5
HMDB0184275	(4aR)-4,4a-dimethyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3,7-triol	C15H24O3	M-H	251.1653	-1.5
HMDB0183498	(4aR)-6-(3-hydroxyprop-1-en-2-yl)-4,4a-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M-H	251.1653	-1.5
HMDB0183500	(4aR)-4,4a-dimethyl-6-(2-methyloxiran-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M-H	251.1653	-1.5
HMDB0183496	(8aS)-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalene-1,2,4-triol	C15H24O3	M-H	251.1653	-1.5
HMDB0183495	(4aR)-4-(hydroxymethyl)-4a-methyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M-H	251.1653	-1.5
HMDB0184273	(4aS)-4a-(hydroxymethyl)-4-methyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene-1,3-diol	C15H24O3	M-H	251.1653	-1.5
HMDB0179268	6-(1,4-dihydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M-H	251.1653	-1.5
HMDB0179266	6-[4-hydroxy-4-(hydroxymethyl)cyclohex-2-en-1-yl]-2-methylhept-2-en-4-one	C15H24O3	M-H	251.1653	-1.5

251.1649

HMDB0179269	1-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M-H	251.1653	-1.5
HMDB0179267	6-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M-H	251.1653	-1.5
HMDB0179272	7-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M-H	251.1653	-1.5
HMDB0179273	5-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylhept-2-en-4-one	C15H24O3	M-H	251.1653	-1.5
HMDB0179271	6-{5-hydroxy-5-methyl-7-oxabicyclo[4.1]heptan-2-yl}-2-methylhept-2-en-4-one	C15H24O3	M-H	251.1653	-1.5
HMDB0179258	3,3a-dihydroxy-3,8-dimethyl-5-(propan-2-yl)-1,2,3,3a,4,5,6,8a-octahydroazulen-6-one	C15H24O3	M-H	251.1653	-1.5
HMDB0179257	1,8a-dihydroxy-1,4-dimethyl-7-(propan-2-ylidene)-decahydroazulen-6-one	C15H24O3	M-H	251.1653	-1.5
HMDB0168751	(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trienal	C15H24O3	M-H	251.1653	-1.5
HMDB0177221	(4aR,7aS,7bR)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4-diol	C15H24O3	M-H	251.1653	-1.5
HMDB0112086	5-(3-methyl-5-pentylfuran-2-yl)-pentanoic acid	C15H24O3	M-H	251.1653	-1.5
HMDB0112094	3-Methyl-5-propyl-2-furanheptanoic acid	C15H24O3	M-H	251.1653	-1.5
HMDB0179139	(6E)-6-(hydroxymethyl)--methyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M-H	251.1653	-1.5
HMDB0179140	(6Z)--(hydroxymethyl)-6-methyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M-H	251.1653	-1.5
HMDB0179142	(6Z)-3-(2-hydroxypropan-2-yl)-6,-dimethylcyclodec-6-ene-1,4-dione	C15H24O3	M-H	251.1653	-1.5
HMDB0179143	(6Z)-8-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M-H	251.1653	-1.5
HMDB0179141	(6Z)--hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M-H	251.1653	-1.5
HMDB0179145	(6Z)-3-(1-hydroxypropan-2-yl)-6,-dimethylcyclodec-6-ene-1,4-dione	C15H24O3	M-H	251.1653	-1.5
HMDB0179147	(6Z)-2-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M-H	251.1653	-1.5
HMDB0179148	(6Z)-3-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M-H	251.1653	-1.5
HMDB0179146	(6Z)-5-hydroxy-6,-dimethyl-3-(propan-2-yl)cyclodec-6-ene-1,4-dione	C15H24O3	M-H	251.1653	-1.5
HMDB0179270	1-(3,3-dimethyloxiran-2-yl)-3-(4-hydroxy-4-methylcyclohex-2-en-1-yl)butan-1-one	C15H24O3	M-H	251.1653	-1.5
HMDB0182313	6-hydroxy--(hydroxymethyl)-6-methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H	251.1653	-1.5
HMDB0182319	6-(hydroxymethyl)--methyl-2-(2-methyloxiran-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H	251.1653	-1.5
HMDB0182318	1-hydroxy-6-(hydroxymethyl)--methyl-3-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H	251.1653	-1.5
HMDB0182316	1-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H	251.1653	-1.5
HMDB0182317	2-hydroxy-6-(hydroxymethyl)--methyl-3-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H	251.1653	-1.5
HMDB0182321	7-hydroxy--(hydroxymethyl)-6-methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H	251.1653	-1.5
HMDB0182315	6-(hydroxymethyl)-2-(3-hydroxyprop-1-en-2-yl)--methylspiro[4.5]decan-8-one	C15H24O3	M-H	251.1653	-1.5
HMDB0179144	1,7-dimethyl-4-(propan-2-yl)-11-oxabicyclo[8.1]undecane-3,6-dione	C15H24O3	M-H	251.1653	-1.5
HMDB0182312	6,-bis(hydroxymethyl)-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H	251.1653	-1.5
HMDB0182314	2-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H	251.1653	-1.5
HMDB0182320	7-hydroxy-6-(hydroxymethyl)--methyl-2-(prop-1-en-2-yl)spiro[4.5]decan-8-one	C15H24O3	M-H	251.1653	-1.5
HMDB0035597	alpha-Carissanol	C15H24O3	M-H	251.1653	-1.5
HMDB0030918	1-Hydroxyepiacorone	C15H24O3	M-H	251.1653	-1.5

	HMDB0035729	Dihydromyoporone	C15H24O3	M-H	251.1653	-1.5
	HMDB0037969	Urodienone	C15H24O3	M-H	251.1653	-1.5
	HMDB0032122	3(4->5)-Abeo-4,11:4,12-diepoxy-3-eudesmanol	C15H24O3	M-H	251.1653	-1.5
	HMDB0037063	Toxin FS2	C15H24O3	M-H	251.1653	-1.5
	HMDB0035613	Epioxylubimin	C15H24O3	M-H	251.1653	-1.5
	HMDB0034574	Apotrichodiol	C15H24O3	M-H	251.1653	-1.5
	HMDB0035767	Piperalol	C15H24O3	M-H	251.1653	-1.5
	HMDB0036448	Zedoarondiol	C15H24O3	M-H	251.1653	-1.5
	HMDB0033149	(4R,5S,7R,11R)-11,12-Dihydroxy-1()-spirovetiven-2-one	C15H24O3	M-H	251.1653	-1.5
	HMDB0035309	6alpha-Carissanol	C15H24O3	M-H	251.1653	-1.5
	HMDB0038502	Bisacurone B	C15H24O3	M-H	251.1653	-1.5
	HMDB0036663	Hydroxypelenolide	C15H24O3	M-H	251.1653	-1.5
	HMDB0040685	2,3-Dihydroabscisic alcohol	C15H24O3	M-H	251.1653	-1.5
	HMDB0030919	Acorusdiol	C15H24O3	M-H	251.1653	-1.5
251.2013	HMDB0160974	9,-Epoxyhexadecanoic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0160973	(9Z)-15-hydroxyhexadec-9-enoic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0160972	8-Hydroxypalmitoleic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0160975	16-hydroxy-9Z-hexadecenoic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0160971	(9Z)-11-hydroxyhexadec-9-enoic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0166466	(3Z)-2-hydroxyhexadec-3-enoic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0030978	11-Oxohexadecanoic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0030972	8-Oxohexadecanoic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0030973	9-Oxohexadecanoic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0166467	4-hydroxy-trans-2-hexadecenoic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0166465	(3Z)-16-hydroxyhexadec-3-enoic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0166462	(3Z)-5-hydroxyhexadec-3-enoic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0166463	(3Z)-15-hydroxyhexadec-3-enoic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0010733	3-Oxohexadecanoic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0160976	hydroxy-palmitoleic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0166464	2-(3-dodecyloxiran-2-yl)acetic acid	C16H30O3	M-H2O-H	251.2011	0.8
	HMDB0061780	1,1,2-Trimethyl-3,5-bis(1-methylethenyl)cyclohexane	C15H26	M+FA-H	251.2017	-1.4
	HMDB0166468	(3Z)-hexadeca-3,15-dienoic acid	C16H28O2	M-H	251.2017	-1.4
	HMDB0032340	Isoambrettolide	C16H28O2	M-H	251.2017	-1.4
	HMDB0038255	Geranyl 2-ethylbutyrate	C16H28O2	M-H	251.2017	-1.4
	HMDB0031086	(Z)-7-Hexadecen-1,16-olide	C16H28O2	M-H	251.2017	-1.4
	HMDB0030429	Linalyl hexanoate	C16H28O2	M-H	251.2017	-1.4
	HMDB0029351	Geranyl hexanoate	C16H28O2	M-H	251.2017	-1.4
	HMDB0037805	D6-Ambrettolide	C16H28O2	M-H	251.2017	-1.4
	HMDB0039131	Ethyl (Z,Z)-5,8-tetradecadienoate	C16H28O2	M-H	251.2017	-1.4
	HMDB0000477	7Z,Z-Hexadecadienoic acid	C16H28O2	M-H	251.2017	-1.4
253.1091	HMDB0094664	Silane, (o-phenylenedioxy)bis(trimethyl-	C12H22O2Si2	M-H	253.1086	2.1
253.1441	HMDB0163191	(2E,4E,7Z)-9-hydroxytrideca-2,4,7-trienal	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0163194	(2E)-3-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}prop-2-enal	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0163190	(2E,4E,7Z)-trideca-2,4,7-trienoic acid	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0132947	1-(4-methoxyphenyl)-4-methylpentan-3-ol	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0163193	3-[(1E,4Z)-deca-1,4-dien-1-yl]oxirane-2-carbaldehyde	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0163196	(2E,4E,7Z)-13-hydroxytrideca-2,4,7-trienal	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0178139	6-[(2Z)-but-2-en-1-yl]-1,5,5-trimethyl-7-oxabicyclo[4.1]heptan-2-one	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0178135	3-[(2Z)-but-2-en-1-yl]-4-(hydroxymethyl)-2,4-dimethylcyclohex-2-en-1-one	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0163195	(2E,4E)-6-(3-pentyloxiran-2-yl)hexa-2,4-dienal	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0163192	(2E,4E,7Z)-12-hydroxytrideca-2,4,7-trienal	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0040233	2,3,5,6,8,8a-Hexahydro-2,5,5,8a-tetramethyl-7H-1-benzopyran-7-one	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0038047	Carvyl propionate	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0029668	Eremopetasinorol	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0041636	(3R,8E)-3-Hydroxy-5,8-megastigmadien-7-one	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0038529	5,9:6,9-Diepoxy-4-megastigmene	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0037776	3-Mercaptohexyl hexanoate	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0035228	Theaspirone A	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0034984	(5R,6S)-5,6-Epoxy-7-megastigmen-9-one	C13H20O2	M+FA-H	253.1445	-1.7

	HMDB0034672	(5alpha,8beta,9beta)-5,9-Epoxy-3,6-megastigmadien-8-ol	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0036824	Acetal R	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0031869	(S,E)-Lyratol propanoate	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0036686	2,2,6,7-Tetramethylbicyclo[4.3]nona-1(9),4-diene-7,8-diol	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0036821	Apo-9-zeaxanthinone	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0178140	3-[(2Z)-but-2-en-1-yl]-6-hydroxy-2,4,4-trimethylcyclohex-2-en-1-one	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0178138	2,4,4-trimethyl-3-[(3-methyloxiran-2-yl)methyl]cyclohex-2-en-1-one	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0178136	3-[(2Z)-but-2-en-1-yl]-2-(hydroxymethyl)-4,4-dimethylcyclohex-2-en-1-one	C13H20O2	M+FA-H	253.1445	-1.7
	HMDB0178137	3-[(2Z)-4-hydroxybut-2-en-1-yl]-2,4,4-trimethylcyclohex-2-en-1-one	C13H20O2	M+FA-H	253.1445	-1.7
253.1808	HMDB0039884	2-Cyclotetradecen-1-one	C14H24O	M+FA-H	253.1809	-0.5
	HMDB0032215	2-Decylfuran	C14H24O	M+FA-H	253.1809	-0.5
	HMDB0035862	(E)-6,-Dimethyl-9-methylene-5-undecen-2-one	C14H24O	M+FA-H	253.1809	-0.5
	HMDB0179280	1-hydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M-H	253.1809	-0.5
	HMDB0179281	3-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylheptan-4-one	C15H26O3	M-H	253.1809	-0.5
	HMDB0179278	2-{5-hydroxy-5-methyl-7-oxabicyclo[4.1]heptan-2-yl}-6-methylheptan-4-one	C15H26O3	M-H	253.1809	-0.5
	HMDB0179279	1-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylheptan-4-one	C15H26O3	M-H	253.1809	-0.5
	HMDB0179277	2-(1,4-dihydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M-H	253.1809	-0.5
	HMDB0179274	2-[4-hydroxy-4-(hydroxymethyl)cyclohex-2-en-1-yl]-6-methylheptan-4-one	C15H26O3	M-H	253.1809	-0.5
	HMDB0179275	2-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylheptan-4-one	C15H26O3	M-H	253.1809	-0.5
	HMDB0179276	2-hydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M-H	253.1809	-0.5
	HMDB0179282	3-hydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M-H	253.1809	-0.5
	HMDB0036053	(3beta,9beta)-7-Drimene-3,11,12-triol	C15H26O3	M-H	253.1809	-0.5
	HMDB0035780	8-Hydroxy-4(6)-lactarene-5,14-diol	C15H26O3	M-H	253.1809	-0.5
	HMDB0040276	5-Acetoxydihydrotheaespirane	C15H26O3	M-H	253.1809	-0.5
	HMDB0037197	Kessyl glycol	C15H26O3	M-H	253.1809	-0.5
	HMDB0036866	7-Drimene-11,12,14-triol	C15H26O3	M-H	253.1809	-0.5
	HMDB0029604	Lubiminol	C15H26O3	M-H	253.1809	-0.5
	HMDB0035918	7(14)-Bisabolene-2,3,,11-tetrol	C15H28O4	M-H2O-H	253.1804	1.7
253.2170	HMDB0031057	2s-hydroxypalmitic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0112191	13-hydroxyhexadecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0155886	15-hydroxypalmitic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0061658	(S)-3-hydroxypalmitic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0112188	-hydroxyhexadecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0112185	7-hydroxyhexadecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0112189	11-hydroxy palmitic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0112184	5-hydroxy-hexadecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0112187	9-Hydroxypalmitic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0184328	13-hydroxy-4,8,12-trimethyltridecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0184178	8-(hydroxymethyl)-4,12-dimethyltridecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0184180	2-hydroxy-4,8,12-trimethyltridecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0184177	4-(hydroxymethyl)-8,12-dimethyltridecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0184176	12-hydroxy-4,8,12-trimethyltridecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0184175	8-hydroxy-4,8,12-trimethyltridecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0184174	4-hydroxy-4,8,12-trimethyltridecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0112192	6-hydroxyhexadecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0112190	12-hydroxyhexadecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0112186	8-hydroxypalmitic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0006294	16-Hydroxy hexadecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0155887	16-Hydroxy hexadecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0
	HMDB0010734	(R)-3-Hydroxy-hexadecanoic acid	C16H32O3	M-H2O-H	253.2168	1.0

	HMDB0062548	2-hydroxyhexadecanoate	C16H31O3	M-H2O-H	253.2168	1.0
	HMDB0032182	Cadinene	C15H28	M+FA-H	253.2173	-1.2
	HMDB0033791	(E)-3-Hexadecenoic acid	C16H30O2	M-H	253.2173	-1.2
	HMDB0038958	Citronellyl hexanoate	C16H30O2	M-H	253.2173	-1.2
	HMDB0031711	15-Hexadecanolide	C16H30O2	M-H	253.2173	-1.2
	HMDB0031145	5-Dodecyldihydro-2(3H)-furanone	C16H30O2	M-H	253.2173	-1.2
	HMDB0002186	Hypogeic acid	C16H30O2	M-H	253.2173	-1.2
	HMDB0171479	2-hydroxy-14-methylcyclopentadecan-1-one	C16H30O2	M-H	253.2173	-1.2
	HMDB0003229	Palmitoleic acid	C16H30O2	M-H	253.2173	-1.2
	HMDB0010735	Trans-Hexa-dec-2-enoic acid	C16H30O2	M-H	253.2173	-1.2
	HMDB0037647	(E)-11-Hexadecenoic acid	C16H30O2	M-H	253.2173	-1.2
	HMDB0041422	(Z)-14-Methyl-6-pentadecenoic acid	C16H30O2	M-H	253.2173	-1.2
	HMDB0032638	(Z)-5-Hexadecenoic acid	C16H30O2	M-H	253.2173	-1.2
	HMDB0171478	2-hydroxy-3-methylcyclopentadecan-1-one	C16H30O2	M-H	253.2173	-1.2
	HMDB0171476	3-(hydroxymethyl)cyclopentadecan-1-one	C16H30O2	M-H	253.2173	-1.2
	HMDB0171477	Cyclopentadecanone, 3-hydroxy-3-methyl-	C16H30O2	M-H	253.2173	-1.2
	HMDB0031053	(E)-6-Hexadecenoic acid	C16H30O2	M-H	253.2173	-1.2
	HMDB0035877	(Z)-13-Hexadecenoic acid	C16H30O2	M-H	253.2173	-1.2
	HMDB0061979	11Z-hexadecenoic acid	C16H30O2	M-H	253.2173	-1.2
	HMDB0012328	Palmitelaidic acid	C16H30O2	M-H	253.2173	-1.2
254.0778	HMDB0060384	4-Acetamido-2-amino-6-nitrotoluene	C9H11N3O3	M+FA-H	254.0782	-1.7
255.1594	HMDB0000394	3-Hydroxytetradecanedioic acid	C14H26O5	M-H2O-H	255.1596	-0.9
	HMDB0040904	Ipomeatetrahydrofuran	C15H28O3	M-H	255.1966	0.5
	HMDB0032525	Tetradec-2-enal	C14H26O	M+FA-H	255.1966	0.5
	HMDB0032526	(Z)-8-Tetradecenal	C14H26O	M+FA-H	255.1966	0.5
255.1967	HMDB0072863	MG(12)	C15H30O4	M-H2O-H	255.1960	2.7
	HMDB0072858	MG(i-12)	C15H30O4	M-H2O-H	255.1960	2.7
	HMDB0072860	MG(i-12)	C15H30O4	M-H2O-H	255.1960	2.7
	HMDB0072869	MG(12)	C15H30O4	M-H2O-H	255.1960	2.7
	HMDB0031082	1-Pentadecene	C15H30	M+FA-H	255.2330	-1.4
	HMDB0031083	(E)-7-Pentadecene	C15H30	M+FA-H	255.2330	-1.4
	HMDB0002396	Trimethyltridecanoic acid	C16H32O2	M-H	255.2330	-1.4
	HMDB0031068	Isopalmitic acid	C16H32O2	M-H	255.2330	-1.4
	HMDB0034153	Ethyl tetradecanoate	C16H32O2	M-H	255.2330	-1.4
	HMDB0036210	Dodecyl 2-methylpropanoate	C16H32O2	M-H	255.2330	-1.4
255.2326	HMDB0032065	Butyl dodecanoate	C16H32O2	M-H	255.2330	-1.4
	HMDB0033166	Octyl octanoate	C16H32O2	M-H	255.2330	-1.4
	HMDB0032249	Dodecyl butyrate	C16H32O2	M-H	255.2330	-1.4
	HMDB0032324	Hexyl decanoate	C16H32O2	M-H	255.2330	-1.4
	HMDB0000220	Palmitic acid	C16H32O2	M-H	255.2330	-1.4
	HMDB0060083	Palmitic acid	C16H32O2	M-H	255.2330	-1.4
	HMDB0061373	Palmitic acid	C16H32O2	M-H	255.2330	-1.4
	HMDB0240577	3-Methylcytidine	C10H15N3O5	M-H	256.0939	0.4
	HMDB0039229	Pyro-L-glutaminy-L-glutamine	C10H15N3O5	M-H	256.0939	0.4
	HMDB0000982	5-Methylcytidine	C10H15N3O5	M-H	256.0939	0.4
	HMDB0015078	Zalcitabine	C9H13N3O3	M+FA-H	256.0939	0.4
	HMDB0240340	N-acetyl-1-methyl-L-histidine	C9H13N3O3	M+FA-H	256.0939	0.4
	HMDB0240341	N-Acetyl-3-methylhistidine	C9H13N3O3	M+FA-H	256.0939	0.4
256.0940	HMDB0005766	Norphthalmic acid	C10H17N3O6	M-H2O-H	256.0933	2.6
	HMDB0011738	N2-gamma-Glutamylglutamine	C10H17N3O6	M-H2O-H	256.0933	2.6
	HMDB0028833	Glutamyl-Gamma-glutamate	C10H17N3O6	M-H2O-H	256.0933	2.6
	HMDB0028796	Glutaminyglutamic acid	C10H17N3O6	M-H2O-H	256.0933	2.6
	HMDB0029147	N-gamma-Glutamylglutamine	C10H17N3O6	M-H2O-H	256.0933	2.6
	HMDB0028817	Glutamylglutamine	C10H17N3O6	M-H2O-H	256.0933	2.6
	HMDB0001127	6-Phosphonoglucono-D-lactone	C6H11O9P	M-H	257.0068	-0.4
	HMDB0001376	2-Keto-3-deoxy-6-phosphogluconic acid	C6H11O9P	M-H	257.0068	-0.4

257.0067	HMDB0062628	[(3,4,5-trihydroxy-6-oxooxan-2-yl)methoxy]phosphonic acid	C6H11O9P	M-H	257.0068	-0.4
	HMDB0062800	2,3,4,5-tetrahydroxy-6-(phosphonoxy)hexanoic acid	C6H13O10P	M-H2O-H	257.0062	1.8
	HMDB0040924	2-Carboxyarabinitol 5-phosphate	C6H13O10P	M-H2O-H	257.0062	1.8
	HMDB0001316	6-Phosphogluconic acid	C6H13O10P	M-H2O-H	257.0062	1.8
257.1755	HMDB0014456	Ethoxzolamide	C9H10N2O3S2	M-H	257.0060	2.7
	HMDB0031017	-Undecenyl acetate	C13H24O2	M+FA-H	257.1758	-1.3
	HMDB0032792	(E)-3-Methyl-4-decen-1-yl acetate	C13H24O2	M+FA-H	257.1758	-1.3
	HMDB0037187	Rhodinyl propionate	C13H24O2	M+FA-H	257.1758	-1.3
	HMDB0039805	4-(3-Hydroxybutyl)-3,3,5-trimethylcyclohexanone	C13H24O2	M+FA-H	257.1758	-1.3
	HMDB0038078	1,1-Diethoxy-2,6-nonadiene	C13H24O2	M+FA-H	257.1758	-1.3
	HMDB0037226	Citronellyl propionate	C13H24O2	M+FA-H	257.1758	-1.3
	HMDB0037626	1-Ethylhexyl tiglate	C13H24O2	M+FA-H	257.1758	-1.3
	HMDB0037907	2,6,-Tetramethyl-1-oxaspiro[4.5]decan-6-ol	C13H24O2	M+FA-H	257.1758	-1.3
	HMDB0034286	Ethyl -undecenoate	C13H24O2	M+FA-H	257.1758	-1.3
	HMDB0031741	Coniferan	C13H24O2	M+FA-H	257.1758	-1.3
	HMDB0031028	Methyl (E)-2-dodecenoate	C13H24O2	M+FA-H	257.1758	-1.3
	HMDB0040451	Oxacyclotetradecan-2-one	C13H24O2	M+FA-H	257.1758	-1.3
	HMDB0176326	14-hydroxy-3-oxotetradecanoic acid	C14H26O4	M-H	257.1758	-1.3
	HMDB0000872	Tetradecanedioic acid	C14H26O4	M-H	257.1758	-1.3
	HMDB0176325	13-hydroxy-3-oxotetradecanoic acid	C14H26O4	M-H	257.1758	-1.3
	HMDB0176327	SCHEMBL886	C14H26O4	M-H	257.1758	-1.3
	HMDB0059946	2-Hydroxypropyl 2-isopropyl-5-methylcyclohexyl carbonate	C14H26O4	M-H	257.1758	-1.3
	HMDB0059947	1-Hydroxypropan-2-yl 2-isopropyl-5-methylcyclohexyl carbonate	C14H26O4	M-H	257.1758	-1.3
	HMDB0040429	Diethyl decanedioate	C14H26O4	M-H	257.1758	-1.3
	HMDB0041618	Diisobutyl adipate	C14H26O4	M-H	257.1758	-1.3
	HMDB0176328	4-hydroxy-3-oxotetradecanoic acid	C14H26O4	M-H	257.1758	-1.3
257.2119	HMDB0030924	2-Tetradecanone	C14H28O	M+FA-H	257.2122	-1.2
	HMDB0034283	Tetradecanal	C14H28O	M+FA-H	257.2122	-1.2
	HMDB0032432	12-Methyltridecanal	C14H28O	M+FA-H	257.2122	-1.2
	HMDB0061955	(E)-9-Tetradecen-1-ol	C14H28O	M+FA-H	257.2122	-1.2
	HMDB0059866	Ethyl 3-hydroxytridecanoate	C15H30O3	M-H	257.2122	-1.2
	HMDB0061657	3-hydroxypentadecanoic acid	C15H30O3	M-H	257.2122	-1.2
	HMDB0031061	-Hydroxymyristic acid methyl ester	C15H30O3	M-H	257.2122	-1.2
259.0224	HMDB0039494	Benzoylmalic acid	C11H10O6	M+Na-2H	259.0224	0.0
	HMDB0137298	3-(7-hydroxy-4-methoxy-2H-1,3-benzodioxol-5-yl)prop-2-enoic acid	C11H10O6	M+Na-2H	259.0224	0.0
	HMDB0137297	3-(4-hydroxy-7-methoxy-2H-1,3-benzodioxol-5-yl)prop-2-enoic acid	C11H10O6	M+Na-2H	259.0224	0.0
	HMDB0128680	3-(7-hydroxy-6-methoxy-2H-1,3-benzodioxol-5-yl)prop-2-enoic acid	C11H10O6	M+Na-2H	259.0224	0.0
	HMDB0128679	3-(6-hydroxy-7-methoxy-2H-1,3-benzodioxol-5-yl)prop-2-enoic acid	C11H10O6	M+Na-2H	259.0224	0.0
	HMDB0059654	Deoxyribose 5-monophosphate	C5H11O7P	M+FA-H	259.0224	-0.2
	HMDB0060393	5-Deoxyribose-1-phosphate	C5H11O7P	M+FA-H	259.0224	-0.2
	HMDB0001213	1-Deoxy-D-xylulose 5-phosphate	C5H11O7P	M+FA-H	259.0224	-0.2
	HMDB0001351	Deoxyribose 1-phosphate	C5H11O7P	M+FA-H	259.0224	-0.2
	HMDB0001031	Deoxyribose 5-phosphate	C5H11O7P	M+FA-H	259.0224	-0.2
	HMDB0060467	D-fructose 1-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0062705	D-Galactopyranose 1-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0000213	1D-myo-inositol 1-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0006814	D-myo-Inositol 3-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0003971	Beta-D-Fructose 6-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0003498	beta-D-Glucose 6-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0002985	Inositol phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0001401	Glucose 6-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0001313	D-myo-Inositol 4-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0001078	Mannose 6-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0001076	Fructose 1-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0000994	Dolichyl phosphate D-mannose	C6H13O9P	M-H	259.0224	-0.2
	HMDB0000124	Fructose 6-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0001586	伪-D-Glucose 1-phosphate	C6H13O9P	M-H	259.0224	-0.2

	HMDB0000645	Galactose 1-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0006328	D-Tagatose 1-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0006797	Sorbose 1-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0006800	Beta-D-Fructose 2-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0006873	D-Tagatose 6-phosphate	C6H13O9P	M-H	259.0224	-0.2
	HMDB0006330	D-Mannose 1-phosphate	C6H13O9P	M-H	259.0224	-0.2
259.1551	HMDB0183243	SCHEMBL1091	C13H24O5	M-H	259.1551	0.0
	HMDB0183241	6-hydroxytridecanedioic acid	C13H24O5	M-H	259.1551	0.0
	HMDB0183240	4-hydroxytridecanedioic acid	C13H24O5	M-H	259.1551	0.0
	HMDB0184194	2-hydroxytridecanedioic acid	C13H24O5	M-H	259.1551	0.0
	HMDB0159934	4-(3-hexyloxiran-2-yl)butanoic acid	C12H22O3	M+FA-H	259.1551	0.0
	HMDB0159935	SCHEMBL14224944	C12H22O3	M+FA-H	259.1551	0.0
	HMDB0159936	(5Z)-2-hydroxydodec-5-enoic acid	C12H22O3	M+FA-H	259.1551	0.0
	HMDB0159931	(5Z)-7-hydroxydodec-5-enoic acid	C12H22O3	M+FA-H	259.1551	0.0
	HMDB0159933	(5Z)-11-hydroxydodec-5-enoic acid	C12H22O3	M+FA-H	259.1551	0.0
	HMDB0159932	(5Z)-4-hydroxydodec-5-enoic acid	C12H22O3	M+FA-H	259.1551	0.0
	HMDB0010727	3-Oxododecanoic acid	C12H22O3	M+FA-H	259.1551	0.0
	HMDB0037398	4-Acetoxy-2-hexyltetrahydrofuran	C12H22O3	M+FA-H	259.1551	0.0
261.1494	HMDB0035028	(x)-2-Heptanol glucoside	C13H26O6	M-H2O-H	259.1545	2.1
	HMDB0059863	(S)-3-Ethyl-4-methylpentanol	C15H20O	M+FA-H	261.1496	-0.8
	HMDB0036589	1,2-Dehydro-alpha-cyperone	C15H20O	M+FA-H	261.1496	-0.8
	HMDB0035965	5beta-1,3,7(11)-Eudesmatrien-8-one	C15H20O	M+FA-H	261.1496	-0.8
	HMDB0038147	Isogermafurene	C15H20O	M+FA-H	261.1496	-0.8
	HMDB0031736	2-Hexyl-3-phenyl-2-propenal	C15H20O	M+FA-H	261.1496	-0.8
	HMDB0036769	Furanodiene	C15H20O	M+FA-H	261.1496	-0.8
	HMDB0035612	(R)-ar-Turmerone	C15H20O	M+FA-H	261.1496	-0.8
	HMDB0036108	1,3,5,11-Bisabolatetraen--one	C15H20O	M+FA-H	261.1496	-0.8
	HMDB0137262	(1E)-1-(3,4-dihydroxyphenyl)dec-1-en-3-one	C16H22O3	M-H	261.1496	-0.8
	HMDB0133034	2,4-bis(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C16H22O3	M-H	261.1496	-0.8
	HMDB0137253	(4E)-1-(3,4-dihydroxyphenyl)dec-4-en-3-one	C16H22O3	M-H	261.1496	-0.8
	HMDB0133061	2-(3,7-dimethylocta-2,6-dien-1-yl)benzene-1,3,5-triol	C16H22O3	M-H	261.1496	-0.8
	HMDB0179992	(3,4-dihydroxyphenyl)methyl 7-methyloctanoate	C16H24O4	M-H2O-H	261.1491	1.3
	HMDB0040755	3b-Hydroxy-6b-methoxy-7(11)-eremophilen-12,8a-olide	C16H24O4	M-H2O-H	261.1491	1.3
	HMDB0036979	6b-Hydroxy-8a-methoxy-7(11)-eremophilen-12,8-olide	C16H24O4	M-H2O-H	261.1491	1.3
	HMDB0041229	Methyl (3b,11x)-3-Hydroxy-8-oxo-6-eremophilen-12-oate	C16H24O4	M-H2O-H	261.1491	1.3
263.1651	HMDB0030148	Prehumulinic acid	C16H24O4	M-H2O-H	261.1491	1.3
	HMDB0134122	(2Z)-2-(phenylmethylidene)octan-1-ol	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0134121	2-benzylactanal	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0094674	1-Phenylnonan-1-one	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0036443	Rotundone	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0037000	alpha-Turmerone	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0038164	Vulgarone B	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0036201	(E)-,11-Dihydro-alpha-atlantone	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0038187	beta-Atlantone	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0036797	Mustakone	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0036733	Vulgarone A	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0036667	Zerumbone	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0036813	alpha-Santalal	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0035081	(5alpha,alpha)-3,7(11)-Eudesmadien-2-one	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0036718	beta-Santalal	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0036109	1,3,5-Bisabolatrien--one	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0035747	Patchoulenone	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0040686	Isohumbertiol	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0038195	Xanthorrhizol	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0038201	4,7(11)-Guaiadien-8-one	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0036071	Dendrolasin	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0035643	beta-Sinensal	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0038215	alpha-Sinensal	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0038200	Calamusenone	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0038511	Bisacumol	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0013687	Nookatone	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0035657	Solavetivone	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0035786	Valerenal	C15H22O	M+FA-H	263.1653	-0.6

	HMDB0037061	(+)-4,11-Eudesmadien-3-one	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0035835	Furanoeremophilane	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0037068	Curlone	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0039637	beta-Elementone	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0035082	(5beta,7beta,beta)-3,11-Eudesmadien-2-one	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0013693	AC1L1WLS	C15H22O	M+FA-H	263.1653	-0.6
	HMDB0032090	12-Oxo-2,3-dinor-,15-phytodienoic acid	C16H24O3	M-H	263.1653	-0.6
	HMDB0061935	3,5-Bis(1,1-dimethylethyl)-4-hydroxy-benzoic acid ethyl ester	C16H24O3	M-H	263.1653	-0.6
	HMDB0033630	Lactapiperanol C	C16H26O4	M-H2O-H	263.1647	1.4
	HMDB0062365	(8R,Z)-8-hydroxy-3-oxohexadeca-6,-dienoic acid	C16H26O4	M-H2O-H	263.1647	1.4
	HMDB0062366	(6E,8S,Z)-8-hydroxy-3-oxohexadecadienoic acid	C16H26O4	M-H2O-H	263.1647	1.4
264.1602	HMDB0060994	alpha-Hydroxymetoprolol	C15H25NO4	M-H2O-H	264.1600	0.9
	HMDB0061122	4-Hydroxy-alprenolol	C15H23NO3	M-H	264.1605	-1.2
	HMDB0015520	Oxprenolol	C15H23NO3	M-H	264.1605	-1.2
	HMDB0175202	Vanillic acid, heptyl ester	C15H22O4	M-H	265.1445	0.6
	HMDB0181829	5-(hydroxymethyl)-3,4a-dimethyl-4H,4aH,5H,6H,7H,8H,8aH,9H-naphtho[2,3-b]furan-4,6-diol	C15H22O4	M-H	265.1445	0.6
	HMDB0182914	2,2a,7-trihydroxy-6,6,7b-trimethyl-1H,2H,2aH,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-3-carbaldehyde	C15H22O4	M-H	265.1445	0.6
	HMDB0182916	2,2a,4a-trihydroxy-6,6,7b-trimethyl-1H,2H,2aH,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-3-carbaldehyde	C15H22O4	M-H	265.1445	0.6
	HMDB0182917	2,2a,7a-trihydroxy-6,6,7b-trimethyl-1H,2H,2aH,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-3-carbaldehyde	C15H22O4	M-H	265.1445	0.6
	HMDB0182913	2,2a,5-trihydroxy-6,6,7b-trimethyl-1H,2H,2aH,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-3-carbaldehyde	C15H22O4	M-H	265.1445	0.6
	HMDB0182912	2,2a-dihydroxy-7b-(hydroxymethyl)-6,6-dimethyl-1H,2H,2aH,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-3-carbaldehyde	C15H22O4	M-H	265.1445	0.6
	HMDB0181828	4a-(hydroxymethyl)-3,5-dimethyl-4H,4aH,5H,6H,7H,8H,8aH,9H-naphtho[2,3-b]furan-4,6-diol	C15H22O4	M-H	265.1445	0.6
	HMDB0181830	3,4a,5-trimethyl-4H,4aH,5H,6H,7H,8H,8aH,9H-naphtho[2,3-b]furan-4,5,6-triol	C15H22O4	M-H	265.1445	0.6
	HMDB0181834	3,4a,5-trimethyl-4H,4aH,5H,6H,7H,8H,8aH,9H-naphtho[2,3-b]furan-4,6,7-triol	C15H22O4	M-H	265.1445	0.6
	HMDB0181833	3,4a,5-trimethyl-4H,4aH,5H,6H,7H,8H,8aH,9H-naphtho[2,3-b]furan-4,6,8-triol	C15H22O4	M-H	265.1445	0.6
	HMDB0181831	3-(hydroxymethyl)-4a,5-dimethyl-4H,4aH,5H,6H,7H,8H,8aH,9H-naphtho[2,3-b]furan-4,6-diol	C15H22O4	M-H	265.1445	0.6
	HMDB0181832	3,4a,5-trimethyl-4H,4aH,5H,6H,7H,8H,8aH,9H-naphtho[2,3-b]furan-4,6,8a-triol	C15H22O4	M-H	265.1445	0.6
	HMDB0182911	2,2a-dihydroxy-6-(hydroxymethyl)-6,7b-dimethyl-1H,2H,2aH,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-3-carbaldehyde	C15H22O4	M-H	265.1445	0.6
	HMDB0182915	5,6-dihydroxy-8,11,11-trimethyl-3-oxatetracyclo[7.3,? 寶]dodecane-4-carbaldehyde	C15H22O4	M-H	265.1445	0.6
	HMDB0182894	3,4-dihydroxy-7,7a-dimethyl-4'-methylidene-octahydrospiro[indene-2,3'-oxolane]-2'-one	C15H22O4	M-H	265.1445	0.6
	HMDB0039516	4'-Dihydroabscisic acid	C15H22O4	M-H	265.1445	0.6
	HMDB0036152	Alkhanol	C15H22O4	M-H	265.1445	0.6
	HMDB0041425	Isoleptospermone	C15H22O4	M-H	265.1445	0.6
	HMDB0038476	5,5-Dibutyl-4,5-dihydro-2(3H)furanone	C15H22O4	M-H	265.1445	0.6
	HMDB0040905	Ipomeamaronolide	C15H22O4	M-H	265.1445	0.6
	HMDB0031902	Blennin D	C15H22O4	M-H	265.1445	0.6
	HMDB0037005	(1alpha,4alpha,5beta,6alpha,11betaH)-1,4-Epoxy-5-hydroxy-(14)-germacren-12,6-olide	C15H22O4	M-H	265.1445	0.6
265.1447	HMDB0030104	Humulinic acid A	C15H22O4	M-H	265.1445	0.6
	HMDB0036151	Arabsin	C15H22O4	M-H	265.1445	0.6

HMDB0037059	1alpha-Hydroxyarbusculin A	C15H22O4	M-H	265.1445	0.6
HMDB0035740	Arlatin	C15H22O4	M-H	265.1445	0.6
HMDB0035647	3,14-Dihydroxy-11,13-dihydrocostunolide	C15H22O4	M-H	265.1445	0.6
HMDB0033229	Absindiol	C15H22O4	M-H	265.1445	0.6
HMDB0033660	(R)-Athanagrandione	C15H22O4	M-H	265.1445	0.6
HMDB0035644	(6beta,8betaOH)-6,8-Dihydroxy-7(11)-eremophilene-12,8-olide	C15H22O4	M-H	265.1445	0.6
HMDB0030137	Adhumulinic acid	C15H22O4	M-H	265.1445	0.6
HMDB0035210	-Hydroxymyoporone	C15H22O4	M-H	265.1445	0.6
HMDB0038148	Ipomeamaranol	C15H22O4	M-H	265.1445	0.6
HMDB0036039	3alpha,15-Dihydroxymarasmene	C15H22O4	M-H	265.1445	0.6
HMDB0036038	Gomphidic acid	C15H22O4	M-H	265.1445	0.6
HMDB0037070	Sporol	C15H22O4	M-H	265.1445	0.6
HMDB0060569	Deoxyartemisinin	C15H22O4	M-H	265.1445	0.6
HMDB0034696	Artemin	C15H22O4	M-H	265.1445	0.6
HMDB0036389	3-Phenylpropyl isovalerate	C14H20O2	M+FA-H	265.1445	0.6
HMDB0126515	2-(phenylmethylidene)heptane-1,3-diol	C14H20O2	M+FA-H	265.1445	0.6
HMDB0040217	3,4-Dihydro-2,2,5,7,8-pentamethyl-2H-1-benzopyran-6-ol	C14H20O2	M+FA-H	265.1445	0.6
HMDB0133167	2-benzyl-6-hydroxyheptanal	C14H20O2	M+FA-H	265.1445	0.6
HMDB0038996	(Z)-6-Tetradecene-1,3-diyne-5,8-diol	C14H20O2	M+FA-H	265.1445	0.6
HMDB0040226	2-Methyl-1-phenyl-2-propanyl butyrate	C14H20O2	M+FA-H	265.1445	0.6
HMDB0126516	3-[(1Z)-3-hydroxy-2-pentylprop-1-en-1-yl]phenol	C14H20O2	M+FA-H	265.1445	0.6
HMDB0126517	4-[(1Z)-3-hydroxy-2-pentylprop-1-en-1-yl]phenol	C14H20O2	M+FA-H	265.1445	0.6
HMDB0133170	2-[(2-hydroxyphenyl)methyl]heptanal	C14H20O2	M+FA-H	265.1445	0.6
HMDB0039539	13-Tetradecene-1,3-diyne-6,7-diol	C14H20O2	M+FA-H	265.1445	0.6
HMDB0037606	13-Nor-6-eremophilene-8,11-dione	C14H20O2	M+FA-H	265.1445	0.6
HMDB0133169	2-benzyl-2-hydroxyheptanal	C14H20O2	M+FA-H	265.1445	0.6
HMDB0133168	2-benzyl-7-hydroxyheptanal	C14H20O2	M+FA-H	265.1445	0.6
HMDB0133166	2-[(4-hydroxyphenyl)methyl]heptanal	C14H20O2	M+FA-H	265.1445	0.6
HMDB0133164	2-[hydroxy(phenyl)methyl]heptanal	C14H20O2	M+FA-H	265.1445	0.6
HMDB0133165	2-[(3-hydroxyphenyl)methyl]heptanal	C14H20O2	M+FA-H	265.1445	0.6
HMDB0126518	(2Z)-2-(phenylmethylidene)heptane-1,6-diol	C14H20O2	M+FA-H	265.1445	0.6
HMDB0126520	(2Z)-2-(phenylmethylidene)heptane-1,7-diol	C14H20O2	M+FA-H	265.1445	0.6
HMDB0133180	2-benzylheptanoic acid	C14H20O2	M+FA-H	265.1445	0.6
HMDB0126519	(2-pentyl-3-phenyloxiran-2-yl)methanol	C14H20O2	M+FA-H	265.1445	0.6
HMDB0013817	2,6-Di-tert-butylbenzoquinone	C14H20O2	M+FA-H	265.1445	0.6
HMDB0037718	2-Phenylethyl hexanoate	C14H20O2	M+FA-H	265.1445	0.6
HMDB0037714	Hexyl phenylacetate	C14H20O2	M+FA-H	265.1445	0.6
HMDB0145053	(4E)-4-{2-[4-(diaminomethylidene)cyclohexa-2,5-dien-1-ylidene]ethylidene}-5-hydroxycyclohex-2-ene-1-carboximidamide	C16H20N4O	M-H2O-H	265.1453	-2.3
HMDB0145049	4-{2-[4-(diaminomethylidene)cyclohexa-2,5-dien-1-ylidene]ethyl}-3-hydroxycyclohexa-1,5-diene-1-carboximidamide	C16H20N4O	M-H2O-H	265.1453	-2.3
HMDB0060593	Alpha-dihydroartemisinin	C15H24O5	M-H2O-H	265.1440	2.7
HMDB0061088	Fluoxetine glucuronide	C15H24O5	M-H2O-H	265.1440	2.7
HMDB0182057	5-{2,3-dimethyltricyclo[2.2.1,]heptan-3-yl}-2-methylpent-2-en-1-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0134152	2-benzyl-octan-1-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182154	1-(6-methylhept-5-en-2-yl)-4-methylidenebicyclo[3.1]hexan-6-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182874	4a-methyl-8-methylidene-2-(prop-1-en-2-yl)-decahydronaphthalen-2-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182875	2-(4a-methyl-8-methylidene-decahydronaphthalen-2-yl)-2-methyloxirane	C15H24O	M+FA-H	265.1809	-1.6
HMDB0036420	spathulenol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182153	5-(6-methylhept-5-en-2-yl)-2-methylidenebicyclo[3.1]hexan-1-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182155	6-methyl-2-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-5-en-1-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182152	2,2-dimethyl-3-(3-{4-methylidenebicyclo[3.1]hexan-1-yl}butyl)oxirane	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182055	[2-methyl-3-(4-methylpent-3-en-1-yl)tricyclo[2.2.1,heptan-3-yl]methanol	C15H24O	M+FA-H	265.1809	-1.6

HMDB0182054	[7-methyl-7-(4-methylpent-3-en-1-yl)tricyclo[2.2.1,heptan-1-yl]methanol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182056	1-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-4-methylpent-3-en-1-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182058	.alpha.-Santalol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182059	1-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-4-methylpent-3-en-2-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182060	1,7-dimethyl-7-(4-methylpent-3-en-1-yl)tricyclo[2.2.1,heptan-3-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182062	santal--en-2-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182147	6-methyl-2-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-5-en-2-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182148	1-(6-methylhept-5-en-2-yl)-4-methylidenebicyclo[3.1]hexan-3-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182150	2-methyl-6-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-2-en-4-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182149	2-methyl-6-{4-methylidenebicyclo[3.1]hexan-1-yl}hept-2-en-1-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0182151	1-(6-methylhept-5-en-2-yl)-4-methylidenebicyclo[3.1]hexan-2-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0037395	11-Copaen-4-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0033826	2,6-Di-tert-butyl-4-methylphenol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0038123	1,5-Epoxy-4(14)-salvialene	C15H24O	M+FA-H	265.1809	-1.6
HMDB0038134	Bisabolene oxide	C15H24O	M+FA-H	265.1809	-1.6
HMDB0039532	(6Z,9Z,12Z)-6,9,12-Pentadecatrien-2-one	C15H24O	M+FA-H	265.1809	-1.6
HMDB0035718	Isocyperol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0038193	Isoshyobunone	C15H24O	M+FA-H	265.1809	-1.6
HMDB0036717	trans-beta-Santalol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0038208	Humuladienone	C15H24O	M+FA-H	265.1809	-1.6
HMDB0036788	beta-Betulenol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0038160	7(14)-Isodaucen--one	C15H24O	M+FA-H	265.1809	-1.6
HMDB0035704	Acorenone	C15H24O	M+FA-H	265.1809	-1.6
HMDB0035645	Epoxyguaiane	C15H24O	M+FA-H	265.1809	-1.6
HMDB0037069	Acoragermacrone	C15H24O	M+FA-H	265.1809	-1.6
HMDB0040763	Neoacrimarine E	C15H24O	M+FA-H	265.1809	-1.6
HMDB0035720	Isoacolamone	C15H24O	M+FA-H	265.1809	-1.6
HMDB0039711	Aromadendrene epoxide	C15H24O	M+FA-H	265.1809	-1.6
HMDB0036118	(3S,6E)-6-Caryophyllen-15-al	C15H24O	M+FA-H	265.1809	-1.6
HMDB0035306	Epishyobunone	C15H24O	M+FA-H	265.1809	-1.6
HMDB0034940	Mammea E/BB	C15H24O	M+FA-H	265.1809	-1.6
HMDB0030232	(2R,6S,7S,Z)-beta-Santala-3(15),-dien-12-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0036793	3,15-Epoxy-6-caryophyllene	C15H24O	M+FA-H	265.1809	-1.6
HMDB0035097	beta-Costol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0036789	Caryophyllene alpha-oxide	C15H24O	M+FA-H	265.1809	-1.6
HMDB0035020	Acolamone	C15H24O	M+FA-H	265.1809	-1.6
HMDB0035026	alpha-Cyperol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0035793	Fukinone	C15H24O	M+FA-H	265.1809	-1.6
HMDB0038512	Bisacurool	C15H24O	M+FA-H	265.1809	-1.6
HMDB0035391	Preisocalamendiol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0038210	Humulene epoxide II	C15H24O	M+FA-H	265.1809	-1.6
HMDB0032220	Dihydronootkatone	C15H24O	M+FA-H	265.1809	-1.6
HMDB0037811	Vetiverol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0013688	Nootkatol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0059836	Cabreuva oxide D	C15H24O	M+FA-H	265.1809	-1.6
HMDB0060295	3,7,7,-tetramethyl-2-oxatetracyclo[7.3.?寶dodecane	C15H24O	M+FA-H	265.1809	-1.6
HMDB0036716	beta-Santalol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0038211	Humulenol I	C15H24O	M+FA-H	265.1809	-1.6
HMDB0038212	Humulenol II	C15H24O	M+FA-H	265.1809	-1.6
HMDB0035739	(R)-2,7(14),9-Bisabolatrien-11-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0038146	Calacone	C15H24O	M+FA-H	265.1809	-1.6
HMDB0036798	8alpha-3-Copaen-8-ol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0036402	alpha-Bergamotenol	C15H24O	M+FA-H	265.1809	-1.6
HMDB0036192	Apritone	C15H24O	M+FA-H	265.1809	-1.6
HMDB0038119	Eremofukinone	C15H24O	M+FA-H	265.1809	-1.6
HMDB0038982	4-Nonylphenol	C15H24O	M+FA-H	265.1809	-1.6

	HMDB0037392	4(15)-Copaen-11-ol	C15H24O	M+FA-H	265.1809	-1.6
	HMDB0060356	2-trans,6-trans-Farnesal	C15H24O	M+FA-H	265.1809	-1.6
	HMDB0034718	Isospathulenol	C15H24O	M+FA-H	265.1809	-1.6
	HMDB0034661	alpha-Valerenol	C15H24O	M+FA-H	265.1809	-1.6
	HMDB0182061	3-(2-{2,3-dimethyltricyclo[2.2.1.]heptan-3-yl}ethyl)-2,2-dimethyloxirane	C15H24O	M+FA-H	265.1809	-1.6
	HMDB0182873	[1-methylidene-7-(prop-1-en-2-yl)-decahydronaphthalen-4a-yl]methanol	C15H24O	M+FA-H	265.1809	-1.6
	HMDB0112089	7-(3,4-dimethyl-5-propylfuran-2-yl)heptanoic acid	C16H26O3	M-H	265.1809	-1.6
	HMDB0112088	6-(5-hexylfuran-2-yl)hexanoic acid	C16H26O3	M-H	265.1809	-1.6
	HMDB0112097	5-Butyl-2-furanheptanoic acid	C16H26O3	M-H	265.1809	-1.6
	HMDB0112092	5-Pentyl-2-furanheptanoic acid	C16H26O3	M-H	265.1809	-1.6
	HMDB0112085	5-(3,4-dimethyl-5-pentylfuran-2-yl)-pentanoic acid	C16H26O3	M-H	265.1809	-1.6
	HMDB0033917	4-Hydroxy-3-methoxy-2,-bisaboladien-9-one	C16H26O3	M-H	265.1809	-1.6
	HMDB0060055	Tetranor 12-HETE	C16H26O3	M-H	265.1809	-1.6
	HMDB0035593	Rishitin	C14H22O2	M+FA-H	267.1602	-0.3
	HMDB0036790	Kobusone	C14H22O2	M+FA-H	267.1602	-0.3
	HMDB0036791	Isokobusone	C14H22O2	M+FA-H	267.1602	-0.3
	HMDB0037820	Acetaldehyde butyl phenethyl acetal	C14H22O2	M+FA-H	267.1602	-0.3
	HMDB0040178	2,6-Di-tert-butyl-1,4-benzenediol	C14H22O2	M+FA-H	267.1602	-0.3
	HMDB0037605	(betaH,11xi)-11-Hydroxy-13-nor-6-eremophilen-8-one	C14H22O2	M+FA-H	267.1602	-0.3
	HMDB0177232	(7bS)-3,7b-bis(hydroxymethyl)-6,6-dimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4-diol	C15H24O4	M-H	267.1602	-0.3
	HMDB0177233	(7bR)-3,6-bis(hydroxymethyl)-6,7b-dimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4-diol	C15H24O4	M-H	267.1602	-0.3
	HMDB0177237	(7bR)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4,4a-triol	C15H24O4	M-H	267.1602	-0.3
	HMDB0177236	(7bS)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4,7a-triol	C15H24O4	M-H	267.1602	-0.3
	HMDB0177235	(7bR)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4,5-triol	C15H24O4	M-H	267.1602	-0.3
	HMDB0177234	(7bR)-3-(hydroxymethyl)-6,6,7b-trimethyl-1H,2H,4H,4aH,5H,6H,7H,7aH,7bH-cyclobuta[e]indene-2,4,7-triol	C15H24O4	M-H	267.1602	-0.3
	HMDB0240213	Prostaglandin lactone-diol	C15H24O4	M-H	267.1602	-0.3
	HMDB0036150	4,11,13,15-Tetrahydridoridentin B	C15H24O4	M-H	267.1602	-0.3
	HMDB0038503	Bisacurone epoxide	C15H24O4	M-H	267.1602	-0.3
	HMDB0038153	1-(3-Furanyl)-6,7-dihydroxy-4,8-dimethyl-1-nonanone	C15H24O4	M-H	267.1602	-0.3
	HMDB0038154	3,11,12-Trihydroxy-1()-spirovetiven-2-one	C15H24O4	M-H	267.1602	-0.3
	HMDB0038165	Acoric acid	C15H24O4	M-H	267.1602	-0.3
	HMDB0060570	Deoxydihydro-artemisinin	C15H24O4	M-H	267.1602	-0.3
	HMDB0059777	2,2,4-Trimethyl-1,3-pentadienol diisobutyrate	C16H30O4	M-H2O-H	267.1960	0.7
	HMDB0061936	Isooctanedioldibutyrate	C16H30O4	M-H2O-H	267.1960	0.7
	HMDB0041287	16-Hydroxy--oxohexadecanoic acid	C16H30O4	M-H2O-H	267.1960	0.7
	HMDB0000672	Hexadecanedioic acid	C16H30O4	M-H2O-H	267.1960	0.7
	HMDB0062018	1-[2-(Isobutyryloxy)-1-methylethyl]-2,2-dimethylpropyl 2-methylpropanoate	C16H30O4	M-H2O-H	267.1960	0.7
	HMDB0036197	(-)-alpha-Bisabolol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0041575	Isokessane	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0036452	alpha-cadinol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0041629	(3S,6E)-nerolidol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0036646	Cedrelanol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0036445	Bulnesol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0035662	Nerolidol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0036579	Carotol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0035711	Panasinsanol A	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0039744	Ginsenosol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0037066	beta-Caryophyllene alcohol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0036679	Faurinone	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0059841	Cubenol	C15H26O	M+FA-H	267.1966	-1.4

267.1962	HMDB0039538	(6Z,9Z)-6,9-Pentadecadien-2-one	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0036447	Guaioxide	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0030938	beta-Triticene	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0036645	Globulol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0035199	Sesquisabinene hydrate	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0036732	Licoagroaurone	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0037031	Epicubenol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0033239	Pogostol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0035351	4beta-8-Daucen-4-ol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0037394	p-Hydroxynonanophenone	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0036642	Isointermedeol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0036198	(+)-alpha-Bisabolol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0035021	(-)-Pacifigorgiol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0035364	6-Epi-beta-bisabolol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0059849	(Z)-Farnesol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0036111	beta-Bisabolol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0035868	Rosifoliol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0036908	Sesquicineol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0038167	Maalialcohol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0038213	Humulol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0035663	(S)-Nerolidol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0036421	(-)-Valeranone	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0037234	Koraiol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0034982	-Epijunenol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0040422	Chamomillol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0037067	Zingiberenol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0030939	alpha-Triticene	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0035383	Panasinsanol B	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0035811	Shyobunol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0034951	Valerianol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0036580	5,8-Epoxydaucane	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0004305	Farnesol	C15H26O	M+FA-H	267.1966	-1.4
	HMDB0159342	FA(16:1)(Ep,cyclo)	C16H28O3	M-H	267.1966	-1.4
	HMDB0159345	(7Z,Z)-2-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M-H	267.1966	-1.4
	HMDB0167945	2-(4-hydroxy-5-methoxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C16H28O3	M-H	267.1966	-1.4
	HMDB0159338	(7Z,9E)-11-hydroxyhexadeca-7,9-dienoic acid	C16H28O3	M-H	267.1966	-1.4
	HMDB0159341	6-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}hexanoic acid	C16H28O3	M-H	267.1966	-1.4
	HMDB0159343	(7Z,Z)-16-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M-H	267.1966	-1.4
	HMDB0159339	(Z)-7-hydroxyhexadeca-8,-dienoic acid	C16H28O3	M-H	267.1966	-1.4
	HMDB0159335	(7Z,Z)-6-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M-H	267.1966	-1.4
	HMDB0159337	(7Z,Z)-9-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M-H	267.1966	-1.4
	HMDB0159336	(7Z,Z)-12-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M-H	267.1966	-1.4
	HMDB0159340	(7Z,Z)-15-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M-H	267.1966	-1.4
267.2326	HMDB0031042	Avocadene	C17H34O3	M-H2O-H	267.2324	0.7
	HMDB0061663	12-hydroxyheptadecanoic acid	C17H34O3	M-H2O-H	267.2324	0.7
	HMDB0062437	(9Z)-heptadecenoic acid	C17H32O2	M-H	267.2330	-1.3
	HMDB0060038	Z-Heptadecenoic acid	C17H32O2	M-H	267.2330	-1.3
	HMDB0061858	7-Hexadecenoic acid, methyl ester	C17H32O2	M-H	267.2330	-1.3
	HMDB0031046	9E-Heptadecenoic acid	C17H32O2	M-H	267.2330	-1.3
	HMDB0040888	2,4-Heptadecanedione	C17H32O2	M-H	267.2330	-1.3
	HMDB0030997	Cyclohexaneundecanoic acid	C17H32O2	M-H	267.2330	-1.3
269.1393	HMDB0163216	(2E,4E)-6-(3-pentyloxiran-2-yl)hexa-2,4-dienoic acid	C13H20O3	M+FA-H	269.1394	-0.5
	HMDB0163215	(2E)-3-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}prop-2-enoic acid	C13H20O3	M+FA-H	269.1394	-0.5
	HMDB0163214	3-[(1E,4Z)-deca-1,4-dien-1-yl]oxirane-2-carboxylic acid	C13H20O3	M+FA-H	269.1394	-0.5
	HMDB0163211	(2E,4E,7Z)-13-hydroxytrideca-2,4,7-trienoic acid	C13H20O3	M+FA-H	269.1394	-0.5
	HMDB0163213	(2E,4E,7Z)-9-hydroxytrideca-2,4,7-trienoic acid	C13H20O3	M+FA-H	269.1394	-0.5
	HMDB0163210	(2E,4E,7Z)-12-hydroxytrideca-2,4,7-trienoic acid	C13H20O3	M+FA-H	269.1394	-0.5
	HMDB0112084	3-(3-methyl-5-pentylfuran-2-yl)propanoic acid	C13H20O3	M+FA-H	269.1394	-0.5
	HMDB0037244	(8alpha,beta,11beta)-3-Hydroxy-4,15-dinor-1(5)-xanthen-12,8-olide	C13H20O3	M+FA-H	269.1394	-0.5
	HMDB0036583	Methyl jasmonate	C13H20O3	M+FA-H	269.1394	-0.5
	HMDB0037726	Octyl 2-furoate	C13H20O3	M+FA-H	269.1394	-0.5

	HMDB0037730	Furfuryl octanoate	C13H20O3	M+FA-H	269.1394	-0.5
	HMDB0032679	Annuiouone A	C13H20O3	M+FA-H	269.1394	-0.5
	HMDB0029670	Epoxyeremopetasinorol	C13H20O3	M+FA-H	269.1394	-0.5
	HMDB0032689	Annuiouone C	C13H20O3	M+FA-H	269.1394	-0.5
	HMDB0034564	13-Oxo-9,11-tridecadienoic acid	C13H20O3	M+FA-H	269.1394	-0.5
269.1756	HMDB0037736	3-Methylbutyl 2-furanbutanoate	C13H20O3	M+FA-H	269.1394	-0.5
	HMDB0030426	Linalyl isobutyrate	C14H24O2	M+FA-H	269.1758	-0.9
	HMDB0032524	Terpinyl isobutyrate	C14H24O2	M+FA-H	269.1758	-0.9
	HMDB0037814	2-Propenyl cyclohexanepentanoate	C14H24O2	M+FA-H	269.1758	-0.9
	HMDB0038260	Geranyl 2-methylpropanoate	C14H24O2	M+FA-H	269.1758	-0.9
	HMDB0038246	Bornyl butyrate	C14H24O2	M+FA-H	269.1758	-0.9
	HMDB0030427	Linalyl butyrate	C14H24O2	M+FA-H	269.1758	-0.9
	HMDB0032342	Isobornyl isobutyrate	C14H24O2	M+FA-H	269.1758	-0.9
	HMDB0031015	Ethyl (2E,6Z)-dodecadienoate	C14H24O2	M+FA-H	269.1758	-0.9
	HMDB0036424	Allyl undecylenate	C14H24O2	M+FA-H	269.1758	-0.9
	HMDB0032053	alpha-Terpineol butanoate	C14H24O2	M+FA-H	269.1758	-0.9
	HMDB0038259	Neryl butyrate	C14H24O2	M+FA-H	269.1758	-0.9
	HMDB0000560	Goshuyic acid	C14H24O2	M+FA-H	269.1758	-0.9
	HMDB0039129	Goshuyic acid	C14H24O2	M+FA-H	269.1758	-0.9
	HMDB0040459	Ethylene brassylate	C15H26O4	M-H	269.1758	-0.9
269.2119	HMDB0031885	6-Hydroxypentadecanedioic acid	C15H28O5	M-H2O-H	269.1753	1.2
	HMDB0072843	MG/a-13)[rac]	C16H32O4	M-H2O-H	269.2117	0.9
	HMDB0072845	MG(13)	C16H32O4	M-H2O-H	269.2117	0.9
	HMDB0072861	MG/13)	C16H32O4	M-H2O-H	269.2117	0.9
	HMDB0072870	MG/i-13)	C16H32O4	M-H2O-H	269.2117	0.9
	HMDB0072841	MG(a-13)[rac]	C16H32O4	M-H2O-H	269.2117	0.9
	HMDB0037798	(S)-,16-Dihydroxyhexadecanoic acid	C16H32O4	M-H2O-H	269.2117	0.9
	HMDB0031111	5,-Pentadecadien-1-ol	C15H28O	M+FA-H	269.2122	-1.2
	HMDB0032218	(+/-)-Dihydrofarnesol	C15H28O	M+FA-H	269.2122	-1.2
	HMDB0040377	3-Pentadecenal	C15H28O	M+FA-H	269.2122	-1.2
	HMDB0166466	(3Z)-2-hydroxyhexadec-3-enoic acid	C16H30O3	M-H	269.2122	-1.2
	HMDB0166467	4-hydroxy-trans-2-hexadecenoic acid	C16H30O3	M-H	269.2122	-1.2
	HMDB0166463	(3Z)-15-hydroxyhexadec-3-enoic acid	C16H30O3	M-H	269.2122	-1.2
	HMDB0166465	(3Z)-16-hydroxyhexadec-3-enoic acid	C16H30O3	M-H	269.2122	-1.2
	HMDB0166464	2-(3-dodecyloxiran-2-yl)acetic acid	C16H30O3	M-H	269.2122	-1.2
	HMDB0160971	(9Z)-11-hydroxyhexadec-9-enoic acid	C16H30O3	M-H	269.2122	-1.2
	HMDB0160975	16-hydroxy-9Z-hexadecenoic acid	C16H30O3	M-H	269.2122	-1.2
	HMDB0160976	hydroxy-palmitoleic acid	C16H30O3	M-H	269.2122	-1.2
	HMDB0166462	(3Z)-5-hydroxyhexadec-3-enoic acid	C16H30O3	M-H	269.2122	-1.2
	HMDB0160972	8-Hydroxypalmitoleic acid	C16H30O3	M-H	269.2122	-1.2
	HMDB0160974	9,-Epoxyhexadecanoic acid	C16H30O3	M-H	269.2122	-1.2
	HMDB0160973	(9Z)-15-hydroxyhexadec-9-enoic acid	C16H30O3	M-H	269.2122	-1.2
	HMDB0010733	3-Oxohehexadecanoic acid	C16H30O3	M-H	269.2122	-1.2
	HMDB0030973	9-Oxohehexadecanoic acid	C16H30O3	M-H	269.2122	-1.2
	HMDB0030972	8-Oxohehexadecanoic acid	C16H30O3	M-H	269.2122	-1.2
	HMDB0030978	11-Oxohehexadecanoic acid	C16H30O3	M-H	269.2122	-1.2
269.2482	HMDB0002259	Heptadecanoic acid	C17H34O2	M-H	269.2486	-1.5
	HMDB0061709	15-Methylpalmitate	C17H34O2	M-H	269.2486	-1.5
	HMDB0031067	(S)-14-Methylhexadecanoic acid	C17H34O2	M-H	269.2486	-1.5
	HMDB0040598	11-Methylhexadecanoic acid	C17H34O2	M-H	269.2486	-1.5
	HMDB0040392	Isopropyl tetradecanoate	C17H34O2	M-H	269.2486	-1.5
	HMDB0061859	Methyl hexadecanoic acid	C17H34O2	M-H	269.2486	-1.5
	HMDB0037372	3-Methylbutyl dodecanoate	C17H34O2	M-H	269.2486	-1.5
	HMDB0034131	Nonyl octanoate	C17H34O2	M-H	269.2486	-1.5
	HMDB0059870	Ethyl pentadecanoate	C17H34O2	M-H	269.2486	-1.5
	HMDB0061969	Pentadecyl acetate	C17H34O2	M-H	269.2486	-1.5
271.1555	HMDB0176430	(9E)-13-oxotridec-9-enoic acid	C13H22O3	M+FA-H	271.1551	1.5
	HMDB0176431	(9E,11E)-13-hydroxytrideca-9,11-dienoic acid	C13H22O3	M+FA-H	271.1551	1.5
	HMDB0037562	Riesling acetal	C13H22O3	M+FA-H	271.1551	1.5
	HMDB0040615	4,5-Dihydrovomifoliol	C13H22O3	M+FA-H	271.1551	1.5
	HMDB0031740	Methyl dihydrojasmonate	C13H22O3	M+FA-H	271.1551	1.5
	HMDB0040168	Glycerol 1-(5-hydroxydodecanoate)	C15H30O5	M-H2O-H	271.1909	0.2
	HMDB0062248	(9E)-tetradecenoic acid	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0094671	cyclohexyl octanoate	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0062243	cis-tetradec-7-enoic acid	C14H26O2	M+FA-H	271.1915	-1.8

271.1910	HMDB0000499	5-Tetradecenoic acid	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0037369	Butyl 2-decenoate	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0037228	Citronellyl isobutyrate	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0037227	Citronellyl butyrate	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0037189	Rhodinyl isobutyrate	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0037188	Rhodinyl butyrate	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0031073	12-Methyl-13-tridecanolide	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0034561	Houttuynin	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0038056	delta-Tetradecalactone	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0030921	(R)-14-Methyloxacyclotetradecan-2-one	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0031029	Ethyl (E)-2-dodecenoate	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0037633	xi-Tetrahydro-3-nonyl-2H-pyran-2-one	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0010732	trans-Tetra-dec-2-enoic acid	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0005051	Tsuzuic acid	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0002000	Myristoleic acid	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0000521	5Z-Tetradecenoic acid	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0040228	1,1-Diethoxy-3,7-dimethyl-2,6-octadiene	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0061991	Menthyl butyrate	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0032152	Acetaldehyde di-cis-3-hexenyl acetal	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0032321	2-Hexenyl octanoate	C14H26O2	M+FA-H	271.1915	-1.8
	HMDB0035918	7(14)-Bisabolene-2,3,,11-tetrol	C15H28O4	M-H	271.1915	-1.8
271.2275	HMDB0061956	Z--Pentadecen-1-ol	C15H30O	M+FA-H	271.2279	-1.4
	HMDB0059813	Heptyl ketone	C15H30O	M+FA-H	271.2279	-1.4
	HMDB0031078	Pentadecanal	C15H30O	M+FA-H	271.2279	-1.4
	HMDB0031081	2-Pentadecanone	C15H30O	M+FA-H	271.2279	-1.4
	HMDB0062548	2-hydroxyhexadecanoate	C16H31O3	M-H	271.2279	-1.4
	HMDB0184177	4-(hydroxymethyl)-8,12-dimethyltridecanoic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0112184	5-hydroxy-hexadecanoic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0061658	(S)-3-hydroxypalmitic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0031057	2s-hydroxypalmitic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0112187	9-Hydroxypalmitic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0112190	12-hydroxyhexadecanoic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0112192	6-hydroxyhexadecanoic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0184178	8-(hydroxymethyl)-4,12-dimethyltridecanoic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0184328	13-hydroxy-4,8,12-trimethyltridecanoic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0184175	8-hydroxy-4,8,12-trimethyltridecanoic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0184176	12-hydroxy-4,8,12-trimethyltridecanoic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0184180	2-hydroxy-4,8,12-trimethyltridecanoic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0184174	4-hydroxy-4,8,12-trimethyltridecanoic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0112191	13-hydroxyhexadecanoic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0006294	16-Hydroxy hexadecanoic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0155887	16-Hydroxy hexadecanoic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0112186	8-hydroxypalmitic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0112189	11-hydroxy palmitic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0112185	7-hydroxyhexadecanoic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0112188	-hydroxyhexadecanoic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0155886	15-hydroxypalmitic acid	C16H32O3	M-H	271.2279	-1.4
	HMDB0010734	(R)-3-Hydroxy-hexadecanoic acid	C16H32O3	M-H	271.2279	-1.4
272.0886	HMDB0000014	Deoxycytidine	C9H13N3O4	M+FA-H	272.0888	-0.8
272.1990	HMDB0030275	Herculin	C16H29NO	M+Na-2H	272.1996	-2.1
273.0917	HMDB0141099	(6Z)-6-hydroxy-1,7-diphenylhepta-1,6-diene-3,5-dione	C19H16O3	M-H2O-H	273.0916	0.5
	HMDB0141080	(6E)-7-(4-hydroxyphenyl)-1-phenylhepta-1,6-diene-3,5-dione	C19H16O3	M-H2O-H	273.0916	0.5
	HMDB0141079	(6E)-1-(4-hydroxyphenyl)-7-phenylhepta-1,6-diene-3,5-dione	C19H16O3	M-H2O-H	273.0916	0.5
	HMDB0141105	1,7-diphenylhept-6-ene-2,3,5-trione	C19H16O3	M-H2O-H	273.0916	0.5
	HMDB0178312	4-phenyl-2,3-dihydro-1H-phenalene-1,2,3-triol	C19H16O3	M-H2O-H	273.0916	0.5
	HMDB0175079	9-(4-hydroxyphenyl)-2,3-dihydro-1H-phenalene-1,2-diol	C19H16O3	M-H2O-H	273.0916	0.5
	HMDB0141160	(6E)-4-hydroxy-1,7-diphenylhepta-1,6-diene-3,5-dione	C19H16O3	M-H2O-H	273.0916	0.5
	HMDB0141149	(6E)-7-(3-hydroxyphenyl)-1-phenylhepta-1,6-diene-3,5-dione	C19H16O3	M-H2O-H	273.0916	0.5
	HMDB0040889	(all-E)-1,7-bis(4-hydroxyphenyl)-1,4,6-heptatrien-3-	C19H16O3	M-H2O-H	273.0916	0.5
	HMDB0141126	(6E)-1-(3-hydroxyphenyl)-7-phenylhepta-1,6-diene-3,5-dione	C19H16O3	M-H2O-H	273.0916	0.5

	HMDB0141119	(1Z,6E)-2-hydroxy-1,7-diphenylhepta-1,6-diene-3,5-dione	C19H16O3	M-H2O-H	273.0916	0.5
	HMDB0141122	(6E)-1,7-diphenylhept-6-ene-2,3,5-trione	C19H16O3	M-H2O-H	273.0916	0.5
	HMDB0168177	9-phenyl-1H-phenalene-1,2-diol	C19H14O2	M-H	273.0921	-1.5
	HMDB0168171	2-hydroxy-9-phenyl-2,3-dihydro-1H-phenalen-1-one	C19H14O2	M-H	273.0921	-1.5
	HMDB0168190	1-hydroxy-9-phenyl-2,3-dihydro-1H-phenalen-2-one	C19H14O2	M-H	273.0921	-1.5
	HMDB0032173	Bakers yeast extract	C19H14O2	M-H	273.0921	-1.5
	HMDB0173636	{3-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-3-carboxypropyl}dimethylsulfanium	C11H21N2O5S	M-H2O-H	273.0909	2.9
	HMDB0039096	N-gamma-Glutamyl-S-propylcysteine	C11H20N2O5S	M-H2O-H	273.0909	2.9
274.1049	HMDB0028817	Glutamylglutamine	C10H17N3O6	M-H	274.1045	1.6
	HMDB0028796	Glutaminylglutamic acid	C10H17N3O6	M-H	274.1045	1.6
	HMDB0029147	N-gamma-Glutamylglutamine	C10H17N3O6	M-H	274.1045	1.6
	HMDB0005766	Norphthalmic acid	C10H17N3O6	M-H	274.1045	1.6
	HMDB0028833	Glutamyl-Gamma-glutamate	C10H17N3O6	M-H	274.1045	1.6
	HMDB0011738	N2-gamma-Glutamylglutamine	C10H17N3O6	M-H	274.1045	1.6
	HMDB0029012	Prolyl-Asparagine	C9H15N3O4	M+FA-H	274.1045	1.6
	HMDB0028739	Asparaginyl-Proline	C9H15N3O4	M+FA-H	274.1045	1.6
	HMDB0240247	Pimethixene	C19H19NS	M-H2O-H	274.1054	-1.9
275.1651	HMDB0168944	heptadeca-1,9-dien-4,6-diyne-3,9,-triol	C17H24O3	M-H	275.1653	-0.6
	HMDB0168365	(7Z)-1-(oxiran-2-yl)pentadec-7-en-2,4-diyne-1,6-diol	C17H24O3	M-H	275.1653	-0.6
	HMDB0171243	(9E)-heptadeca-1,9-dien-4,6-diyne-3,8,11-triol	C17H24O3	M-H	275.1653	-0.6
	HMDB0015586	Cyclandelate	C17H24O3	M-H	275.1653	-0.6
	HMDB0040375	Ginsenoynes K	C17H24O3	M-H	275.1653	-0.6
	HMDB0041201	Panaquinquecol 7	C17H24O3	M-H	275.1653	-0.6
	HMDB0171246	(8E)-heptadeca-8,16-dien-11,13-diyne-1,,15-triol	C17H24O3	M-H	275.1653	-0.6
	HMDB0038994	Ginsenoynes C	C17H24O3	M-H	275.1653	-0.6
	HMDB0038938	Panaquinquecol 2	C17H24O3	M-H	275.1653	-0.6
	HMDB0031463	[8]-Shogaol	C17H24O3	M-H	275.1653	-0.6
	HMDB0171244	(8E)-heptadeca-8,16-dien-11,13-diyne-2,,15-triol	C17H24O3	M-H	275.1653	-0.6
	HMDB0171245	(7E)-1-(oxiran-2-yl)pentadec-7-en-2,4-diyne-1,6-diol	C17H24O3	M-H	275.1653	-0.6
	HMDB0168364	(8Z)-heptadeca-8,16-dien-11,13-diyne-2,,15-triol	C17H24O3	M-H	275.1653	-0.6
	HMDB0137236	Shogaols	C17H24O3	M-H	275.1653	-0.6
	HMDB0168366	(8Z)-heptadeca-8,16-dien-11,13-diyne-1,,15-triol	C17H24O3	M-H	275.1653	-0.6
	HMDB0137237	(1E)-1-(4-hydroxy-3-methoxyphenyl)dec-1-en-3-one	C17H24O3	M-H	275.1653	-0.6
	HMDB0137250	4-[(1E,4E)-3-hydroxydeca-1,4-dien-1-yl]-2-methoxyphenol	C17H24O3	M-H	275.1653	-0.6
	HMDB0168363	CHEMBL1719	C17H24O3	M-H	275.1653	-0.6
	HMDB0180101	(3,4-dihydroxyphenyl)methyl 8-methylnonanoate	C17H26O4	M-H2O-H	275.1647	1.4
	HMDB0005783	Gingerol	C17H26O4	M-H2O-H	275.1647	1.4
	HMDB0034779	Nordihydrocapsiate	C17H26O4	M-H2O-H	275.1647	1.4
	HMDB0035722	Tanacetol A	C17H26O4	M-H2O-H	275.1647	1.4
	HMDB0035754	Phytuberin	C17H26O4	M-H2O-H	275.1647	1.4
	HMDB0040646	Myrsinone	C17H26O4	M-H2O-H	275.1647	1.4
	HMDB0039376	Methyl dihydrophaseate	C16H24O5	M-H2O-H	277.1440	0.8
	HMDB0038120	Ovalicin	C16H24O5	M-H2O-H	277.1440	0.8
	HMDB0041551	3,8-Dihydroxy-6-methoxy-7(11)-eremophilene-12,8-olide	C16H24O5	M-H2O-H	277.1440	0.8
	HMDB0134125	(2Z)-2-[(3-hydroxyphenyl)methylidene]octanal	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0134128	2-hexyl-3-phenyloxirane-2-carbaldehyde	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0134129	(2Z)-8-hydroxy-2-(phenylmethylidene)octanal	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0134127	(2Z)-7-hydroxy-2-(phenylmethylidene)octanal	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0134123	(2Z)-2-(phenylmethylidene)octanoic acid	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0134124	3-hydroxy-2-(phenylmethylidene)octanal	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0134126	(2Z)-2-[(4-hydroxyphenyl)methylidene]octanal	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0134130	(2Z)-2-[(2-hydroxyphenyl)methylidene]octanal	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0176371	(9E)-11-hydroxypentadec-9-en-12,14-diyne	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0036688	Costunolide	C15H20O2	M+FA-H	277.1445	-1.2

277.1442	HMDB0036766	Furanogermenone	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0036119	Alloalantolactone	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0036881	Germacone-13-al	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0035906	Alantolactone	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0035934	Isoalantolactone	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0039011	1,3,11(13)-Eudesmatrien-12-oic acid	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0041038	Collybial	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0041062	,11-Epidioxycalamene	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0036206	alpha-Amylcinnamyl formate	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0040902	(E)-9-(3-Furanyl)-2,6-dimethyl-2,6-nonadien-4-one	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0036110	(S)-Bilobanone	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0031000	(Z)-8-Decene-4,6-diyn-1-yl 3-methylbutanoate	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0035412	1(),11-Eremophiladiene-2,9-dione	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0037563	Turmeronol B	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0040981	(7b,a)-3-Hydroxy-1,3,5-cadinatrien-9-one	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0030761	Pterisin O	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0037608	Turmeronol A	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0030790	6-[(3,4-Methylenedioxy)phenyl]-3,3-dimethyl-1-	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0036148	Furoeremophilone 1	C15H20O2	M+FA-H	277.1445	-1.2
	HMDB0013248	Monoethylhexyl phthalic acid	C16H22O4	M-H	277.1445	-1.2
	HMDB0168847	3,4,5-trihydroxy-2,4-bis(3-methylbut-2-en-1-yl)cyclohexa-2,5-dien-1-one	C16H22O4	M-H	277.1445	-1.2
	HMDB0013835	Diisobutyl phthalate	C16H22O4	M-H	277.1445	-1.2
	HMDB0133047	bis(3-methylbut-2-en-1-yl)benzene-1,2,3,5-tetrol	C16H22O4	M-H	277.1445	-1.2
	HMDB0133048	2-[(3,3-dimethyloxiran-2-yl)methyl]-4-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C16H22O4	M-H	277.1445	-1.2
	HMDB0133084	4-(3,7-dimethylocta-2,6-dien-1-yl)benzene-1,2,3,5-tetrol	C16H22O4	M-H	277.1445	-1.2
	HMDB0133085	2-[[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]methyl]benzene-1,3,5-triol	C16H22O4	M-H	277.1445	-1.2
	HMDB0133087	2-[(2Z)-4-hydroxy-3-(4-methylpent-3-en-1-yl)but-2-en-1-yl]benzene-1,3,5-triol	C16H22O4	M-H	277.1445	-1.2
	HMDB0133089	2-(5-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)benzene-1,3,5-triol	C16H22O4	M-H	277.1445	-1.2
	HMDB0133091	2-(8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)benzene-1,3,5-triol	C16H22O4	M-H	277.1445	-1.2
	HMDB0133086	2-[5-(3,3-dimethyloxiran-2-yl)-3-methylpent-2-en-1-yl]benzene-1,3,5-triol	C16H22O4	M-H	277.1445	-1.2
	HMDB0133090	2-[(6E)-8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl]benzene-1,3,5-triol	C16H22O4	M-H	277.1445	-1.2
	HMDB0033244	Dibutyl phthalate	C16H22O4	M-H	277.1445	-1.2
	HMDB0133046	2-(4-hydroxy-3-methylbut-2-en-1-yl)-4-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C16H22O4	M-H	277.1445	-1.2
	HMDB0133045	2-(4-hydroxy-3-methylbut-2-en-1-yl)-4-(3-methylbut-2-en-1-yl)benzene-1,3,5-triol	C16H22O4	M-H	277.1445	-1.2
	HMDB0133088	2-(4-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)benzene-1,3,5-triol	C16H22O4	M-H	277.1445	-1.2
	HMDB0001518	alpha-CEHC	C16H22O4	M-H	277.1445	-1.2
277.1806	HMDB0134775	5-formyl-6-hydroxy-1,1,4a,6-tetramethyl-decahydronaphthalen-2-yl acetate	C17H28O4	M-H2O-H	277.1804	0.8
	HMDB0038798	(1(E,4a,5E)-1(),5-Germacradiene-12-acetoxy-4,11-diol	C17H28O4	M-H2O-H	277.1804	0.8
	HMDB0035075	Tanacetol B	C17H28O4	M-H2O-H	277.1804	0.8
	HMDB0029704	1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1,6-heptadien-3-one	C16H24O	M+FA-H	277.1809	-1.1
	HMDB0168550	(8E,13E)-heptadeca-8,13,16-trien-11-yne-2,,15-triol	C17H26O3	M-H	277.1809	-1.2
	HMDB0168549	(4E,9E)-heptadeca-1,4,9-trien-6-yne-3,8,11-triol	C17H26O3	M-H	277.1809	-1.2
	HMDB0168552	(4E)-1-[3-(1-hydroxyprop-2-en-1-yl)oxiran-2-yl]dodec-4-en-1-yn-3-ol	C17H26O3	M-H	277.1809	-1.2
	HMDB0168554	(8E,13E)-heptadeca-8,13,16-trien-11-yne-1,,15-triol	C17H26O3	M-H	277.1809	-1.2
	HMDB0168553	(4E)-1-(3-heptyloxiran-2-yl)octa-4,7-dien-2-yne-1,6-diol	C17H26O3	M-H	277.1809	-1.2
	HMDB0168551	(2E,7E)-1-(oxiran-2-yl)pentadeca-2,7-dien-4-yne-1,6-diol	C17H26O3	M-H	277.1809	-1.2
	HMDB0030974	8-Acetoxy-4-acoren-3-one	C17H26O3	M-H	277.1809	-1.2

	HMDB0137260	4-[(4E)-3-hydroxydec-4-en-1-yl]-2-methoxyphenol	C17H26O3	M-H	277.1809	-1.2
	HMDB0137271	4-[(1E)-3-hydroxydec-1-en-1-yl]-2-methoxyphenol	C17H26O3	M-H	277.1809	-1.2
	HMDB0031928	Panaxatriol	C17H26O3	M-H	277.1809	-1.2
	HMDB0030801	[6]-Paradol	C17H26O3	M-H	277.1809	-1.2
	HMDB0039251	Panaxacol	C17H26O3	M-H	277.1809	-1.2
279.1600	HMDB0240643	3,5-di-tert-butyl-4-hydroxybenzaldehyde	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0134131	2-[hydroxy(phenyl)methyl]octanal	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0150675	2,5,5,8a-tetramethyl-6-oxo-1,4,4a,5,6,7,8,8a-octahydronaphthalene-1-carbaldehyde	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0177624	(1Z)-1-ethylidene-5-hydroxy-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0177700	(1E)-1-ethylidene-5-hydroxy-4-methylidene-7-(propan-2-yl)-octahydro-1H-inden-2-one	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0183493	(8aR)-4-hydroxy-1,8a-dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-one	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0134153	2-benzyl-octanoic acid	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0134142	(2-hexyl-3-phenyloxiran-2-yl)methanol	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0134132	2-[(3-hydroxyphenyl)methyl]octanal	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0134133	2-[(4-hydroxyphenyl)methyl]octanal	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0134134	2-benzyl-7-hydroxyoctanal	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0134135	2-benzyl-8-hydroxyoctanal	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0134139	3-[(1Z)-2-hexyl-3-hydroxyprop-1-en-1-yl]phenol	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0134137	2-[(2-hydroxyphenyl)methyl]octanal	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0134136	2-benzyl-2-hydroxyoctanal	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0134138	2-(phenylmethylidene)octane-1,3-diol	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0134141	(2Z)-2-(phenylmethylidene)octane-1,7-diol	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0134143	(2Z)-2-(phenylmethylidene)octane-1,8-diol	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0134140	4-[(1Z)-2-hexyl-3-hydroxyprop-1-en-1-yl]phenol	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0036466	Zerumbone oxide	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0036647	Isocurcumenol	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0038698	xi-2-Hydroxy-1,3,5-bisabolatrien-9-one	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0037710	4-Methylphenyl octanoate	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0035639	Petasalbin	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0037391	p-Hydroxynonanophenone	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0038190	Rishitinol	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0038795	7,9-Illudadiene-3,14-diol	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0033252	Curcumanolide A	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0038914	4,6-Decadiyn-1-ol isovalerate	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0035408	1,-Epoxygermacrone	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0039621	beta-Santalal acid	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0034562	9-Pentadecene-12,14-diyne-1,11-diol	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0036449	(1alpha,4beta,5beta)-4-Hydroxy-7(11),(14)-guaia dien-8-one	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0033960	Curcumenol	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0035935	Dihydroisoolantolactone	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0031349	Epiacoronene	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0035413	(4alpha,5alpha)-11-Eremophilene-2,9-dione	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0036392	(Z)-alpha-Bergamotenoic acid	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0034956	Oxysolavetivone	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0035869	alpha-Rotunol	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0036390	3-Phenylpropyl hexanoate	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0041036	Sugeonol	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0035889	Germacrone 4,5-epoxide	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0037739	7-(1,3-Cyclohexadienyl)-5-hydroxy-2,6-dimethyl-2-hepten-4-one	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0036427	Procucumenol	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0035794	beta-Costic acid	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0036035	Acutissimin A	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0032081	4,-Longipinanedione	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0038796	2,7(14)-Illudadiene-,15-diol	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0034742	Saussurea lactone	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0033253	Curcumenone	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0030016	Valerenic acid	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0037640	2-Methyl-4-phenyl-2-butyl 2-methylpropanoate	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0035202	7-Hydroxycostal	C15H22O2	M+FA-H	279.1602	-0.6

	HMDB0038198	3,7-Bisaboladiene-2,8-dione	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0037038	Cyclodehydroisolubimin	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0035407	Dehydrocurdione	C15H22O2	M+FA-H	279.1602	-0.6
	HMDB0040755	3b-Hydroxy-6b-methoxy-7(11)-eremophilen-12,8a-olide	C16H24O4	M-H	279.1602	-0.7
	HMDB0041229	Methyl (3b,11x)-3-Hydroxy-8-oxo-6-eremophilen-12-oate	C16H24O4	M-H	279.1602	-0.7
	HMDB0036979	6b-Hydroxy-8a-methoxy-7(11)-eremophilen-12,8-olide	C16H24O4	M-H	279.1602	-0.7
	HMDB0179992	(3,4-dihydroxyphenyl)methyl 7-methyloctanoate	C16H24O4	M-H	279.1602	-0.7
	HMDB0030148	Prehumulinic acid	C16H24O4	M-H	279.1602	-0.7
279.1962	HMDB0015643	Artemether	C16H26O5	M-H2O-H	279.1596	1.3
	HMDB0175561	2-[(1E,5Z)-2,6,-trimethylundeca-1,5,9-trien-1-yl]oxirane	C16H26O	M+FA-H	279.1966	-1.3
	HMDB0175554	(6Z,E)-2,6,-trimethyltrideca-2,6,,12-tetraen-5-ol	C16H26O	M+FA-H	279.1966	-1.3
	HMDB0175552	(3E,7Z)-4,8,12-trimethyltrideca-1,3,7,11-tetraen-5-ol	C16H26O	M+FA-H	279.1966	-1.3
	HMDB0175557	(2E,6Z,E)-2,6,-trimethyltrideca-2,6,,12-tetraen-1-ol	C16H26O	M+FA-H	279.1966	-1.3
	HMDB0175559	(6Z,E)-2,6,-trimethyltrideca-2,6,,12-tetraen-4-ol	C16H26O	M+FA-H	279.1966	-1.3
	HMDB0175558	(3E,7Z)-4,8,12-trimethyltrideca-1,3,7,11-tetraen-6-ol	C16H26O	M+FA-H	279.1966	-1.3
	HMDB0175556	(6Z,E)-2,6,-trimethyltrideca-2,6,,12-tetraen-1-ol	C16H26O	M+FA-H	279.1966	-1.3
	HMDB0175563	3-[(3Z,7E)-3,7-dimethyldeca-3,7,9-trien-1-yl]-2,2-dimethyloxirane	C16H26O	M+FA-H	279.1966	-1.3
	HMDB0175560	2-[(3Z)-4,8-dimethylnona-3,7-dien-1-yl]-3-ethenyl-2-methyloxirane	C16H26O	M+FA-H	279.1966	-1.3
	HMDB0175562	2-methyl-3-[(3E)-3-methylhexa-3,5-dien-1-yl]-2-(4-methylpent-3-en-1-yl)oxirane	C16H26O	M+FA-H	279.1966	-1.3
	HMDB0040179	2,6-Di-tert-butyl-4-ethylphenol	C16H26O	M+FA-H	279.1966	-1.3
	HMDB0175555	(2E,6E)-6-methyl-2-(4-methylpent-3-en-1-yl)nona-2,6,8-trien-1-ol	C16H26O	M+FA-H	279.1966	-1.3
	HMDB0175553	(2Z,5Z)-6,-dimethyl-2-(prop-2-en-1-ylidene)undeca-5,9-dien-1-ol	C16H26O	M+FA-H	279.1966	-1.3
	HMDB0112087	5-(3-methyl-5-heptylfuran-2-yl)-pentanoic acid	C17H28O3	M-H	279.1966	-1.3
	HMDB0094642	9-(3-methyl-5-propylfuran-2-yl)-nonanoic acid	C17H28O3	M-H	279.1966	-1.3
	HMDB0112095	7-(3-methyl-5-pentylfuran-2-yl)-heptanoic acid	C17H28O3	M-H	279.1966	-1.3
	HMDB0112098	5-Pentyl-2-furanoctanoic acid	C17H28O3	M-H	279.1966	-1.3
	HMDB0032675	Dihydropanaxacol	C17H28O3	M-H	279.1966	-1.3
	HMDB0041388	Valeracetate	C17H28O3	M-H	279.1966	-1.3
	HMDB0036422	Fauronyl acetate	C17H28O3	M-H	279.1966	-1.3
	HMDB0012535	12S-HHT	C17H28O3	M-H	279.1966	-1.3
279.2326	HMDB0187014	(11Z)-18-hydroxyoctadec-11-enoic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0187015	2-Hydroxy-cis-vaccensaure	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0187013	Oxiranedecanoic acid, 3-hexyl-	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0187011	-hydroxy-cis-vaccenic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0187012	(11Z)-17-hydroxyoctadec-11-enoic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0187010	(11Z)-13-hydroxyoctadec-11-enoic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0160380	18-Hydroxy-9-octadecenoic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0160378	8-home(9)	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0160379	17-hydroxy-9-octadecenoic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0160381	SCHEMBL378128	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0160377	11-hydroxy-9-octadecenoic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0155792	17-Hydroxyoleic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0155793	18-hydroxyoleic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0155791	8-Hydroxyoleic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0155794	2-hydroxyoleic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0155790	(9Z)-11-hydroxyoctadec-9-enoic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0030979	9-Oxoctadecanoic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0010736	3-keto stearic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0030980	-Oxoctadecanoic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0034074	5-Oxoctadecanoic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0030981	11-Oxoctadecanoic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0031127	5-Hexyltetrahydro-2-furanoctanoic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0034297	Ricinoleic acid	C18H34O3	M-H2O-H	279.2324	0.7
	HMDB0041082	(5Z,8Z)-1,5,8-Heptadecatriene	C17H30	M+FA-H	279.2330	-1.3
	HMDB0006270	Linoelaidic acid	C18H32O2	M-H	279.2330	-1.3
	HMDB0005047	9E,11E-Octadecadienoic acid	C18H32O2	M-H	279.2330	-1.3
	HMDB0031051	Ethyl 2E,4Z-hexadecadienoate	C18H32O2	M-H	279.2330	-1.3

	HMDB0031097	5-Octadecynoic acid	C18H32O2	M-H	279.2330	-1.3
	HMDB0061864	Dihomolinoleic acid	C18H32O2	M-H	279.2330	-1.3
	HMDB0005048	E,12Z-Octadecadienoic acid	C18H32O2	M-H	279.2330	-1.3
	HMDB0000673	Linoleic acid	C18H32O2	M-H	279.2330	-1.3
	HMDB0173874	Linoleic acid	C18H32O2	M-H	279.2330	-1.3
	HMDB0003797	Bovinic acid	C18H32O2	M-H	279.2330	-1.3
	HMDB0029800	Mangiferic acid	C18H32O2	M-H	279.2330	-1.3
	HMDB0062238	(6Z,9Z)-octadecadienoic acid	C18H32O2	M-H	279.2330	-1.3
	HMDB0030430	Linalyl caprylate	C18H32O2	M-H	279.2330	-1.3
	HMDB0062784	Octadecadienoate	C18H32O2	M-H	279.2330	-1.3
281.1752	HMDB0182083	2-(3-{2,3-dimethyltricyclo[2.2.1]heptan-3-yl}propylidene)propane-1,3-diol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0166723	396--2	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0137903	6-hydroxy-5,5,8a-trimethyl-2-methylidene-decahydronaphthalene-1-carbaldehyde	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0150688	5-(hydroxymethyl)-1,1,4a,6-tetramethyl-1,2,3,4,4a,5,8,8a-octahydronaphthalen-2-one	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0163044	(2Z)-5-(5-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl)-3-methylpent-2-enal	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0166721	2,4-di-tert-butyl-6-methylbenzene-1,3-diol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0166722	UNII-7B7Y8CEM7E	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0177914	(2E)-3-[3-(hydroxymethyl)-7-methyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl]-2-methylprop-2-en-1-ol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0177916	4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-7-ol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0177917	2-[(3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl)methylidene]propane-1,3-diol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0182080	(2Z)-5-[2-(hydroxymethyl)-3-methyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-en-1-ol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0182081	(2Z)-5-[3-(hydroxymethyl)-2-methyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-en-1-ol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0182082	(2Z)-5-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-ene-1,5-diol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0182086	[3-(2-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]ethyl)-2-methyloxiran-2-yl]methanol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0182084	(2Z)-5-{2,3-dimethyltricyclo[2.2.1,heptan-3-yl]-2-methylpent-2-ene-1,4-diol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0182085	7-[(3Z)-5-hydroxy-4-methylpent-3-en-1-yl]-1,7-dimethyltricyclo[2.2.1,heptan-3-ol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0182087	3-[(3Z)-5-hydroxy-4-methylpent-3-en-1-yl]-2,3-dimethyltricyclo[2.2.1,heptan-1-ol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0179230	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,7a-diol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0179231	1,1,4,7-tetramethyl-1H,1aH,2H,3H,5H,6H,7H,7aH,7bH-cyclopropa[e]azulene-7,7b-diol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0179227	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,4-diol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0177915	(2E)-3-[7-(hydroxymethyl)-3-methyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl]-2-methylprop-2-en-1-ol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0177920	[3-(3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl)-2-methyloxiran-2-yl]methanol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0177919	4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-1-ol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0177918	4-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-2-ol	C15H24O2	M+FA-H	281.1758	-2.2
	HMDB0179224	1-(hydroxymethyl)-1,2,5-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2-ol	C15H24O2	M+FA-H	281.1758	-2.2

HMDB0179225	2-(hydroxymethyl)-1,1,5-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-ol	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0179226	5-(hydroxymethyl)-1,1,2-trimethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulen-2-ol	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0179228	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,6-diol	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0179229	1,1,2,5-tetramethyl-1H,1aH,1bH,2H,3H,4H,6H,7H,7aH-cyclopropa[e]azulene-2,3-diol	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0035032	Epilubimin	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0036680	Cyperolone	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0032048	2,6-Di-tert-butyl-4-hydroxymethylphenol	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0030916	2-Hydroxyacorenone	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0035827	Aubergenone	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0037393	(3xi,7(11)Z)-7(11)-Copaene-4,12-diol	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0035040	7-Hydroxycostol	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0033104	Calamensesquiterpinenol	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0037906	Hernandulcin	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0033083	(4S)-Dihydrocurcumenone	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0040712	Humulene diepoxide A	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0038027	beta-Ionyl acetate	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0034714	Curdione	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0038122	5-Methyl-5-hexen-2-one	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0032292	Geranyl tiglate	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0036549	Apotrichothecene	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0036687	Tanavulgarol	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0038178	Davanone	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0034722	3-Hydroxy-1,-bisaboladien-9-one	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0038144	Petasitolone	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0030891	(2E,6E)-1-Hydroxy-2,6,-farnesatrien-9-one	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0031348	Epiacorone	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0002352	Capsidiol	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0036446	(4alpha, alpha)-1(5),6-Guaiadiene	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0032681	alpha-4,5-Seco-11-eudesmene-4,5-dione	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0035301	4alpha,5alpha-Epoxy-11-eudesmen-3a-ol	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0035648	Isolubimin	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0035127	(-)-Myrtenyl isovalerate	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0039525	Isomelitic acid A	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0030920	Acorusnol	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0035147	Rishitinone	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0039688	Tuberone	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0036668	Humulene-8-hydroperoxide	C15H24O2	M+FA-H	281.1758	-2.2
HMDB0062365	(8R,Z)-8-hydroxy-3-oxohexadeca-6,-dienoic acid	C16H26O4	M-H	281.1758	-2.3
HMDB0062366	(6E,8S,Z)-8-hydroxy-3-oxohexadecadienoic acid	C16H26O4	M-H	281.1758	-2.3
HMDB0033630	Lactapiperanol C	C16H26O4	M-H	281.1758	-2.3
HMDB0036831	Ambtronide	C16H28O	M+FA-H	281.2122	-0.1
HMDB0031851	3-(5,6,6-Trimethylbicyclo[2.2.1]hept-1-yl)cyclohexanol	C16H28O	M+FA-H	281.2122	-0.1
HMDB0011562	MG(14:1(9Z))	C17H32O4	M-H2O-H	281.2117	1.9
HMDB0011531	MG/14:1(9Z))	C17H32O4	M-H2O-H	281.2117	1.9
HMDB0061662	13-hydroxyoctadecanoic acid	C18H36O3	M-H2O-H	281.2481	0.5
HMDB0171068	17-hydroxy stearic acid	C18H36O3	M-H2O-H	281.2481	0.5
HMDB0112183	DI-11-hydroxy stearic acid	C18H36O3	M-H2O-H	281.2481	0.5
HMDB0171069	18-Hydroxyoctadecanoic acid	C18H36O3	M-H2O-H	281.2481	0.5
HMDB0061706	12-Hydroxystearic acid	C18H36O3	M-H2O-H	281.2481	0.5
HMDB0061661	9-hydroxyoctadecanoic acid	C18H36O3	M-H2O-H	281.2481	0.5
HMDB0062549	(S)-2-hydroxyoctadecanoic acid	C18H36O3	M-H2O-H	281.2481	0.5
HMDB0240330	3-hydroxystearate	C18H35O3	M-H2O-H	281.2481	0.5
HMDB0010737	(R)-3-Hydroxy-Octadecanoic acid	C18H36O3	M-H2O-H	281.2481	0.5
HMDB0240324	-hydroxystearate	C18H35O3	M-H2O-H	281.2481	0.5
HMDB0037396	xi--Hydroxyoctadecanoic acid	C18H36O3	M-H2O-H	281.2481	0.5
HMDB0112180	5-hydroxyoctadecanoic acid	C18H36O3	M-H2O-H	281.2481	0.5
HMDB0112181	DI-7-hydroxy stearic acid	C18H36O3	M-H2O-H	281.2481	0.5

HMDB0112182	DI-8-hydroxy stearic acid	C18H36O3	M-H2O-H	281.2481	0.5
HMDB0112193	DI-6-hydroxy stearic acid	C18H36O3	M-H2O-H	281.2481	0.5
HMDB0003231	Vaccenic acid	C18H34O2	M-H	281.2486	-1.4
HMDB0002080	Petroselinic acid	C18H34O2	M-H	281.2486	-1.4
HMDB0062703	octadec-9-enoic acid	C18H34O2	M-H	281.2486	-1.4
HMDB0062242	7z-octadecenoic acid	C18H34O2	M-H	281.2486	-1.4
HMDB0041480	(Z)-13-Octadecenoic acid	C18H34O2	M-H	281.2486	-1.4
HMDB0062218	(Z)-13-Octadecenoic acid	C18H34O2	M-H	281.2486	-1.4
HMDB0062093	octadec-13-enoic acid	C18H34O2	M-H	281.2486	-1.4
HMDB0000207	Oleic acid	C18H34O2	M-H	281.2486	-1.4
HMDB0240219	cis-Vaccenic acid	C18H34O2	M-H	281.2486	-1.4
HMDB0059871	Ethyl 9-hexadecenoate	C18H34O2	M-H	281.2486	-1.4
HMDB0000573	Elaidic acid	C18H34O2	M-H	281.2486	-1.4
HMDB0161063	5-hydroxy-1,16-hexadecanedioic acid	C16H30O5	M-H2O-H	283.1909	0.2
HMDB0161062	SCHEMBL76124	C16H30O5	M-H2O-H	283.1909	0.2
HMDB0161065	hydroxyhexadecanedioic acid	C16H30O5	M-H2O-H	283.1909	0.2
HMDB0161064	6-hydroxyhexadecanedioic acid	C16H30O5	M-H2O-H	283.1909	0.2
HMDB0037831	xi-8-Hydroxyhexadecanedioic acid	C16H30O5	M-H2O-H	283.1909	0.2
HMDB0161061	3-hydroxythapsic acid	C16H30O5	M-H2O-H	283.1909	0.2
HMDB0037830	xi-7-Hydroxyhexadecanedioic acid	C16H30O5	M-H2O-H	283.1909	0.2
HMDB0182767	2-(1-hydroxypropan-2-yl)-4a-methyl-8-methylidene-decahydronaphthalen-1-ol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0182764	4a-(hydroxymethyl)-8-methylidene-2-(propan-2-yl)-decahydronaphthalen-1-ol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0182220	3-(2-hydroxypropan-2-yl)-4a,5-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalen-1-ol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0182219	7-(2-hydroxypropan-2-yl)-1,8a-dimethyl-1,2,3,5,6,7,8,8a-octahydronaphthalen-1-ol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0182221	6-(2-hydroxypropan-2-yl)-4,4a-dimethyl-2,3,4,4a,5,6,7,8-octahydronaphthalen-2-ol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0182217	2-[8a-(hydroxymethyl)-8-methyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl]propan-2-ol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0182218	2-[8-(hydroxymethyl)-8a-methyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl]propan-2-ol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0179265	2-(4-hydroxy-4-methylcyclohex-en-1-yl)-6-methylheptan-4-one	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0041589	alpha-Kessyl alcohol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0040273	Terpenyl isovalerate	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0038247	Bornyl valerate	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0036730	Tricyclohumuladiol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0038196	alpha-Bisabolol oxide A	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0037284	5(1->)-Abeo-1,12-patchoulanediol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0036880	1,6,9-Farnesatriene-3,11-diol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0037279	2,-Bisaboladiene-1,4-diol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0034673	Calamendiol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0031383	(3S,4S,6R,7S)-1,-Bisaboladiene-3,4-diol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0038250	Isobornyl isovalerate	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0033228	Guaidiol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0036032	3beta-7-Drimene-3,11-diol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0031384	beta-Kessyl alcohol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0035887	Germacrenone	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0038248	Bornyl isovalerate	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0032054	alpha-Terpinyl pentanoate	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0039745	(2E,6E,9xi)-Farnesol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0062130	methyl tetradec-13-ynoate	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0032343	Isobornyl 2-methylbutyrate	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0032209	Citronellyl trans-2-methyl-2-butenate	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0032291	Geranyl 2-methylbutyrate	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0035287	Daucol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0038136	Curcumadiol	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0038138	alpha-Bisabolol oxide C	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0038197	alpha-Bisabolol oxide B	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0030428	Linalyl isovalerate	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0037195	2-Propenyl cyclohexanhexanoate	C15H26O2	M+FA-H	283.1915	-1.7
HMDB0040281	Geranyl valerate	C15H26O2	M+FA-H	283.1915	-1.7

	HMDB0029350	Geranyl 3-methylbutanoate	C15H26O2	M+FA-H	283.1915	-1.7
	HMDB0039130	Methyl (Z,Z)-5,8-tetradecadienoate	C15H26O2	M+FA-H	283.1915	-1.7
	HMDB0182766	4a-methyl-8-methylidene-2-(propan-2-yl)-decahydronaphthalene-1,7-diol	C15H26O2	M+FA-H	283.1915	-1.7
	HMDB0182222	2-(8,8a-dimethyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl)propane-1,2-diol	C15H26O2	M+FA-H	283.1915	-1.7
	HMDB0182765	2-(2-hydroxypropan-2-yl)-4a-methyl-8-methylidene-decahydronaphthalen-1-ol	C15H26O2	M+FA-H	283.1915	-1.7
283.2277	HMDB0060482	Hexadecenal	C16H30O	M+FA-H	283.2279	-0.6
	HMDB0037544	2-Dodecylcyclobutanone	C16H30O	M+FA-H	283.2279	-0.6
	HMDB0034181	3-Methylcyclopentadecanone	C16H30O	M+FA-H	283.2279	-0.6
	HMDB0038685	Muricatacin	C17H32O3	M-H	283.2279	-0.6
	HMDB0035473	Avocadyne	C17H32O3	M-H	283.2279	-0.6
	HMDB0011561	MG(14)	C17H34O4	M-H20-H	283.2273	1.3
	HMDB0072853	MG(i-14)	C17H34O4	M-H20-H	283.2273	1.3
	HMDB0072867	MG(i-14)	C17H34O4	M-H20-H	283.2273	1.3
	HMDB0011530	MG(14)	C17H34O4	M-H20-H	283.2273	1.3
283.2638	HMDB0183479	17-hydroxyoctadecanal	C18H36O2	M-H	283.2643	-1.6
	HMDB0183481	2-hydroxyoctadecanal	C18H36O2	M-H	283.2643	-1.6
	HMDB0183480	SCHEMBL8	C18H36O2	M-H	283.2643	-1.6
	HMDB0000827	Stearic acid	C18H36O2	M-H	283.2643	-1.6
	HMDB0031066	16-Methylheptadecanoic acid	C18H36O2	M-H	283.2643	-1.6
	HMDB0029811	Ethyl hexadecanoate	C18H36O2	M-H	283.2643	-1.6
	HMDB0061946	Hexyl dodecanoate	C18H36O2	M-H	283.2643	-1.6
285.1347	HMDB0176437	(9E,11E)-4-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M+FA-H	285.1344	1.2
	HMDB0176432	SCHEMBL2554147	C13H20O4	M+FA-H	285.1344	1.2
	HMDB0176436	(9E,11E)-5-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M+FA-H	285.1344	1.2
	HMDB0176441	8-{3-[(1E)-3-oxoprop-1-en-1-yl]oxiran-2-yl}octanoic acid	C13H20O4	M+FA-H	285.1344	1.2
	HMDB0176442	(9E,11E)-2-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M+FA-H	285.1344	1.2
	HMDB0176434	(9E,11E)-7-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M+FA-H	285.1344	1.2
	HMDB0176440	(9E)--(3-formyloxiran-2-yl)dec-9-enoic acid	C13H20O4	M+FA-H	285.1344	1.2
	HMDB0176438	(9E,11E)-3-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M+FA-H	285.1344	1.2
	HMDB0176439	(9E,11E)-8-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M+FA-H	285.1344	1.2
	HMDB0176435	(9E,11E)-6-hydroxy-13-oxotrideca-9,11-dienoic acid	C13H20O4	M+FA-H	285.1344	1.2
285.2068	HMDB0032347	Isobutyl -undecenoate	C15H28O2	M+FA-H	285.2071	-1.2
	HMDB0037190	Rhodinyl isovalerate	C15H28O2	M+FA-H	285.2071	-1.2
	HMDB0039715	Auberganol	C15H28O2	M+FA-H	285.2071	-1.2
	HMDB0034455	Exaltolide	C15H28O2	M+FA-H	285.2071	-1.2
	HMDB0036426	Butyl undecylenate	C15H28O2	M+FA-H	285.2071	-1.2
	HMDB0038954	Citronellyl isovalerate	C15H28O2	M+FA-H	285.2071	-1.2
	HMDB0037211	Menthyl isovalerate	C15H28O2	M+FA-H	285.2071	-1.2
	HMDB0037229	Citronellyl pentanoate	C15H28O2	M+FA-H	285.2071	-1.2
	HMDB0040997	15,5-Farnesanolide	C15H28O2	M+FA-H	285.2071	-1.2
	HMDB0029765	9-Pentadecenoic acid	C15H28O2	M+FA-H	285.2071	-1.2
	HMDB0041287	16-Hydroxy--oxohexadecanoic acid	C16H30O4	M-H	285.2071	-1.2
	HMDB0062018	1-[2-(Isobutyryloxy)-1-methylethyl]-2,2-dimethylpropyl 2-methylpropanoate	C16H30O4	M-H	285.2071	-1.2
	HMDB0059777	2,2,4-Trimethyl-1,3-pentadienol diisobutyrate	C16H30O4	M-H	285.2071	-1.2
	HMDB0000672	Hexadecanedioic acid	C16H30O4	M-H	285.2071	-1.2
	HMDB0061936	Isooctanedioldibutyrate	C16H30O4	M-H	285.2071	-1.2
285.2435	HMDB0001551	Palmitaldehyde	C16H32O	M+FA-H	285.2435	-0.1
	HMDB0062168	1-Hexadecenol	C16H32O	M+FA-H	285.2435	-0.1
	HMDB0031052	2-Hexadecanone	C16H32O	M+FA-H	285.2435	-0.1
	HMDB0031042	Avocadene	C17H34O3	M-H	285.2435	-0.1
	HMDB0061663	12-hydroxyheptadecanoic acid	C17H34O3	M-H	285.2435	-0.1
286.0792	HMDB0033718	Clitocine	C9H13N5O6	M-H	286.0793	-0.4
286.9238	HMDB0157723	2-(phosphonoxy)-3-(sulfoxy)propanoic acid	C3H7O10PS	M+Na-2H	286.9244	-2.2
286.9859	HMDB0174253	2-({[(1Z)-3-(prop-2-ene-1-sulfonyl)prop-1-en-1-yl]disulfanyl}methyl)oxirane	C9H14O3S3	M+Na-2H	286.9852	2.5
	HMDB0174252	2-({[(2Z)-3-(prop-2-en-1-yl)disulfanyl]prop-2-ene-1-sulfonyl}methyl)oxirane	C9H14O3S3	M+Na-2H	286.9852	2.5
	HMDB0183682	3-[3-(sulfoxy)phenyl]prop-2-ynoic acid	C9H6O6S	M+FA-H	286.9867	-2.8
	HMDB0183685	3-[4-(sulfoxy)phenyl]prop-2-ynoic acid	C9H6O6S	M+FA-H	286.9867	-2.8
	HMDB0240565	Umbelliferone sulfate	C9H5O6S	M+FA-H	286.9867	-2.8

287.0623	HMDB0144633	Des-N,N-diethylethanamine 4-Hydroxyclophenone	C20H15ClO	M-H2O-H	287.0628	-1.6
287.0799	HMDB0164647	[(1,7-dihydroxyoctan-3-yl)oxy]sulfonic acid	C8H18O6S	M+FA-H	287.0806	-2.5
	HMDB0164646	[(3,7-dihydroxyoctyl)oxy]sulfonic acid	C8H18O6S	M+FA-H	287.0806	-2.5
	HMDB0164648	[(6,8-dihydroxyoctan-2-yl)oxy]sulfonic acid	C8H18O6S	M+FA-H	287.0806	-2.5
287.0903	HMDB0133196	2,3-dihydroxy-3-[4-hydroxy-3-(3-methylbut-2-en-1-yl)phenyl]propanoic acid	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0133195	2-hydroxy-3-[4-hydroxy-3-(4-hydroxy-3-methylbut-2-en-1-yl)phenyl]propanoic acid	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0125455	2-[4,6-dihydroxy-2-methoxy-3-(3-methylbut-2-en-1-yl)phenyl]acetic acid	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0133197	3-{3-[(3,3-dimethyloxiran-2-yl)methyl]-4-hydroxyphenyl}-2-hydroxypropanoic acid	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0133198	3-[3,4-dihydroxy-5-(3-methylbut-2-en-1-yl)phenyl]-2-hydroxypropanoic acid	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0169146	3-(4,7-dihydroxy-2,2-dimethyl-3,4-dihydro-2H-1-benzopyran-6-yl)propanoic acid	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0162483	2-[(2,3-dihydroxy-5-methoxyphenyl)methyl]-6-methyloxan-4-one	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0162480	3-hydroxy-6-[(3-hydroxy-5-methoxyphenyl)methyl]-2-methyloxan-4-one	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0162479	2-[(2,5-dihydroxy-3-methoxyphenyl)methyl]-6-methyloxan-4-one	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0162482	2-[(3,4-dihydroxy-5-methoxyphenyl)methyl]-6-methyloxan-4-one	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0162481	3-hydroxy-2-[(3-hydroxy-5-methoxyphenyl)methyl]-6-methyloxan-4-one	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0162478	2-[hydroxy(3-hydroxy-5-methoxyphenyl)methyl]-6-methyloxan-4-one	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0162476	2-[(3-hydroxy-5-methoxyphenyl)methyl]-6-(hydroxymethyl)oxan-4-one	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0149851	2-[2,4,6-trihydroxy-3-(3-methylbut-2-en-1-yl)phenyl]propanoic acid	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0148585	2-[2,4,5-trihydroxy-3-(3-methylbut-2-en-1-yl)phenyl]propanoic acid	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0148582	2-{3-[(3,3-dimethyloxiran-2-yl)methyl]-2,4-dihydroxyphenyl} propanoic acid	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0148579	2-{2,4-dihydroxy-3-[(2E)-4-hydroxy-3-methylbut-2-en-1-yl]phenyl} propanoic acid	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0148576	2-[2,4-dihydroxy-3-(4-hydroxy-3-methylbut-2-en-1-yl)phenyl]propanoic acid	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0041582	Sapidolide A	C14H18O5	M+Na-2H	287.0901	0.7
	HMDB0040891	3',4',5'-Trimethoxycinnamyl alcohol acetate	C14H18O5	M+Na-2H	287.0901	0.7
287.1192	HMDB0041518	Nb-p-Coumaroyltryptamine	C19H18N2O2	M-H2O-H	287.1184	2.7
	HMDB0041543	2,5-Dibenzyl-3-hydroxy-6-methoxypyrazine	C19H18N2O2	M-H2O-H	287.1184	2.7
	HMDB0039105	3-Oxo-14,15-dehydrorhazinilam	C19H18N2O2	M-H2O-H	287.1184	2.7
	HMDB0030308	O-Isopentenylhalfordinol	C19H18N2O2	M-H2O-H	287.1184	2.7
287.1494	HMDB0031315	1-(beta-D-Glucopyranosyloxy)-3-octanone	C14H26O7	M-H2O-H	287.1495	-0.2
	HMDB0172315	3,4,5-trihydroxy-6-(octan-2-yloxy)oxane-2-carboxylic acid	C14H26O7	M-H2O-H	287.1495	-0.2
	HMDB0170963	3,4,5-trihydroxy-6-(octyloxy)oxane-2-carboxylic acid	C14H26O7	M-H2O-H	287.1495	-0.2
	HMDB0176459	(9E)--[3-(hydroxymethyl)oxiran-2-yl]dec-9-enoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176461	(9E,11E)-2,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176443	(9E)-7-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176444	(9E)-6-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176446	(9E)-4-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176447	(9E)-3-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176445	(9E)-5-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176448	(9E)-8-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176451	(9E)-12-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176450	8-[3-(3-oxopropyl)oxiran-2-yl]octanoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176449	(9E)-11-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+FA-H	287.1500	-2.1

	HMDB0176458	(9E,11E)-8,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176453	(9E,11E)-7,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176454	(9E,11E)-6,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176455	(9E,11E)-5,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176456	(9E,11E)-4,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176457	(9E,11E)-3,13-dihydroxytrideca-9,11-dienoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176460	8-{3-[(1E)-3-hydroxyprop-1-en-1-yl]oxiran-2-yl}octanoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0176452	(9E)-2-hydroxy-13-oxotridec-9-enoic acid	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0038736	(3S,5R,6R,7E)-3,5,6-Trihydroxy-7-megastigmen-9-one	C13H22O4	M+FA-H	287.1500	-2.1
	HMDB0030987	2-Carboxy-4-dodecanolide	C13H22O4	M+FA-H	287.1500	-2.1
287.1628	HMDB0112097	5-Butyl-2-furanoctanoic acid	C16H26O3	M+Na-2H	287.1629	-0.2
	HMDB0112092	5-Pentyl-2-furanheptanoic acid	C16H26O3	M+Na-2H	287.1629	-0.2
	HMDB0112088	6-(5-hexylfuran-2-yl)hexanoic acid	C16H26O3	M+Na-2H	287.1629	-0.2
	HMDB0112085	5-(3,4-dimethyl-5-pentylfuran-2-yl)-pentanoic acid	C16H26O3	M+Na-2H	287.1629	-0.2
	HMDB0112089	7-(3,4-dimethyl-5-propylfuran-2-yl)heptanoic acid	C16H26O3	M+Na-2H	287.1629	-0.2
	HMDB0060055	Tetranor 12-HETE	C16H26O3	M+Na-2H	287.1629	-0.2
	HMDB0033917	4-Hydroxy-3-methoxy-2,-bisaboladien-9-one	C16H26O3	M+Na-2H	287.1629	-0.2
287.2007	HMDB0137390	4-[(4E)-3-hydroxydodec-4-en-1-yl]-2-methoxyphenol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0137401	4-[(1E)-3-hydroxydodec-1-en-1-yl]-2-methoxyphenol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0154820	(1S,2S,7S,R,11S,15S)-5,13-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0154818	(1S,2S,7R,R,11S,15S)-5,9-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0154819	(1S,2R,7S,R,11S,15S)-5,8-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0154822	(1S,2S,7S,R,11S,15S)-5-hydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadecan-14-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0154821	(1S,2R,7S,R,11S,15S)-5-hydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-14-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0155967	(2R,15S)-8,14-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0155969	(2R,15S)-14-hydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-5-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0155968	(2S,15S)-13,14-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0155970	(2S,15S)-14-hydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadecan-5-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0155984	(2S,15S)-14,17-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0156130	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,14,16-triol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0156600	(1S,2S,S,11S,15R)-5,13-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-3-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0159470	(1S,2S,5R,7S,R,11S,15S)-5,9-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0159472	(1S,2R,5R,7R,R,11S,15S)-5,8-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0159473	(1S,2S,5R,7R,R,11S,15S)-5,13-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0159471	SCHEMBL1799883	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0159474	(1S,2R,5R,7R,R,11S,15S)-5-hydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-14-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0159475	(1S,2S,5R,7R,R,11S,15S)-5-hydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadecan-14-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0185968	(2S,15S)-4,14-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0185969	(2R,15S)-6,14-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-one	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0013199	5-Androstene-3alpha-16beta,17beta-triol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0156131	(2R,15R)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,11,14-triol	C19H30O3	M-H2O-H	287.2011	-1.4

	HMDB0156127	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5.,14-triol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0156119	STL525817	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0156121	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,6,14-triol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0156118	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,13,14-triol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0156120	(2R,15S)-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadec-7-ene-5,14-diol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0156125	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-3,5,14-triol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0156122	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,9,14-triol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0156123	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,14,14-triol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0156124	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,12,14-triol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0156129	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,14,17-triol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0156128	(2S,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-1,5,14-triol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0156126	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-4,5,14-triol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0014759	Oxandrolone	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0000523	5-Androstene-3b,16b,17a-triol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0000540	5-Androstene-3b,16a,17a-triol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0000550	5-Androstenetriol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0002984	11-Hydroxyandrosterone	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0040640	[8]-Paradol	C19H30O3	M-H2O-H	287.2011	-1.4
	HMDB0013156	1-Hydroxypyrene	C19H30O3	M-H2O-H	287.2011	-1.4
287.2750	HMDB0005943	5b-Pregnanediol	C21H36	M-H	287.2744	2.0
	HMDB0040180	Pentadecylbenzene	C21H36	M-H	287.2744	2.0
288.0662	HMDB0033247	Grevilline D	C18H13NO4	M-H2O-H	288.0661	0.5
	HMDB0029826	Hallacridone	C18H13NO4	M-H2O-H	288.0661	0.5
	HMDB0173599	9-hydroxy-11-methyl-3,5-dioxo-11-azapentacyclo[.7.1,??]icosa-1(),2(6),7,12,14,16,18-heptaen--one	C18H13NO4	M-H2O-H	288.0661	0.5
	HMDB0000125	Glutathione	C10H17N3O6S	M-H2O-H	288.0654	2.7
	HMDB0062697	gamma-Glutamylcysteinylglycine	C10H17N3O6S	M-H2O-H	288.0654	2.7
288.0827	HMDB0029450	Aspergillomarasmine A	C10H17N3O8	M-H2O-H	288.0832	-1.6
	HMDB0155070	3,4,5-trihydroxy-6-{[2-(N-methylcarbamimidamido)acetyl]oxy}oxane-2-carboxylic acid	C10H17N3O8	M-H2O-H	288.0832	-1.6
288.1104	HMDB0059780	1,N2-propanodeoxyguanosine	C13H17N5O4	M-H2O-H	288.1097	2.6
288.1557	HMDB0029022	Prolyl-Lysine	C11H21N3O3	M+FA-H	288.1565	-2.8
	HMDB0028959	Lys-Pro	C11H21N3O3	M+FA-H	288.1565	-2.8
	HMDB0179991	(4-hydroxy-3-methoxyphenyl)methyl 2-hydroxy-7-methyloctanoate	C17H26O5	M-H2O-H	291.1596	0.2
	HMDB0040756	3-Hydroxy-6,8-dimethoxy-7(11)-eremophilen-12,8-olide	C17H26O5	M-H2O-H	291.1596	0.2
	HMDB0040980	Valdiate	C17H26O5	M-H2O-H	291.1596	0.2
	HMDB0179993	(3,4-dihydroxy-5-methoxyphenyl)methyl 7-methyloctanoate	C17H26O5	M-H2O-H	291.1596	0.2
	HMDB0179989	(4-hydroxy-3-methoxyphenyl)methyl 7-hydroxy-7-methyloctanoate	C17H26O5	M-H2O-H	291.1596	0.2
	HMDB0179990	(4-hydroxy-3-methoxyphenyl)methyl 8-hydroxy-7-methyloctanoate	C17H26O5	M-H2O-H	291.1596	0.2
	HMDB0037705	Heptyl cinnamate	C16H22O2	M+FA-H	291.1602	-1.7
	HMDB0036207	alpha-Amylcinnamyl acetate	C16H22O2	M+FA-H	291.1602	-1.7

291.1597	HMDB0041250	Demethoxyshogaol	C16H22O2	M+FA-H	291.1602	-1.7
	HMDB0180049	(3,4-dihydroxyphenyl)methyl (6E)-8-methylnon-6-enoate	C17H24O4	M-H	291.1602	-1.7
	HMDB0137265	(1E)-1-(2,4-dihydroxy-3-methoxyphenyl)dec-1-en-3-one	C17H24O4	M-H	291.1602	-1.7
	HMDB0137268	(1E)--hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-1-en-3-one	C17H24O4	M-H	291.1602	-1.7
	HMDB0137267	1-[3-(4-hydroxy-3-methoxyphenyl)oxiran-2-yl]octan-1-one	C17H24O4	M-H	291.1602	-1.7
	HMDB0137266	(1E)-9-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-1-en-3-one	C17H24O4	M-H	291.1602	-1.7
	HMDB0137270	(1E)-4-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-1-en-3-one	C17H24O4	M-H	291.1602	-1.7
	HMDB0179994	(4-hydroxy-3-methoxyphenyl)methyl 7-methyloct-7-enoate	C17H24O4	M-H	291.1602	-1.7
	HMDB0137261	(1Z)-2-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-1-en-3-one	C17H24O4	M-H	291.1602	-1.7
	HMDB0137264	(1E)-1-(3,4-dihydroxy-5-methoxyphenyl)dec-1-en-3-one	C17H24O4	M-H	291.1602	-1.7
	HMDB0137251	(4Z)-4-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-4-en-3-one	C17H24O4	M-H	291.1602	-1.7
	HMDB0137252	(4E)-1-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-4-en-3-one	C17H24O4	M-H	291.1602	-1.7
	HMDB0137263	(1E)-1-(2,4-dihydroxy-5-methoxyphenyl)dec-1-en-3-one	C17H24O4	M-H	291.1602	-1.7
	HMDB0137257	(4E)--hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-4-en-3-one	C17H24O4	M-H	291.1602	-1.7
	HMDB0137259	(4E)-2-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-4-en-3-one	C17H24O4	M-H	291.1602	-1.7
	HMDB0137256	3-(4-hydroxy-3-methoxyphenyl)-1-(3-pentyloxiran-2-yl)propan-1-one	C17H24O4	M-H	291.1602	-1.7
	HMDB0137254	(4E)-1-(3,4-dihydroxy-5-methoxyphenyl)dec-4-en-3-one	C17H24O4	M-H	291.1602	-1.7
	HMDB0137255	(4E)-9-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dec-4-en-3-one	C17H24O4	M-H	291.1602	-1.7
	HMDB0036693	Acetylbalchanolide	C17H24O4	M-H	291.1602	-1.7
	HMDB0034930	(3beta,6beta)-Furanoeremophilane-3,6-diol 6-acetate	C17H24O4	M-H	291.1602	-1.7
	HMDB0034738	Isotrichodermin	C17H24O4	M-H	291.1602	-1.7
	HMDB0035687	Acetylvalerenolic acid	C17H24O4	M-H	291.1602	-1.7
	HMDB0039275	[6]-Gingerdione	C17H24O4	M-H	291.1602	-1.7
	HMDB0034658	9-Acetoxyfukinanolide	C17H24O4	M-H	291.1602	-1.7
	HMDB0041249	6-Hydroxyshogaol	C17H24O4	M-H	291.1602	-1.7
293.1758	HMDB0037713	Octyl phenylacetate	C16H24O2	M+FA-H	293.1758	-0.1
	HMDB0037719	2-Phenylethyl octanoate	C16H24O2	M+FA-H	293.1758	-0.1
	HMDB0032228	Dimethylbenzyl carbiny hexanoate	C16H24O2	M+FA-H	293.1758	-0.1
	HMDB0036221	[2-(Dimethoxymethyl)-1-heptenyl]benzene	C16H24O2	M+FA-H	293.1758	-0.1
	HMDB0036640	Furanofukinin	C16H24O2	M+FA-H	293.1758	-0.1
	HMDB0180101	(3,4-dihydroxyphenyl)methyl 8-methylnonanoate	C17H26O4	M-H	293.1758	-0.1
	HMDB0034779	Nordihydrocapsiate	C17H26O4	M-H	293.1758	-0.1
	HMDB0005783	Gingerol	C17H26O4	M-H	293.1758	-0.1
	HMDB0035722	Tanacetol A	C17H26O4	M-H	293.1758	-0.1
	HMDB0035754	Phytuberin	C17H26O4	M-H	293.1758	-0.1
	HMDB0040646	Myrsinone	C17H26O4	M-H	293.1758	-0.1
	HMDB0015026	Granisetron	C18H24N4O	M-H2O-H	293.1766	-2.8
	HMDB0060512	Sterol	C17H28O	M+FA-H	293.2122	-0.4
	HMDB0030932	Avocadenofuran	C17H28O	M+FA-H	293.2122	-0.4
	HMDB0041333	(all-Z)-8,11,14-Heptadecatrienal	C17H28O	M+FA-H	293.2122	-0.4
	HMDB0112099	8-(5-hexylfuran-2-yl)octanoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0186498	(6Z,9Z,12Z)-14-hydroxyoctadeca-6,9,12-trienoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0186497	(6Z,12Z)-5-hydroxyoctadeca-6,9,12-trienoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0186499	(6Z,9Z,12Z)-8-hydroxyoctadeca-6,9,12-trienoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0186501	(6Z,8E,12Z)--hydroxyoctadeca-6,8,12-trienoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0186500	(6Z,9Z,12Z)-11-hydroxyoctadeca-6,9,12-trienoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0186503	13-hydroxy-6Z,9Z,11E-octadecatrienoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0186504	(6Z,12Z)-9-hydroxyoctadeca-6,,12-trienoic acid	C18H30O3	M-H	293.2122	-0.4

293.2121	HMDB0186507	gamma- 9()-EpODE	C18H30O3	M-H	293.2122	-0.4
	HMDB0186506	gamma- 6(7)-EpODE	C18H30O3	M-H	293.2122	-0.4
	HMDB0186505	17-hydroxy-linolenic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0186510	(6Z,12Z)-2-hydroxyoctadeca-6,9,12-trienoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0186508	SCHEMBL14956948	C18H30O3	M-H	293.2122	-0.4
	HMDB0112093	5-heptylfuran-2-yl-heptanoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0112102	9-(5-pentylfuran-2-yl)-nonanoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0062288	Gamma- 12(13)-epode	C18H30O3	M-H	293.2122	-0.4
	HMDB0186502	(9Z,12Z)-6-hydroxyoctadeca-7,9,12-trienoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0004669	9-OxoODE	C18H30O3	M-H	293.2122	-0.4
	HMDB0030995	(2'E,4'Z,8E)-Colneleic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0039603	3,4-Dimethyl-5-pentyl-2-furanheptanoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0010220	9()-EpODE	C18H30O3	M-H	293.2122	-0.4
	HMDB0061644	3,4-Dimethyl-5-propyl-2-furannonanoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0031934	(9S,E,12Z,15Z)-9-Hydroxy-,12,15-octadecatrienoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0112103	9-(5-butyl-3-methylfuran-2-yl)nonanoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0004668	13-OxoODE	C18H30O3	M-H	293.2122	-0.4
	HMDB0010200	A-12(13)-EpODE	C18H30O3	M-H	293.2122	-0.4
	HMDB0010203	13-HOTE	C18H30O3	M-H	293.2122	-0.4
	HMDB0010206	15(16)-EpODE	C18H30O3	M-H	293.2122	-0.4
	HMDB0010224	9-HOTE	C18H30O3	M-H	293.2122	-0.4
	HMDB0011108	17-Hydroxylinolenic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0029786	-Oxo-11-octadecen-13-olide	C18H30O3	M-H	293.2122	-0.4
	HMDB0030950	15,16-Epoxy-9,12-octadecadienoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0036832	Sterebin D	C18H30O3	M-H	293.2122	-0.4
	HMDB0031103	2-Hydroxylinolenic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0029969	Squamostanal A	C18H30O3	M-H	293.2122	-0.4
	HMDB0031088	12,13-Epoxy-9,15-octadecadienoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0034586	(9Z,12Z,14E)-16-Hydroxy-9,12,14-octadecatrienoic acid	C18H30O3	M-H	293.2122	-0.4
	HMDB0062281	(11S)-11-hydroperoxylinoleic acid	C18H32O4	M-H2O-H	293.2117	1.5
	HMDB0062637	13(S)-HPODE	C18H32O4	M-H2O-H	293.2117	1.5
	HMDB0003871	13-L-Hydroperoxylinoleic acid	C18H32O4	M-H2O-H	293.2117	1.5
	HMDB0010221	9,-DiHODE	C18H32O4	M-H2O-H	293.2117	1.5
	HMDB0004706	8(R)-Hydroperoxylinoleic acid	C18H32O4	M-H2O-H	293.2117	1.5
	HMDB0006940	9(S)-HPODE	C18H32O4	M-H2O-H	293.2117	1.5
	HMDB0010201	12,13-DiHODE	C18H32O4	M-H2O-H	293.2117	1.5
	HMDB0010208	15,16-DiHODE	C18H32O4	M-H2O-H	293.2117	1.5
	HMDB0062434	(9S,E,12Z,15Z)-9-hydroperoxy-,12,15-octadecadienoate	C18H32O4	M-H2O-H	293.2117	1.5
	HMDB0040900	(E)-13-Hydroxy--oxo-11-octadecenoic acid	C18H32O4	M-H2O-H	293.2117	1.5
295.1910	HMDB0061952	AC1LBPUV	C16H26O2	M+FA-H	295.1915	-1.6
	HMDB0035293	Norambreinolide	C16H26O2	M+FA-H	295.1915	-1.6
	HMDB0037631	3-Methyl-alpha-ionyl acetate	C16H26O2	M+FA-H	295.1915	-1.6
	HMDB0037712	[2,2-Bis(2-methylpropoxy)ethyl]benzene	C16H26O2	M+FA-H	295.1915	-1.6
	HMDB0240361	(7Z,Z,13Z)-hexadecatrienoate	C16H25O2	M+FA-H	295.1915	-1.6
	HMDB0159344	(7Z,Z)-hexadeca-7,,15-trienoic acid	C16H26O2	M+FA-H	295.1915	-1.6
	HMDB0134775	5-formyl-6-hydroxy-1,1,4a,6-tetramethyl-decahydronaphthalen-2-yl acetate	C17H28O4	M-H	295.1915	-1.6
	HMDB0038798	(1(E,4a,5E)-1(),5-Germacradiene-12-acetoxy-4,11-diol	C17H28O4	M-H	295.1915	-1.6
	HMDB0035075	Tanacetol B	C17H28O4	M-H	295.1915	-1.6
	HMDB0061650	(9R,S)-9,-epoxy-18-hydroxyoctadecanoic acid	C18H34O4	M-H2O-H	295.2273	0.3
	HMDB0170226	17-hydroxy-5-oxooctadecanoic acid	C18H34O4	M-H2O-H	295.2273	0.3
	HMDB0004705	12,13-DHOME	C18H34O4	M-H2O-H	295.2273	0.3
	HMDB0004704	9,-DHOME	C18H34O4	M-H2O-H	295.2273	0.3
	HMDB0170230	6-hydroxy-5-oxooctadecanoic acid	C18H34O4	M-H2O-H	295.2273	0.3
	HMDB0170227	18-hydroxy-5-oxooctadecanoic acid	C18H34O4	M-H2O-H	295.2273	0.3
	HMDB0170228	2-hydroxy-5-oxooctadecanoic acid	C18H34O4	M-H2O-H	295.2273	0.3
	HMDB0170229	4-hydroxy-5-oxooctadecanoic acid	C18H34O4	M-H2O-H	295.2273	0.3
	HMDB0041220	Dibutyl decanedioate	C18H34O4	M-H2O-H	295.2273	0.3
	HMDB0000782	Octadecanedioic acid	C18H34O4	M-H2O-H	295.2273	0.3
	HMDB0031679	(9xi,xi,12xi)-9,-Dihydroxy-12-octadecenoic acid	C18H34O4	M-H2O-H	295.2273	0.3
	HMDB0041334	8,11-Heptadecadienal	C17H30O	M+FA-H	295.2279	-1.6

295.2274	HMDB0062074	CHEMBL48139	C17H30O	M+FA-H	295.2279	-1.6
	HMDB0031336	(Z)-9-Cycloheptadecen-1-one	C17H30O	M+FA-H	295.2279	-1.6
	HMDB0004701	9,-Epoxyoctadecenoic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0062652	9-HODE	C18H32O3	M-H	295.2279	-1.6
	HMDB0004670	alpha-Dimorphecolic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0029998	12-Hydroxy-8,-octadecadienoic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0004667	13-HODE	C18H32O3	M-H	295.2279	-1.6
	HMDB0061708	13-HODE	C18H32O3	M-H	295.2279	-1.6
	HMDB0173893	(9E,12Z)-2-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0029796	(Z)-13-Oxo-9-octadecenoic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0160588	8-Hydroxylinoleic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0112194	13-HODE	C18H32O3	M-H	295.2279	-1.6
	HMDB0160590	11-Hode	C18H32O3	M-H	295.2279	-1.6
	HMDB0173886	(9E,12Z)-14-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0173885	(9E,12Z)-8-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0173889	(9E,12Z)-17-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0004702	12,13-EpOME	C18H32O3	M-H	295.2279	-1.6
	HMDB0010223	9-HODE	C18H32O3	M-H	295.2279	-1.6
	HMDB0029978	Avenoleic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0160595	alpha-Hydroxylinoleic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0173888	alpha-artemismic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0173891	(9E,12Z)-18-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0160592	17-hydroxylinoleic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0160591	(12Z)-9-hydroxyoctadeca-,12-dienoic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0160593	18-hydroxylinoleic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0160589	(9Z,12Z)-14-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0173887	(9E,12Z)-11-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M-H	295.2279	-1.6
	HMDB0173890	12,13-epome(9)	C18H32O3	M-H	295.2279	-1.6
297.0468	HMDB0014642	Flutamide	C11H11F3N2O3	M+Na-2H	297.0468	-0.1
	HMDB0124938	6-(carboxymethoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C8H12O9	M+FA-H	297.0463	1.6
	HMDB0124939	3,4,5-trihydroxy-6-[(2-hydroxyacetyl)oxy]oxane-2-carboxylic acid	C8H12O9	M+FA-H	297.0463	1.6
	HMDB0159746	2-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]acetate	C8H11O9	M+FA-H	297.0463	1.6
297.2066	HMDB0032340	Isoambrettolide	C16H28O2	M+FA-H	297.2071	-1.8
	HMDB0038255	Geranyl 2-ethylbutyrate	C16H28O2	M+FA-H	297.2071	-1.8
	HMDB0031086	(Z)-7-Hexadecen-1,16-olide	C16H28O2	M+FA-H	297.2071	-1.8
	HMDB0030429	Linalyl hexanoate	C16H28O2	M+FA-H	297.2071	-1.8
	HMDB0029351	Geranyl hexanoate	C16H28O2	M+FA-H	297.2071	-1.8
	HMDB0037805	D6-Ambrettolide	C16H28O2	M+FA-H	297.2071	-1.8
	HMDB0039131	Ethyl (Z,Z)-5,8-tetradecadienoate	C16H28O2	M+FA-H	297.2071	-1.8
	HMDB0000477	7Z,Z-Hexadecadienoic acid	C16H28O2	M+FA-H	297.2071	-1.8
297.2431	HMDB0166468	(3Z)-hexadeca-3,15-dienoic acid	C16H28O2	M+FA-H	297.2071	-1.8
	HMDB0059633	(9S,S)-9,-dihydroxyoctadecanoate	C18H36O4	M-H2O-H	297.2430	0.4
	HMDB0072849	MG/i-15)	C18H36O4	M-H2O-H	297.2430	0.4
	HMDB0072862	MG/a-15)[rac]	C18H36O4	M-H2O-H	297.2430	0.4
	HMDB0072878	MG(i-15)	C18H36O4	M-H2O-H	297.2430	0.4
	HMDB0011532	MG/15)	C18H36O4	M-H2O-H	297.2430	0.4
	HMDB0011563	MG(15)	C18H36O4	M-H2O-H	297.2430	0.4
	HMDB0031008	(+)-15,16-Dihydroxyoctadecanoic acid	C18H36O4	M-H2O-H	297.2430	0.4
	HMDB0072865	MG(a-15)[rac]	C18H36O4	M-H2O-H	297.2430	0.4
	HMDB0013813	13-Heptadecyn-1-ol	C17H32O	M+FA-H	297.2435	-1.4
	HMDB0041335	8-Heptadecenal	C17H32O	M+FA-H	297.2435	-1.4
	HMDB0187010	(11Z)-13-hydroxyoctadec-11-enoic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0187012	(11Z)-17-hydroxyoctadec-11-enoic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0187011	-hydroxy-cis-vaccenic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0187014	(11Z)-18-hydroxyoctadec-11-enoic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0187015	2-Hydroxy-cis-vaccensaure	C18H34O3	M-H	297.2435	-1.4
	HMDB0160380	18-Hydroxy-9-octadecenoic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0187013	Oxiranedecanoic acid, 3-hexyl-	C18H34O3	M-H	297.2435	-1.4
	HMDB0155790	(9Z)-11-hydroxyoctadec-9-enoic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0155794	2-hydroxyoleic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0155791	8-Hydroxyoleic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0155793	18-hydroxyoleic acid	C18H34O3	M-H	297.2435	-1.4

	HMDB0155792	17-Hydroxyoleic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0160377	11-hydroxy-9-octadecenoic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0160381	SCHEMBL378128	C18H34O3	M-H	297.2435	-1.4
	HMDB0160379	17-hydroxy-9-octadecenoic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0160378	8-home(9)	C18H34O3	M-H	297.2435	-1.4
	HMDB0030979	9-Oxoctadecanoic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0034074	5-Oxoctadecanoic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0030980	-Oxoctadecanoic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0031127	5-Hexyltetrahydro-2-furanoctanoic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0034297	Ricinoleic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0030981	11-Oxoctadecanoic acid	C18H34O3	M-H	297.2435	-1.4
	HMDB0010736	3-keto stearic acid	C18H34O3	M-H	297.2435	-1.4
297.2796	HMDB0032112	1,2,4-Nonadecanetriol	C19H40O3	M-H20-H	297.2794	0.8
	HMDB0036345	3-Cyclohexyldodecane	C18H36	M+FA-H	297.2799	-1.0
	HMDB0175454	6,,14-trimethyl-2-methylidenepentadecane-1,6-diol	C19H38O2	M-H	297.2799	-1.0
	HMDB0175460	6-methyl-2-methylidene--(4-methylpentyl)undecane-1,11-diol	C19H38O2	M-H	297.2799	-1.0
	HMDB0175456	6,,14-trimethyl-2-methylidenepentadecane-1,14-diol	C19H38O2	M-H	297.2799	-1.0
	HMDB0175458	[2-(4,8,12-trimethyltridecyl)oxiran-2-yl]methanol	C19H38O2	M-H	297.2799	-1.0
	HMDB0175459	2-(4,8-dimethylnonyl)-6-methylideneheptane-1,7-diol	C19H38O2	M-H	297.2799	-1.0
	HMDB0175455	6,,14-trimethyl-2-methylidenepentadecane-1,-diol	C19H38O2	M-H	297.2799	-1.0
	HMDB0175457	6,,14-trimethyl-2-methylidenepentadecane-1,3-diol	C19H38O2	M-H	297.2799	-1.0
	HMDB0000772	Nonadecanoic acid	C19H38O2	M-H	297.2799	-1.0
	HMDB0000795	Pristanic acid	C19H38O2	M-H	297.2799	-1.0
	HMDB0004085	Tuberculostearic acid	C19H38O2	M-H	297.2799	-1.0
	HMDB0035675	6-Hydroxy-4-nonadecanone	C19H38O2	M-H	297.2799	-1.0
	HMDB0035674	4-Hydroxy-6-nonadecanone	C19H38O2	M-H	297.2799	-1.0
	HMDB0037397	欽?7-Methyloctadecanoic acid	C19H38O2	M-H	297.2799	-1.0
	HMDB0061710	欽?7-Methyloctadecanoic acid	C19H38O2	M-H	297.2799	-1.0
	HMDB0038070	xi-16-Methyloctadecanoic acid	C19H38O2	M-H	297.2799	-1.0
	HMDB0034154	Methyl stearate	C19H38O2	M-H	297.2799	-1.0
	HMDB0035474	Isopropyl hexadecanoate	C19H38O2	M-H	297.2799	-1.0
	HMDB0061964	Heptadecyl acetate	C19H38O2	M-H	297.2799	-1.0
	HMDB0175461	2,6,-trimethyl-14-methylidenepentadecane-1,15-diol	C19H38O2	M-H	297.2799	-1.0
299.1862	HMDB0179275	2-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylheptan-4-one	C15H26O3	M+FA-H	299.1864	-0.7
	HMDB0179276	2-hydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M+FA-H	299.1864	-0.7
	HMDB0179274	2-[4-hydroxy-4-(hydroxymethyl)cyclohex-2-en-1-yl]-6-methylheptan-4-one	C15H26O3	M+FA-H	299.1864	-0.7
	HMDB0179277	2-(1,4-dihydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M+FA-H	299.1864	-0.7
	HMDB0179279	1-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylheptan-4-one	C15H26O3	M+FA-H	299.1864	-0.7
	HMDB0179278	2-{5-hydroxy-5-methyl-7-oxabicyclo[4.1]heptan-2-yl}-6-methylheptan-4-one	C15H26O3	M+FA-H	299.1864	-0.7
	HMDB0179280	1-hydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M+FA-H	299.1864	-0.7
	HMDB0179281	3-hydroxy-6-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-2-methylheptan-4-one	C15H26O3	M+FA-H	299.1864	-0.7
	HMDB0179282	3-hydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C15H26O3	M+FA-H	299.1864	-0.7
	HMDB0036053	(3beta,9beta)-7-Drimene-3,11,12-triol	C15H26O3	M+FA-H	299.1864	-0.7
	HMDB0029604	Lubiminol	C15H26O3	M+FA-H	299.1864	-0.7
	HMDB0036866	7-Drimene-11,12,14-triol	C15H26O3	M+FA-H	299.1864	-0.7
	HMDB0037197	Kessyl glycol	C15H26O3	M+FA-H	299.1864	-0.7
	HMDB0040276	5-Acetoxydihydrotheaespirane	C15H26O3	M+FA-H	299.1864	-0.7
	HMDB0035780	8-Hydroxy-4(6)-lactarene-5,14-diol	C15H26O3	M+FA-H	299.1864	-0.7
	HMDB0032368	Menthyl pyrrolidone carboxylate	C16H30O6	M-H20-H	299.1858	1.2
	HMDB0029850	L-Citronellol glucoside	C16H30O6	M-H20-H	299.1858	1.2
	HMDB0061980	14-methyl-8-hexadecen-1-ol	C17H34O	M+FA-H	299.2592	-1.6
	HMDB0031039	Heptadecanal	C17H34O	M+FA-H	299.2592	-1.6
	HMDB0031040	2-Heptadecanone	C17H34O	M+FA-H	299.2592	-1.6
	HMDB0010737	(R)-3-Hydroxy-Octadecanoic acid	C18H36O3	M-H	299.2592	-1.6
	HMDB0112180	5-hydroxyoctadecanoic acid	C18H36O3	M-H	299.2592	-1.6

299.2587	HMDB0112182	DI-8-hydroxy stearic acid	C18H36O3	M-H	299.2592	-1.6
	HMDB0112193	DI-6-hydroxy stearic acid	C18H36O3	M-H	299.2592	-1.6
	HMDB0240324	-hydroxystearate	C18H35O3	M-H	299.2592	-1.6
	HMDB0240330	3-hydroxystearate	C18H35O3	M-H	299.2592	-1.6
	HMDB0112181	DI-7-hydroxy stearic acid	C18H36O3	M-H	299.2592	-1.6
	HMDB0037396	xi--Hydroxyoctadecanoic acid	C18H36O3	M-H	299.2592	-1.6
	HMDB0061662	13-hydroxyoctadecanoic acid	C18H36O3	M-H	299.2592	-1.6
	HMDB0061661	9-hydroxyoctadecanoic acid	C18H36O3	M-H	299.2592	-1.6
	HMDB0061706	12-Hydroxystearic acid	C18H36O3	M-H	299.2592	-1.6
	HMDB0171068	17-hydroxy stearic acid	C18H36O3	M-H	299.2592	-1.6
	HMDB0171069	18-Hydroxyoctadecanoic acid	C18H36O3	M-H	299.2592	-1.6
	HMDB0112183	DI-11-hydroxy stearic acid	C18H36O3	M-H	299.2592	-1.6
	HMDB0062549	(S)-2-hydroxyoctadecanoic acid	C18H36O3	M-H	299.2592	-1.6
300.0482	HMDB0032294	N-Gluconyl ethanolamine phosphate	C8H18NO10P	M-H2O-H	300.0484	-0.8
	HMDB0061249	2- {[(2-formylphenyl)(hydroxy)methylidene]amino } pentanedioic acid	C13H13NO6	M+Na-2H	300.0490	-2.5
	HMDB0176564	3-[(1-carboxy-2-phenylethyl)carbamoyl]-3-oxopropanoic acid	C13H13NO6	M+Na-2H	300.0490	-2.5
	HMDB0029234	N-[4'-hydroxy-(E)-cinnamoyl]-L-aspartic acid	C13H13NO6	M+Na-2H	300.0490	-2.5
	HMDB0029294	N-[4'-hydroxy-(E)-cinnamoyl]-L-aspartic acid	C13H13NO6	M+Na-2H	300.0490	-2.5
	HMDB0062500	ZINC7257	C8H16NO9P	M-H	300.0490	-2.6
	HMDB0001062	N-Acetyl-D-Glucosamine 6-Phosphate	C8H16NO9P	M-H	300.0490	-2.6
	HMDB0001121	N-Acetyl-D-mannosamine 6-phosphate	C8H16NO9P	M-H	300.0490	-2.6
	HMDB0001367	N-Acetyl-glucosamine 1-phosphate	C8H16NO9P	M-H	300.0490	-2.6
	HMDB0002817	N-Acetylglucosamine 6-phosphate	C8H16NO9P	M-H	300.0490	-2.6
	HMDB0006480	N-Acetyl-D-galactosamine 1-phosphate	C8H16NO9P	M-H	300.0490	-2.6
	HMDB0059626	N-acetyl-alpha-D-galactosamine 1-phosphate	C8H16NO9P	M-H	300.0490	-2.6
300.2300	HMDB0062656	linoleamide	C18H33NO	M+Na-2H	300.2309	-2.9
300.2302	HMDB0062656	linoleamide	C18H33NO	M+Na-2H	300.2309	-2.3
	HMDB0141328	3-hydroxy-3-(3,4,5-trimethoxyphenyl)propanoic acid	C12H16O6	M+FA-H	301.0929	-0.3
	HMDB0142088	3-(6-hydroxy-2,3,4-trimethoxyphenyl)propanoic acid	C12H16O6	M+FA-H	301.0929	-0.3
	HMDB0142082	2-hydroxy-3-(2,3,4-trimethoxyphenyl)propanoic acid	C12H16O6	M+FA-H	301.0929	-0.3
	HMDB0141330	2-hydroxy-3-(3,4,5-trimethoxyphenyl)propanoic acid	C12H16O6	M+FA-H	301.0929	-0.3
	HMDB0142079	3-hydroxy-3-(2,3,4-trimethoxyphenyl)propanoic acid	C12H16O6	M+FA-H	301.0929	-0.3
	HMDB0141333	3-(2-hydroxy-3,4,5-trimethoxyphenyl)propanoic acid	C12H16O6	M+FA-H	301.0929	-0.3
	HMDB0164730	3,4,5-trihydroxy-6-[(1-methyl-4-oxocyclohex-2-en-1-yl)oxy]oxane-2-carboxylic acid	C13H18O8	M-H	301.0929	-0.3
	HMDB0165497	1-{5-hydroxy-4-methoxy-6-methyl-2H,5H,6H,7H,8H-6H-1,3-dioxolo[4,5-g]isoquinolin-6-yl}ethan-1-one	C14H18NO5	M+Na-2H	301.0932	-1.2
	HMDB0165498	1-{8-hydroxy-4-methoxy-6-methyl-2H,5H,6H,7H,8H-6H-1,3-dioxolo[4,5-g]isoquinolin-6-yl}ethan-1-one	C14H18NO5	M+Na-2H	301.0932	-1.2
	HMDB0165499	2-hydroxy-1-{4-methoxy-6-methyl-2H,5H,6H,7H,8H-6H-1,3-dioxolo[4,5-g]isoquinolin-6-yl}ethan-1-one	C14H18NO5	M+Na-2H	301.0932	-1.2
	HMDB0165496	1-{7-hydroxy-4-methoxy-6-methyl-2H,5H,6H,7H,8H-6H-1,3-dioxolo[4,5-g]isoquinolin-6-yl}ethan-1-one	C14H18NO5	M+Na-2H	301.0932	-1.2
	HMDB0166779	6-[[(1E)-1-carboxyhex-1-en-3-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0166780	3,4,5-trihydroxy-6-[[(2E)-4-hydroxyhept-2-enoyl]oxy]oxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0166516	3,4,5-trihydroxy-6-[[(4Z)-2-hydroxyhept-4-enoyl]oxy]oxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0166515	6-[[(3Z)-1-carboxyhex-3-en-1-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0180342	3,4,5-trihydroxy-6-[[(2E)-3-[3-(1-hydroxyethyl)oxiran-2-yl]prop-2-en-1-yl]oxy]oxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5

301.0928	HMDB0166783	3,4,5-trihydroxy-6-[[2(E)-6-hydroxyhept-2-enoyl]oxy]oxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0180347	3,4,5-trihydroxy-6-(2-{3-[(1E)-3-hydroxyprop-1-en-1-yl]oxiran-2-yl}ethoxy)oxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0180348	3,4,5-trihydroxy-6-[[2(E)-3-[3-(2-hydroxyethyl)oxiran-2-yl]prop-2-en-1-yl]oxy]oxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0180341	3,4,5-trihydroxy-6-(1-{3-[(1E)-3-hydroxyprop-1-en-1-yl]oxiran-2-yl}ethoxy)oxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0166788	6-[[5(E)-6-carboxyhex-5-en-1-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0166503	6-[(6-carboxyhex-3-en-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0166789	3,4,5-trihydroxy-6-[[2(E)-7-hydroxyhept-2-enoyl]oxy]oxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0166785	6-(3-butyloxirane-2-carbonyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0166782	6-[[5(E)-6-carboxyhex-5-en-2-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0166513	3,4,5-trihydroxy-6-[[4(Z)-7-hydroxyhept-4-enoyl]oxy]oxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0166512	6-[[3(Z)-6-carboxyhex-3-en-1-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0166509	6-{[3-(3-ethyloxiran-2-yl)propanoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0164741	3,4,5-trihydroxy-6-[(1-hydroxy-4-oxocyclohexyl)methoxy]oxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0163410	6-[(5-ethyl-4-methyl-2-oxoxolan-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0164742	3,4,5-trihydroxy-6-{[1-(hydroxymethyl)-4-oxocyclohexyl]oxy}oxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0164745	3,4,5-trihydroxy-6-[(3-hydroxy-1-methyl-4-oxocyclohexyl)oxy]oxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0164744	3,4,5-trihydroxy-6-[(5-hydroxy-5-methyl-2-oxocyclohexyl)oxy]oxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0165788	6-[(5-ethyl-2-methyl-4-oxoxolan-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0166506	6-[[3(Z)-1-carboxyhex-3-en-2-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0166507	3,4,5-trihydroxy-6-[[4(Z)-3-hydroxyhept-4-enoyl]oxy]oxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
	HMDB0166504	3,4,5-trihydroxy-6-[[4(Z)-6-hydroxyhept-4-enoyl]oxy]oxane-2-carboxylic acid	C13H20O9	M-H2O-H	301.0923	1.5
301.2012	HMDB0040904	Ipomeatetrahydrofuran	C15H28O3	M+FA-H	301.2020	-2.8
	HMDB0161061	3-hydroxythapsic acid	C16H30O5	M-H	301.2020	-2.8
	HMDB0161063	5-hydroxy-1,16-hexadecanedioic acid	C16H30O5	M-H	301.2020	-2.8
	HMDB0161064	6-hydroxyhexadecanedioic acid	C16H30O5	M-H	301.2020	-2.8
	HMDB0161062	SCHEMBL76124	C16H30O5	M-H	301.2020	-2.8
	HMDB0161065	hydroxyhexadecanedioic acid	C16H30O5	M-H	301.2020	-2.8
	HMDB0037830	xi-7-Hydroxyhexadecanedioic acid	C16H30O5	M-H	301.2020	-2.8
	HMDB0037831	xi-8-Hydroxyhexadecanedioic acid	C16H30O5	M-H	301.2020	-2.8
301.2024	HMDB0161063	5-hydroxy-1,16-hexadecanedioic acid	C16H30O5	M-H	301.2020	1.2
	HMDB0161064	6-hydroxyhexadecanedioic acid	C16H30O5	M-H	301.2020	1.2
	HMDB0161062	SCHEMBL76124	C16H30O5	M-H	301.2020	1.2
	HMDB0161065	hydroxyhexadecanedioic acid	C16H30O5	M-H	301.2020	1.2
	HMDB0161061	3-hydroxythapsic acid	C16H30O5	M-H	301.2020	1.2
	HMDB0037830	xi-7-Hydroxyhexadecanedioic acid	C16H30O5	M-H	301.2020	1.2
	HMDB0037831	xi-8-Hydroxyhexadecanedioic acid	C16H30O5	M-H	301.2020	1.2
	HMDB0040904	Ipomeatetrahydrofuran	C15H28O3	M+FA-H	301.2020	1.2
	HMDB0061119	12(R)-HETE	C20H32O3	M-H2O-H	301.2168	-0.5
	HMDB0061111	12-HETE	C20H32O3	M-H2O-H	301.2168	-0.5
	HMDB0061118	12-HETE	C20H32O3	M-H2O-H	301.2168	-0.5
	HMDB0060101	12 Hydroxy arachidonic acid	C20H32O3	M-H2O-H	301.2168	-0.5
	HMDB0012508	-HETE	C20H32O3	M-H2O-H	301.2168	-0.5
	HMDB0012567	13-HETE	C20H32O3	M-H2O-H	301.2168	-0.5
	HMDB0012598	17-HETE	C20H32O3	M-H2O-H	301.2168	-0.5

HMDB0010222	9-HETE	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0010409	11,12-EpETrE	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0011134	5-HETE	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0011136	19(S)-HETE	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0036262	Annoglabasin E	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0036810	8alpha,13R-Epoxy-14-labden-19-oic acid	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0006245	18-Hydroxyarachidonic acid	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0005998	-Hydroxyeicosatetraenoic acid	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0002190	5,6-Epoxy-8,11,14-eicosatrienoic acid	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0002232	8,9-Epoxyeicosatrienoic acid	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0002283	14R,15S-EpETrE	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0003876	15-HETE	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0004264	14,15-Epoxy-5,8,11-eicosatrienoic acid	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0004680	16(R)-HETE	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0004682	11(R)-HETE	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0004679	8-HETE	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0038694	Crispane	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0038520	2-Hydroxy-6-tridecylbenzoic acid	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0036705	8-Ocimenyl acetate	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0038688	(ent-2alpha,3beta,15beta,16beta)-15,16-Epoxy-2,3-kauranediol	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0004673	11,12-Epoxyeicosatrienoic acid	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0038689	(ent-2alpha,3beta,15beta)-16-Kaurene-2,3,15-triol	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0112071	11-{3,4-dimethyl-5-[(1E)-prop-1-en-1-yl]furan-2-yl}undecanoic acid	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0112068	(E)-11-(3,4-dimethyl-5-propylfuran-2-yl)undec--enoic acid	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0062433	8-HETE	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0062431	(5Z,8Z,14Z)-7-hydroxyicosa-5,8,11,14-tetraenoic acid	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0062302	18-HETE	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0062294	15(R)-HETE	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0062287	(5E,12S,14Z)-12-hydroxyicosa-5,8,,14-tetraenoic acid	C20H32O3	M-H2O-H	301.2168	-0.5
HMDB0156395	(2E,4E,6E)-3-methyl-7-[3-(2,6,6-trimethylcyclohex-1-en-1-yl)oxiran-2-yl]octa-2,4,6-trien-1-ol	C20H30O2	M-H	301.2173	-2.3
HMDB0156394	3-Hydroxyretinol	C20H30O2	M-H	301.2173	-2.3
HMDB0156392	(2Z)-2-[(1E,3E,5E)-4-methyl-6-(2,6,6-trimethylcyclohex-1-en-1-yl)hexa-1,3,5-trien-1-yl]but-2-ene-1,4-diol	C20H30O2	M-H	301.2173	-2.3
HMDB0156393	SCHEMBL3411787	C20H30O2	M-H	301.2173	-2.3
HMDB0156398	SCHEMBL8523586	C20H30O2	M-H	301.2173	-2.3
HMDB0156399	Hepaxanthin	C20H30O2	M-H	301.2173	-2.3
HMDB0156396	(2E,4E)-3-methyl-5-{3-methyl-3-[(E)-2-(2,6,6-trimethylcyclohex-1-en-1-yl)ethenyl]oxiran-2-yl}penta-2,4-dien-1-ol	C20H30O2	M-H	301.2173	-2.3
HMDB0156397	(2E)-3-{3-[(1E,3E)-2-methyl-4-(2,6,6-trimethylcyclohex-1-en-1-yl)buta-1,3-dien-1-yl]oxiran-2-yl}but-2-en-1-ol	C20H30O2	M-H	301.2173	-2.3
HMDB0156400	(2E,4E,6E,8E)-9-[6-(hydroxymethyl)-2,6-dimethylcyclohex-1-en-1-yl]-3,7-dimethylnona-2,4,6,8-tetraen-1-ol	C20H30O2	M-H	301.2173	-2.3
HMDB0156390	(2E,4E,6E,8E)-9-[2-(hydroxymethyl)-6,6-dimethylcyclohex-1-en-1-yl]-3,7-dimethylnona-2,4,6,8-tetraen-1-ol	C20H30O2	M-H	301.2173	-2.3
HMDB0156391	(2Z,4E,6E)-6-methyl-2-[(E)-2-(2,6,6-trimethylcyclohex-1-en-1-yl)ethenyl]octa-2,4,6-triene-1,8-diol	C20H30O2	M-H	301.2173	-2.3
HMDB0156389	4-Hydroxyretinol	C20H30O2	M-H	301.2173	-2.3
HMDB0179578	7-(1-hydroxypropan-2-yl)-1,4a-dimethyl-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-2.3
HMDB0156415	(4E,6E,8E)-2-hydroxy-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-4,6,8-trienal	C20H30O2	M-H	301.2173	-2.3
HMDB0156416	(2Z,4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraene-1,2-diol	C20H30O2	M-H	301.2173	-2.3

301.2166

HMDB0179572	4a-(hydroxymethyl)-1-methyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-2.3
HMDB0183789	17191-5	C20H30O2	M-H	301.2173	-2.3
HMDB0179581	4-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-2.3
HMDB0179582	3-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-2.3
HMDB0179575	6-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-2.3
HMDB0179573	1-(hydroxymethyl)-4a-methyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-2.3
HMDB0179574	7-(2-hydroxypropan-2-yl)-1,4a-dimethyl-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-2.3
HMDB0179576	-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-2.3
HMDB0179580	4b-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-2.3
HMDB0179579	5-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-2.3
HMDB0179577	2,6-dimethyl-13-(propan-2-yl)-12-oxatetracyclo[8.5.,]pentadec-9-ene-6-carbaldehyde	C20H30O2	M-H	301.2173	-2.3
HMDB0179583	2-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-2.3
HMDB0179584	a-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-2.3
HMDB0036811	Isopimaric acid	C20H30O2	M-H	301.2173	-2.3
HMDB0003598	Retinyl ester	C20H30O2	M-H	301.2173	-2.3
HMDB0041928	Methenolone	C20H30O2	M-H	301.2173	-2.3
HMDB0179571	Resin acid	C20H30O2	M-H	301.2173	-2.3
HMDB0036709	Yucalexin B14	C20H30O2	M-H	301.2173	-2.3
HMDB0036703	Siderone	C20H30O2	M-H	301.2173	-2.3
HMDB0039486	ent-8(17),13(16),14-Labdatrien-18-oic acid	C20H30O2	M-H	301.2173	-2.3
HMDB0036775	Yucalexin A16	C20H30O2	M-H	301.2173	-2.3
HMDB0038687	(ent-15beta,16beta)-15,16-Epoxy-3-kauranone	C20H30O2	M-H	301.2173	-2.3
HMDB0036826	Cascarillone	C20H30O2	M-H	301.2173	-2.3
HMDB0036805	8(17),12-Labdadiene-15,16-dial	C20H30O2	M-H	301.2173	-2.3
HMDB0015655	Methyltestosterone	C20H30O2	M-H	301.2173	-2.3
HMDB0038172	8,13-Abietadien-18-oic acid	C20H30O2	M-H	301.2173	-2.3
HMDB0035692	8,15-Isopimaradien-18-oic acid	C20H30O2	M-H	301.2173	-2.3
HMDB0001999	Eicosapentaenoic acid	C20H30O2	M-H	301.2173	-2.3
HMDB0061119	12(R)-HETE	C20H32O3	M-H20-H	301.2168	0.5
HMDB0006111	12-HETE	C20H32O3	M-H20-H	301.2168	0.5
HMDB0061118	12-HETE	C20H32O3	M-H20-H	301.2168	0.5
HMDB0060101	12 Hydroxy arachidonic acid	C20H32O3	M-H20-H	301.2168	0.5
HMDB0012508	-HETE	C20H32O3	M-H20-H	301.2168	0.5
HMDB0012567	13-HETE	C20H32O3	M-H20-H	301.2168	0.5
HMDB0012598	17-HETE	C20H32O3	M-H20-H	301.2168	0.5
HMDB0010222	9-HETE	C20H32O3	M-H20-H	301.2168	0.5
HMDB0010409	11,12-EpETrE	C20H32O3	M-H20-H	301.2168	0.5
HMDB0011134	5-HETE	C20H32O3	M-H20-H	301.2168	0.5
HMDB0011136	19(S)-HETE	C20H32O3	M-H20-H	301.2168	0.5
HMDB0036262	Annoglabasin E	C20H32O3	M-H20-H	301.2168	0.5
HMDB0036810	8alpha,13R-Epoxy-14-labden-19-oic acid	C20H32O3	M-H20-H	301.2168	0.5
HMDB0006245	18-Hydroxyarachidonic acid	C20H32O3	M-H20-H	301.2168	0.5

301.2169

HMDB0005998	-Hydroxyeicosatetraenoic acid	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0002190	5,6-Epoxy-8,11,14-icosatrienoic acid	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0002232	8,9-Epoxyeicosatrienoic acid	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0002283	14R,15S-EpETrE	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0003876	15-HETE	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0004264	14,15-Epoxy-5,8,11-eicosatrienoic acid	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0004680	16(R)-HETE	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0004682	11(R)-HETE	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0004679	8-HETE	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0038694	Crispane	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0038520	2-Hydroxy-6-tridecylbenzoic acid	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0036705	8-Ocimenyl acetate	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0038688	(ent-2alpha,3beta,15beta,16beta)-15,16-Epoxy-2,3-kauranediol	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0004673	11,12-Epoxyeicosatrienoic acid	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0038689	(ent-2alpha,3beta,15beta)-16-Kaurene-2,3,15-triol	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0112071	11-{3,4-dimethyl-5-[(1E)-prop-1-en-1-yl]furan-2-yl}undecanoic acid	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0112068	(E)-11-(3,4-dimethyl-5-propylfuran-2-yl)undec--enoic acid	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0062433	8-HETE	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0062431	(5Z,8Z,14Z)-7-hydroxyicosa-5,8,11,14-tetraenoic acid	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0062302	18-HETE	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0062294	15(R)-HETE	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0062287	(5E,12S,14Z)-12-hydroxyicosa-5,8,,14-tetraenoic acid	C20H32O3	M-H2O-H	301.2168	0.5
HMDB0156395	(2E,4E,6E)-3-methyl-7-[3-(2,6,6-trimethylcyclohex-1-en-1-yl)oxiran-2-yl]octa-2,4,6-trien-1-ol	C20H30O2	M-H	301.2173	-1.3
HMDB0156394	3-Hydroxyretinol	C20H30O2	M-H	301.2173	-1.3
HMDB0156392	(2Z)-2-[(1E,3E,5E)-4-methyl-6-(2,6,6-trimethylcyclohex-1-en-1-yl)hexa-1,3,5-trien-1-yl]but-2-ene-1,4-diol	C20H30O2	M-H	301.2173	-1.3
HMDB0156393	SCHEMBL3411787	C20H30O2	M-H	301.2173	-1.3
HMDB0156398	SCHEMBL8523586	C20H30O2	M-H	301.2173	-1.3
HMDB0156399	Hepaxanthin	C20H30O2	M-H	301.2173	-1.3
HMDB0156396	(2E,4E)-3-methyl-5-{3-methyl-3-[(E)-2-(2,6,6-trimethylcyclohex-1-en-1-yl)ethenyl]oxiran-2-yl}penta-2,4-dien-1-ol	C20H30O2	M-H	301.2173	-1.3
HMDB0156397	(2E)-3-{3-[(1E,3E)-2-methyl-4-(2,6,6-trimethylcyclohex-1-en-1-yl)buta-1,3-dien-1-yl]oxiran-2-yl}but-2-en-1-ol	C20H30O2	M-H	301.2173	-1.3
HMDB0156400	(2E,4E,6E,8E)-9-[6-(hydroxymethyl)-2,6-dimethylcyclohex-1-en-1-yl]-3,7-dimethylnona-2,4,6,8-tetraen-1-ol	C20H30O2	M-H	301.2173	-1.3
HMDB0156390	(2E,4E,6E,8E)-9-[2-(hydroxymethyl)-6,6-dimethylcyclohex-1-en-1-yl]-3,7-dimethylnona-2,4,6,8-tetraen-1-ol	C20H30O2	M-H	301.2173	-1.3
HMDB0156391	(2Z,4E,6E)-6-methyl-2-[(E)-2-(2,6,6-trimethylcyclohex-1-en-1-yl)ethenyl]octa-2,4,6-triene-1,8-diol	C20H30O2	M-H	301.2173	-1.3
HMDB0156389	4-Hydroxyretinol	C20H30O2	M-H	301.2173	-1.3
HMDB0179578	7-(1-hydroxypropan-2-yl)-1,4a-dimethyl-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-1.3
HMDB0156415	(4E,6E,8E)-2-hydroxy-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-4,6,8-trienal	C20H30O2	M-H	301.2173	-1.3
HMDB0156416	(2Z,4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraene-1,2-diol	C20H30O2	M-H	301.2173	-1.3
HMDB0179572	4a-(hydroxymethyl)-1-methyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-1.3
HMDB0183789	17191-5	C20H30O2	M-H	301.2173	-1.3
HMDB0179581	4-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-1.3

HMDB0179582	3-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-1.3
HMDB0179575	6-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-1.3
HMDB0179573	1-(hydroxymethyl)-4a-methyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-1.3
HMDB0179574	7-(2-hydroxypropan-2-yl)-1,4a-dimethyl-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-1.3
HMDB0179576	-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-1.3
HMDB0179580	4b-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-1.3
HMDB0179579	5-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-1.3
HMDB0179577	2,6-dimethyl-13-(propan-2-yl)-12-oxatetracyclo[8.5,,]pentadec-9-ene-6-carbaldehyde	C20H30O2	M-H	301.2173	-1.3
HMDB0179583	2-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-1.3
HMDB0179584	a-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carbaldehyde	C20H30O2	M-H	301.2173	-1.3
HMDB0036811	Isopimaric acid	C20H30O2	M-H	301.2173	-1.3
HMDB0003598	Retinyl ester	C20H30O2	M-H	301.2173	-1.3
HMDB0041928	Methenolone	C20H30O2	M-H	301.2173	-1.3
HMDB0179571	Resin acid	C20H30O2	M-H	301.2173	-1.3
HMDB0036709	Yucalexin B14	C20H30O2	M-H	301.2173	-1.3
HMDB0036703	Siderone	C20H30O2	M-H	301.2173	-1.3
HMDB0039486	ent-8(17),13(16),14-Labdatrien-18-oic acid	C20H30O2	M-H	301.2173	-1.3
HMDB0036775	Yucalexin A16	C20H30O2	M-H	301.2173	-1.3
HMDB0038687	(ent-15beta,16beta)-15,16-Epoxy-3-kauranone	C20H30O2	M-H	301.2173	-1.3
HMDB0036826	Cascarillone	C20H30O2	M-H	301.2173	-1.3
HMDB0036805	8(17),12-Labdadiene-15,16-dial	C20H30O2	M-H	301.2173	-1.3
HMDB0015655	Methyltestosterone	C20H30O2	M-H	301.2173	-1.3
HMDB0038172	8,13-Abietadien-18-oic acid	C20H30O2	M-H	301.2173	-1.3
HMDB0035692	8,15-Isopimaradien-18-oic acid	C20H30O2	M-H	301.2173	-1.3
HMDB0001999	Eicosapentaenoic acid	C20H30O2	M-H	301.2173	-1.3
HMDB0173638	3,4,5-trihydroxy-6-(4-hydroxy-1H-pyrrole-2-carbonyloxy)oxane-2-carboxylic acid	C11H13NO9	M-H	302.0518	-0.8
HMDB0173637	4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1H-pyrrole-2-carboxylic acid	C11H13NO9	M-H	302.0518	-0.8
HMDB0013220	Beta-Citryl-L-glutamic acid	C11H15NO10	M-H20-H	302.0512	1.0
HMDB0061860	2-Acetyl-3,5,5,6,8,8-hexamethyl-5,6,7,8-tetrahydronaphthalene	C18H26O	M+FA-H	303.1966	-0.9
HMDB0155961	Androst-4-en-3-one,6,17-dihydroxy-, (6b,17b)-	C19H28O3	M-H	303.1966	-0.9
HMDB0155960	CTK4G5541	C19H28O3	M-H	303.1966	-0.9
HMDB0155963	(1S,2R,R,11S,15S)-14-hydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7,,heptadec-6-en-5-one	C19H28O3	M-H	303.1966	-0.9
HMDB0155965	(1S,2R,R,11S,15S)-4,14-dihydroxy-2,15-dimethyltetracyclo[8.7,,heptadec-6-en-5-one	C19H28O3	M-H	303.1966	-0.9
HMDB0155962	16,17-Dihydroxyandrost-4-en-3-one	C19H28O3	M-H	303.1966	-0.9
HMDB0155966	4,17-Dihydroxyandrost-4-en-3-one	C19H28O3	M-H	303.1966	-0.9
HMDB0156602	(1S,2S,S,11S,15R)-13-hydroxy-2,15-dimethyltetracyclo[8.7,,heptadecane-3,5-dione	C19H28O3	M-H	303.1966	-0.9
HMDB0156968	(2S,15S)-14-hydroxy-2,15-dimethyl-13-oxotetracyclo[8.7,,heptadecan-7-ylum-5-olate	C19H28O3	M-H	303.1966	-0.9

303.1963

HMDB0159843	(1S,2R,R,11S,15S)-13,14-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-one	C19H28O3	M-H	303.1966	-0.9
HMDB0169093	3-[(2E)-3,7-dimethylocta-2,6-dien-1-yl]-4-(1-hydroxyethyl)-5-methoxyphenol	C19H28O3	M-H	303.1966	-0.9
HMDB0174397	8,17-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-13-en-5-one	C19H28O3	M-H	303.1966	-0.9
HMDB0174401	9-hydroxy-7,11-dimethyl-5-oxapentacyclo[8.8.?,octadecan-14-one	C19H28O3	M-H	303.1966	-0.9
HMDB0174399	17-hydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadec-13-en-5-one	C19H28O3	M-H	303.1966	-0.9
HMDB0174398	17-hydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadec-13-en-5-one	C19H28O3	M-H	303.1966	-0.9
HMDB0174400	12,17-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-13-en-5-one	C19H28O3	M-H	303.1966	-0.9
HMDB0186115	(2S,7S,S,11S,15S)-5-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecane-14,17-dione	C19H28O3	M-H	303.1966	-0.9
HMDB0155186	(2R,15S)-5,6-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-one	C19H28O3	M-H	303.1966	-0.9
HMDB0155187	(2R,15S)-5,12-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-one	C19H28O3	M-H	303.1966	-0.9
HMDB0154836	(2S,15S)-9-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecane-5,14-dione	C19H28O3	M-H	303.1966	-0.9
HMDB0137366	SCHEMBL668211	C19H28O3	M-H	303.1966	-0.9
HMDB0137379	4-[(1E,4E)-3-hydroxydodeca-1,4-dien-1-yl]-2-methoxyphenol	C19H28O3	M-H	303.1966	-0.9
HMDB0154824	(2S,15S)-13-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecane-5,14-dione	C19H28O3	M-H	303.1966	-0.9
HMDB0154823	(2R,15S)-8-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecane-5,14-dione	C19H28O3	M-H	303.1966	-0.9
HMDB0154826	(2S,15S)-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadecane-5,14-dione	C19H28O3	M-H	303.1966	-0.9
HMDB0000309	3a,16b-dihydroxyandrostenone	C19H28O3	M-H	303.1966	-0.9
HMDB0154825	(2R,15S)-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecane-5,14-dione	C19H28O3	M-H	303.1966	-0.9
HMDB0154837	(2S,15S)-17-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecane-5,14-dione	C19H28O3	M-H	303.1966	-0.9
HMDB0154992	(2R,15S)-6-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecane-5,14-dione	C19H28O3	M-H	303.1966	-0.9
HMDB0155184	(2S,15S)-5-hydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadec-7-en-14-one	C19H28O3	M-H	303.1966	-0.9
HMDB0155182	(2R,15S)-5,17-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-one	C19H28O3	M-H	303.1966	-0.9
HMDB0155181	(2R,15S)-5,9-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-one	C19H28O3	M-H	303.1966	-0.9
HMDB0155183	(2R,15S)-5,13-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-one	C19H28O3	M-H	303.1966	-0.9
HMDB0155185	(2R,15S)-5-hydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadec-7-en-14-one	C19H28O3	M-H	303.1966	-0.9
HMDB0155188	(2R,15S)-4,5-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-one	C19H28O3	M-H	303.1966	-0.9
HMDB0000324	3a,16a-dihydroxyandrostenone	C19H28O3	M-H	303.1966	-0.9
HMDB0000322	16-Oxoandrostenediol	C19H28O3	M-H	303.1966	-0.9
HMDB0000352	16a-Hydroxydehydroisoandrosterone	C19H28O3	M-H	303.1966	-0.9
HMDB0000388	3a,16-Dihydroxyandrostenone	C19H28O3	M-H	303.1966	-0.9
HMDB0003956	7a-Hydroxytestosterone	C19H28O3	M-H	303.1966	-0.9
HMDB0004611	7a-Hydroxydehydroepiandrosterone	C19H28O3	M-H	303.1966	-0.9
HMDB0004624	7b-Hydroxydehydroepiandrosterone	C19H28O3	M-H	303.1966	-0.9
HMDB0006259	DG(O-16/18)	C19H28O3	M-H	303.1966	-0.9
HMDB0006769	Indole-5,6-quinone	C19H28O3	M-H	303.1966	-0.9
HMDB0039589	Ginsenoside G	C19H28O3	M-H	303.1966	-0.9
HMDB0039735	-Acetoxy-8-heptadecene-4,6-diyn-3-ol	C19H28O3	M-H	303.1966	-0.9
HMDB0031464	cis-[8]-Shogaol	C19H28O3	M-H	303.1966	-0.9
HMDB0012533	11beta-Hydroxytestosterone	C19H28O3	M-H	303.1966	-0.9
HMDB0012654	SM(d18/24:1(15Z)(OH))	C19H28O3	M-H	303.1966	-0.9
HMDB0060089	w Hydroxy testosterone	C19H28O3	M-H	303.1966	-0.9

HMDB0060339	11beta,17beta-Dihydroxy-4-androsten-3-one	C19H28O3	M-H	303.1966	-0.9
HMDB0006031	11-Ketoetiocholanolone	C19H28O3	M-H	303.1966	-0.9
HMDB0033615	(S)-[8]-Gingerol	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0156606	(2R,15R)-5,8,13-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-3-one	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0156608	(2S,15S)-5,13-dihydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadecan-3-one	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0185970	(2S,15S)-8,14,17-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-one	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0185972	(2R,15S)-14,17-dihydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-5-one	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0185971	(2S,15S)-13,14,17-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-one	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0185973	(2S,15S)-14,17-dihydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadecan-5-one	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0159845	(1S,2R,S,11S,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,13,14,17-tetrol	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0156607	(2S,15R)-5,13-dihydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-3-one	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0154827	(2R,15S)-5,8,9-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-one	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0154828	(2S,15S)-5,9,13-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-one	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0154834	(2S,15S)-5,17-dihydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadecan-14-one	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0154833	(2R,15S)-5,17-dihydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-14-one	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0154829	(2R,15S)-5,9-dihydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-14-one	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0154831	(2S,15S)-5,8,17-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-one	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0154832	(2S,15S)-5,13,17-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-one	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0154830	(2S,15S)-5,9-dihydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadecan-14-one	C19H30O4	M-H2O-H	303.1960	0.9
HMDB0112104	9-(5-hexyl-3-methylfuran-2-yl)nonanoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0112091	7-(5-heptyl-3,4-dimethylfuran-2-yl)heptanoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0060052	8-HETrE	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0062747	12(S)-HETrE	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0062290	12r-hetre	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0185645	(11Z,14Z)-8,9-Epoxy-11,14-icosadienoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0185643	(8Z,14Z)-11-hydroxyicosa-8,12,14-trienoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0005045	15(S)-Hydroxyeicosatrienoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0185641	(11Z,14Z)-8-hydroxyicosa-9,11,14-trienoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0185639	(8Z,11Z,14Z)-13-hydroxyicosa-8,11,14-trienoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0185647	(8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-8,11-dienoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0185644	(8Z,11Z,14Z)-19-hydroxyicosa-8,11,14-trienoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0185650	(8Z,11Z,14Z)-2-hydroxyicosa-8,11,14-trienoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0185646	CHEMBL132396	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0036802	Austroinulin	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0185648	(8Z,11Z,14Z)--hydroxyicosa-8,11,14-trienoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0061645	3,4-Dimethyl-5-pentyl-2-furannonanoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0185637	(8Z,11Z,14Z)-16-hydroxyicosa-8,11,14-trienoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0061647	3,鈇?-鈇婦imethyl-鈇?-鈇嫗ropyl-2-鈇嫗uranundecanoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0185636	(8Z,14Z)-7-hydroxyicosa-8,11,14-trienoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0185640	(8Z,E,14Z)-12-hydroxyicosa-8.,14-trienoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0185638	(8Z,11Z,14Z)--hydroxyicosa-8,11,14-trienoic acid	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0185642	15-Hetre	C20H34O3	M-H2O-H	303.2324	-0.7
HMDB0185649	(8Z,11Z,14Z)-icosa-8,11,14,19-tetraenoic acid	C20H32O2	M-H	303.2330	-2.5
HMDB0179588	2-[8-(hydroxymethyl)-4b,8-dimethyl-3,4,4a,4b,5,6,7,8,8a,9-decahydrophenanthren-2-yl]propan-2-ol	C20H32O2	M-H	303.2330	-2.5

HMDB0179587	[1-(hydroxymethyl)-4a-methyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthren-1-yl]methanol	C20H32O2	M-H	303.2330	-2.5
HMDB0179586	[1-(hydroxymethyl)-1-methyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthren-4a-yl]methanol	C20H32O2	M-H	303.2330	-2.5
HMDB0179590	8-(hydroxymethyl)-4b,8-dimethyl-2-(propan-2-yl)-3,4,4a,4b,5,6,7,8,8a,9-decahydrophenanthren-9-ol	C20H32O2	M-H	303.2330	-2.5
HMDB0179589	8-(hydroxymethyl)-4b,8-dimethyl-2-(propan-2-yl)-3,4,4a,4b,5,6,7,8,8a,9-decahydrophenanthren-3-ol	C20H32O2	M-H	303.2330	-2.5
HMDB0179592	2-[8-(hydroxymethyl)-4b,8-dimethyl-3,4,4a,4b,5,6,7,8,8a,9-decahydrophenanthren-2-yl]propan-1-ol	C20H32O2	M-H	303.2330	-2.5
HMDB0179591	[2,6-dimethyl-13-(propan-2-yl)-12-oxatetracyclo[8.5.,,pentadec-9-en-6-yl]methanol	C20H32O2	M-H	303.2330	-2.5
HMDB0014996	Drostanolone	C20H32O2	M-H	303.2330	-2.5
HMDB0001043	Arachidonic acid	C20H32O2	M-H	303.2330	-2.5
HMDB0060102	Arachidonic acid	C20H32O2	M-H	303.2330	-2.5
HMDB0002177	Cis-8,11,14,17-Eicosatetraenoic acid	C20H32O2	M-H	303.2330	-2.5
HMDB0006036	Mesterolone	C20H32O2	M-H	303.2330	-2.5
HMDB0036830	Junicedral	C20H32O2	M-H	303.2330	-2.5
HMDB0037824	7,13-Eperudien-15-oic acid	C20H32O2	M-H	303.2330	-2.5
HMDB0036721	ent-17-Hydroxy-16beta-kauran-19-al	C20H32O2	M-H	303.2330	-2.5
HMDB0036754	Yucalexin P21	C20H32O2	M-H	303.2330	-2.5
HMDB0039687	Oryzalexin S	C20H32O2	M-H	303.2330	-2.5
HMDB0036702	Sideridiol	C20H32O2	M-H	303.2330	-2.5
HMDB0039702	Oryzalexin E	C20H32O2	M-H	303.2330	-2.5
HMDB0036829	Copalic acid	C20H32O2	M-H	303.2330	-2.5
HMDB0181753	16-hydroxy-3,5-dioxa-11-azapentacyclo[.7.1,??]icosa-1(),2(6),7,12,14(19),15,17-heptaene-13-carboxylic acid	C18H13NO5	M-H20-H	304.0610	-1.3
HMDB0181752	17-hydroxy-3,5-dioxa-11-azapentacyclo[.7.1,??]icosa-1(),2(6),7,12,14(19),15,17-heptaene-13-carboxylic acid	C18H13NO5	M-H20-H	304.0610	-1.3
HMDB0173593	2-[9-(methylamino)-14,16-dioxatetracyclo[8.7.,,heptadeca-1(),2,4,6,8,11,13(17)-heptaen-11-yl]-2-oxoacetic acid	C18H13NO5	M-H20-H	304.0610	-1.3
HMDB0181754	18-hydroxy-3,5-dioxa-11-azapentacyclo[.7.1,??]icosa-1(),2(6),7,12,14(19),15,17-heptaene-13-carboxylic acid	C18H13NO5	M-H20-H	304.0610	-1.3
HMDB0028821	Glutamylhistidine	C11H16N4O5	M+Na-2H	305.0867	-1.8
HMDB0029151	gamma-Glutamylhistidine	C11H16N4O5	M+Na-2H	305.0867	-1.8
HMDB0028884	His-Glu	C11H16N4O5	M+Na-2H	305.0867	-1.8
HMDB0040985	Polixetonium chloride	C10H28Cl2N2OP2	M-H20-H	305.0870	-2.6
HMDB0165423	8-(3-heptyloxiran-2-yl)octa-4,6-diyn-3-one	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165261	heptadeca-4,6-diyne-3,8-dione	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165426	(4E,9E)-11-hydroxyheptadeca-1,4,9-trien-6-yn-3-one	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165425	(9E)-17-hydroxyheptadec-9-en-4,6-diyn-3-one	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165430	(4E)-8-(3-heptyloxiran-2-yl)octa-1,4-dien-6-yn-3-one	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165429	1-{3-[(4E)-dodec-4-en-1-yn-1-yl]oxiran-2-yl}prop-2-en-1-one	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165427	(4E,9E)-16-hydroxyheptadeca-1,4,9-trien-6-yn-3-one	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165431	(4E,9E)-17-hydroxyheptadeca-1,4,9-trien-6-yn-3-one	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0171236	Falcarindiol	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165424	(9E)-1-hydroxyheptadec-9-en-4,6-diyn-3-one	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165422	(9E)-16-hydroxyheptadec-9-en-4,6-diyn-3-one	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165421	(9E)-2-hydroxyheptadec-9-en-4,6-diyn-3-one	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165262	(9E)-heptadeca-6,9-dien-4-yne-3,8-dione	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165263	(4E,9E)-heptadeca-4,9-dien-6-yne-3,8-dione	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165265	(4E)-heptadeca-1,4-dien-6-yne-3,8-dione	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165267	(4E,9E)-heptadeca-1,4,6,9-tetraene-3,8-dione	C17H24O2	M+FA-H	305.1758	-0.8

305.1756

HMDB0165264	heptadeca-1,6-dien-4-yne-3,8-dione	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165266	(9E)-heptadeca-1,9-dien-4-yne-3,8-dione	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165268	(9E)-heptadeca-1,9-dien-6-yne-3,8-dione	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165420	(9E)-11-hydroxyheptadec-9-en-4,6-diyn-3-one	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0033941	Falcarindiol	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0038781	1,8-Heptadecadiene-4,6-diyne-3,-diol	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0034000	Panaxydol	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0060355	2-Polyprenyl-6-methoxyphenol	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0165428	(2E,7E)-1-(oxiran-2-yl)pentadeca-2,7-dien-4-yn-1-one	C17H24O2	M+FA-H	305.1758	-0.8
HMDB0034780	Capsiate	C18H26O4	M-H	305.1758	-0.8
HMDB0184953	(15S)-2,14,17-trihydroxy-15-methyltetracyclo[8.7,,heptadec-6-en-5-one	C18H26O4	M-H	305.1758	-0.8
HMDB0184954	(15S)-4,14,17-trihydroxy-15-methyltetracyclo[8.7,,heptadec-6-en-5-one	C18H26O4	M-H	305.1758	-0.8
HMDB0184949	(15S)-8,14,17-trihydroxy-15-methyltetracyclo[8.7,,heptadec-6-en-5-one	C18H26O4	M-H	305.1758	-0.8
HMDB0184951	(15S)-14,17-dihydroxy-15-(hydroxymethyl)tetracyclo[8.7,,heptadec-6-en-5-one	C18H26O4	M-H	305.1758	-0.8
HMDB0180103	(4-hydroxy-3-methoxyphenyl)methyl 8-methylnon-8-enoate	C18H26O4	M-H	305.1758	-0.8
HMDB0012799	5'-Carboxy-gamma-chromanol	C18H26O4	M-H	305.1758	-0.8
HMDB0184950	(15S)-13,14,17-trihydroxy-15-methyltetracyclo[8.7,,heptadec-6-en-5-one	C18H26O4	M-H	305.1758	-0.8
HMDB0033631	Lactapiperanol D	C18H28O5	M-H2O-H	305.1753	1.0
HMDB0180021	(4-hydroxy-3,5-dimethoxyphenyl)methyl 7-methyloctanoate	C18H28O5	M-H2O-H	305.1753	1.0
HMDB0180098	(4-hydroxy-3-methoxyphenyl)methyl 8-hydroxy-8-methylnonanoate	C18H28O5	M-H2O-H	305.1753	1.0
HMDB0180099	(4-hydroxy-3-methoxyphenyl)methyl 9-hydroxy-8-methylnonanoate	C18H28O5	M-H2O-H	305.1753	1.0
HMDB0180102	(3,4-dihydroxy-5-methoxyphenyl)methyl 8-methylnonanoate	C18H28O5	M-H2O-H	305.1753	1.0
HMDB0180100	(4-hydroxy-3-methoxyphenyl)methyl 2-hydroxy-8-methylnonanoate	C18H28O5	M-H2O-H	305.1753	1.0
HMDB0038580	Cibacic acid	C18H28O5	M-H2O-H	305.1753	1.0
HMDB0164465	1-(4-hydroxy-3-methoxyphenyl)dodecane-3,5-diol	C19H32O4	M-H2O-H	305.2117	-0.9
HMDB0031007	1-Acetoxy-2-hydroxy-16-heptadecyn-4-one	C19H32O4	M-H2O-H	305.2117	-0.9
HMDB0154822	(1S,2S,7S,R,11S,15S)-5-hydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7,,heptadecan-14-one	C19H30O3	M-H	305.2122	-2.7
HMDB0154819	(1S,2R,7S,R,11S,15S)-5,8-dihydroxy-2,15-dimethyltetracyclo[8.7,,heptadecan-14-one	C19H30O3	M-H	305.2122	-2.7
HMDB0154818	(1S,2S,7R,R,11S,15S)-5,9-dihydroxy-2,15-dimethyltetracyclo[8.7,,heptadecan-14-one	C19H30O3	M-H	305.2122	-2.7
HMDB0154820	(1S,2S,7S,R,11S,15S)-5,13-dihydroxy-2,15-dimethyltetracyclo[8.7,,heptadecan-14-one	C19H30O3	M-H	305.2122	-2.7
HMDB0137401	4-[(1E)-3-hydroxydodec-1-en-1-yl]-2-methoxyphenol	C19H30O3	M-H	305.2122	-2.7
HMDB0137390	4-[(4E)-3-hydroxydodec-4-en-1-yl]-2-methoxyphenol	C19H30O3	M-H	305.2122	-2.7
HMDB0154821	(1S,2R,7S,R,11S,15S)-5-hydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7,,heptadecan-14-one	C19H30O3	M-H	305.2122	-2.7
HMDB0155967	(2R,15S)-8,14-dihydroxy-2,15-dimethyltetracyclo[8.7,,heptadecan-5-one	C19H30O3	M-H	305.2122	-2.7
HMDB0156127	(2R,15S)-2,15-dimethyltetracyclo[8.7,,heptadec-7-ene-5,,14-triol	C19H30O3	M-H	305.2122	-2.7
HMDB0156131	(2R,15R)-2,15-dimethyltetracyclo[8.7,,heptadec-7-ene-5,11,14-triol	C19H30O3	M-H	305.2122	-2.7
HMDB0156130	(2R,15S)-2,15-dimethyltetracyclo[8.7,,heptadec-7-ene-5,14,16-triol	C19H30O3	M-H	305.2122	-2.7
HMDB0156600	(1S,2S,S,11S,15R)-5,13-dihydroxy-2,15-dimethyltetracyclo[8.7,,heptadecan-3-one	C19H30O3	M-H	305.2122	-2.7
HMDB0159470	(1S,2S,5R,7S,R,11S,15S)-5,9-dihydroxy-2,15-dimethyltetracyclo[8.7,,heptadecan-14-one	C19H30O3	M-H	305.2122	-2.7
HMDB0159472	(1S,2R,5R,7R,R,11S,15S)-5,8-dihydroxy-2,15-dimethyltetracyclo[8.7,,heptadecan-14-one	C19H30O3	M-H	305.2122	-2.7
HMDB0159473	(1S,2S,5R,7R,R,11S,15S)-5,13-dihydroxy-2,15-dimethyltetracyclo[8.7,,heptadecan-14-one	C19H30O3	M-H	305.2122	-2.7

305.2114

HMDB0159471	SCHEMBL1799883	C19H30O3	M-H	305.2122	-2.7
HMDB0159474	(1S,2R,5R,7R,R,11S,15S)-5-hydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-14-one	C19H30O3	M-H	305.2122	-2.7
HMDB0159475	(1S,2S,5R,7R,R,11S,15S)-5-hydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadecan-14-one	C19H30O3	M-H	305.2122	-2.7
HMDB0185968	(2S,15S)-4,14-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-one	C19H30O3	M-H	305.2122	-2.7
HMDB0185969	(2R,15S)-6,14-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-one	C19H30O3	M-H	305.2122	-2.7
HMDB0013199	5-Androstene-3alpha-16beta,17beta-triol	C19H30O3	M-H	305.2122	-2.7
HMDB0156126	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-4,5,14-triol	C19H30O3	M-H	305.2122	-2.7
HMDB0156128	(2S,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-1,5,14-triol	C19H30O3	M-H	305.2122	-2.7
HMDB0155969	(2R,15S)-14-hydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-5-one	C19H30O3	M-H	305.2122	-2.7
HMDB0155968	(2S,15S)-13,14-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-one	C19H30O3	M-H	305.2122	-2.7
HMDB0155970	(2S,15S)-14-hydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadecan-5-one	C19H30O3	M-H	305.2122	-2.7
HMDB0155984	(2S,15S)-14,17-dihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-one	C19H30O3	M-H	305.2122	-2.7
HMDB0156119	STL525817	C19H30O3	M-H	305.2122	-2.7
HMDB0156118	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,13,14-triol	C19H30O3	M-H	305.2122	-2.7
HMDB0156121	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,6,14-triol	C19H30O3	M-H	305.2122	-2.7
HMDB0156120	(2R,15S)-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadec-7-ene-5,14-diol	C19H30O3	M-H	305.2122	-2.7
HMDB0156125	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-3,5,14-triol	C19H30O3	M-H	305.2122	-2.7
HMDB0156122	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,9,14-triol	C19H30O3	M-H	305.2122	-2.7
HMDB0156123	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,14,14-triol	C19H30O3	M-H	305.2122	-2.7
HMDB0156124	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,12,14-triol	C19H30O3	M-H	305.2122	-2.7
HMDB0156129	(2R,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,14,17-triol	C19H30O3	M-H	305.2122	-2.7
HMDB0000523	5-Androstene-3b,16b,17a-triol	C19H30O3	M-H	305.2122	-2.7
HMDB0014759	Oxandrolone	C19H30O3	M-H	305.2122	-2.7
HMDB0000540	5-Androstene-3b,16a,17a-triol	C19H30O3	M-H	305.2122	-2.7
HMDB0000550	5-Androstenetriol	C19H30O3	M-H	305.2122	-2.7
HMDB0002984	11-Hydroxyandrosterone	C19H30O3	M-H	305.2122	-2.7
HMDB0040640	[8]-Paradol	C19H30O3	M-H	305.2122	-2.7
HMDB0013156	1-Hydroxypyrene	C19H30O3	M-H	305.2122	-2.7
HMDB0029797	(Z)-15-Oxo-11-eicosenoic acid	C20H36O3	M-H20-H	305.2481	-0.8
HMDB0034958	(13R,14R)-7-Labdene-13,14,15-triol	C20H36O3	M-H20-H	305.2481	-0.8
HMDB0034957	(13R,14R)-8-Labdene-13,14,15-triol	C20H36O3	M-H20-H	305.2481	-0.8
HMDB0174149	(6E,E,14E)-2,6,,14-tetramethylhexadeca-2,6,,14-tetraene-1,16-diol	C20H34O2	M-H	305.2486	-2.6
HMDB0174098	(2E)-2-[(3E,7E)-4,8,12-trimethyltrideca-3,7,11-trien-1-yl]but-2-ene-1,4-diol	C20H34O2	M-H	305.2486	-2.6
HMDB0174099	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,4-diol	C20H34O2	M-H	305.2486	-2.6
HMDB0174097	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,8-diol	C20H34O2	M-H	305.2486	-2.6
HMDB0174096	SCHEMBL116891	C20H34O2	M-H	305.2486	-2.6
HMDB0174102	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,5-diol	C20H34O2	M-H	305.2486	-2.6
HMDB0174103	147-52-2	C20H34O2	M-H	305.2486	-2.6
HMDB0174101	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,9-diol	C20H34O2	M-H	305.2486	-2.6

305.2478	HMDB0174100	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,13-diol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174093	(6E,E,14Z)-2,6,,14-tetramethylhexadeca-2,6,,14-tetraene-1,16-diol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174094	(2Z,6E,Z)-6,-dimethyl-2-(4-methylpent-3-en-1-yl)dodeca-2,6,-triene-1,12-diol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174095	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,12-diol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174106	{3-methyl-3-[(3E,7E)-4,8,12-trimethyltrideca-3,7,11-trien-1-yl]oxiran-2-yl}methanol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174104	(2Z,6E)-3,7-dimethyl-9-[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]nona-2,6-dien-1-ol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174158	(2E,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,5-diol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174159	14,15-Epoxygeranylgeraniol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174161	6,7-Epoxygeranylgeraniol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174160	(2E,6E)-3,7-dimethyl-9-[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]nona-2,6-dien-1-ol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174157	May-64	C20H34O2	M-H	305.2486	-2.6
	HMDB0174105	(2Z)-3-Methyl-5-[3-methyl-3-(4,8-dimethyl-3,7-nonadienyl)oxiranyl]-2-pentene-1-ol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174152	plaunotol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174150	SCHEMBL8576448	C20H34O2	M-H	305.2486	-2.6
	HMDB0174151	(2E,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,12-diol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174153	(2E,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,8-diol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174154	(2Z)-2-[(3E,7E)-4,8,12-trimethyltrideca-3,7,11-trien-1-yl]but-2-ene-1,4-diol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174156	(2E,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,13-diol	C20H34O2	M-H	305.2486	-2.6
	HMDB0174155	(2E,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,4-diol	C20H34O2	M-H	305.2486	-2.6
	HMDB0060039	Dihomo-alpha-linolenic acid	C20H34O2	M-H	305.2486	-2.6
	HMDB0036835	Sagittariol	C20H34O2	M-H	305.2486	-2.6
	HMDB0031058	Sciadonic acid	C20H34O2	M-H	305.2486	-2.6
	HMDB0010378	5,8,11-Eicosatrienoic acid	C20H34O2	M-H	305.2486	-2.6
	HMDB0002925	Dihomo-gamma-linolenic acid	C20H34O2	M-H	305.2486	-2.6
306.0760	HMDB0015141	Letrozole	C17H11N5	M+Na-2H	306.0761	-0.4
	HMDB0000125	Glutathione	C10H17N3O6S	M-H	306.0765	-1.7
	HMDB0062697	gamma-Glutamylcysteinylglycine	C10H17N3O6S	M-H	306.0765	-1.7
	HMDB0173606	2-hydroxy-2-[9-(methylamino)-14,16-dioxatetracyclo[8.7,,heptadeca-1(0),2,4,6,8,11,13(17)-heptaen-11-yl]acetic acid	C18H15NO5	M-H20-H	306.0766	-2.1
	HMDB0033193	Avenanthramide L	C18H15NO5	M-H20-H	306.0766	-2.1
306.0940	HMDB0028730	Asparaginyllutamic acid	C9H15N3O6	M+FA-H	306.0943	-0.9
	HMDB0028814	Glutamylasparagine	C9H15N3O6	M+FA-H	306.0943	-0.9
	HMDB0029144	gamma-Glutamylasparagine	C9H15N3O6	M+FA-H	306.0943	-0.9
	HMDB0028793	Glutaminylaspartic acid	C9H15N3O6	M+FA-H	306.0943	-0.9
	HMDB0028751	Aspartyl-Glutamine	C9H15N3O6	M+FA-H	306.0943	-0.9
	HMDB0028767	Aspartyl-Gamma-glutamate	C9H15N3O6	M+FA-H	306.0943	-0.9
	HMDB0029450	Aspergillomarasmine A	C10H17N3O8	M-H	306.0943	-0.9
	HMDB0155070	3,4,5-trihydroxy-6-{[2-(N-methylcarbamiimidamido)acetyl]oxy}oxane-2-carboxylic acid	C10H17N3O8	M-H	306.0943	-0.9
307.0793	HMDB0003546	Salicin	C13H18O7	M+Na-2H	307.0799	-2.0
	HMDB0034023	Isosalicin	C13H18O7	M+Na-2H	307.0799	-2.0
	HMDB0038331	3-Hydroxybenzyl alcohol glucoside	C13H18O7	M+Na-2H	307.0799	-2.0
	HMDB0038964	3-Hydroxy-4,6-heptadiyne-1-yl 1-glucoside	C13H18O7	M+Na-2H	307.0799	-2.0
	HMDB0061378	(3Z)-5-[(1S,2R)-3,5-dihydroxy-2-[(1E)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoic acid	C18H30O5	M-H20-H	307.1909	-0.4

307.1908	HMDB0162418	(9E,15Z)-11,12,13-trihydroxyoctadeca-9,12,15-trienoic acid	C18H30O5	M-H2O-H	307.1909	-0.4
	HMDB0031963	(3b,6b,8a,12a)-8,12-Epoxy-7(11)-eremophilene-6,8,12-trimethoxy-3-ol	C18H30O5	M-H2O-H	307.1909	-0.4
	HMDB0032501	Santalyl acetate	C17H26O2	M+FA-H	307.1915	-2.2
	HMDB0037209	D-Galactose	C17H26O2	M+FA-H	307.1915	-2.2
	HMDB0038782	1-Heptadecene-4,6-diyne-3,9-diol	C17H26O2	M+FA-H	307.1915	-2.2
	HMDB0037832	Vetiveryl acetate	C17H26O2	M+FA-H	307.1915	-2.2
	HMDB0062021	1-(3,5-di-tert-butyl-4-hydroxyphenyl)propan-1-one	C17H26O2	M+FA-H	307.1915	-2.2
	HMDB0038024	beta-Santalyl acetate	C17H26O2	M+FA-H	307.1915	-2.2
	HMDB0040374	Ginsenoside I	C17H26O2	M+FA-H	307.1915	-2.2
	HMDB0039358	Ginsenoside D	C17H26O2	M+FA-H	307.1915	-2.2
	HMDB0033957	Crithmumdiol	C17H26O2	M+FA-H	307.1915	-2.2
	HMDB0062357	(6E,R,12Z)--hydroxy-3-oxooctadeca-6,8,12-trienoic acid	C18H28O4	M-H	307.1915	-2.2
	HMDB0031471	Diplodiatxin	C18H28O4	M-H	307.1915	-2.2
	HMDB0062359	(6E,S,12Z)--hydroxy-3-oxooctadeca-6,8,12-trienoic acid	C18H28O4	M-H	307.1915	-2.2
	HMDB0029852	Methylgingerol	C18H28O4	M-H	307.1915	-2.2
	HMDB0184806	(15S)-5,13,17-trihydroxy-15-methyltetracyclo[8.7,,heptadecan-14-one	C18H28O4	M-H	307.1915	-2.2
	HMDB0164463	1-(3,4-dihydroxyphenyl)-5-hydroxydodecan-3-one	C18H28O4	M-H	307.1915	-2.2
	HMDB0032664	Corchorifatty acid A	C18H28O4	M-H	307.1915	-2.2
	HMDB0184805	(15S)-5,8,17-trihydroxy-15-methyltetracyclo[8.7,,heptadecan-14-one	C18H28O4	M-H	307.1915	-2.2
	HMDB0033243	Corchorifatty acid D	C18H28O4	M-H	307.1915	-2.2
	HMDB0184807	(15S)-5,17-dihydroxy-15-(hydroxymethyl)tetracyclo[8.7,,heptadecan-14-one	C18H28O4	M-H	307.1915	-2.2
	HMDB0040867	5-O-Methylembelin	C18H28O4	M-H	307.1915	-2.2
	HMDB0034781	Dihydrocapsiate	C18H28O4	M-H	307.1915	-2.2
307.2272	HMDB0031049	Avocadyne 4-acetate	C19H34O4	M-H2O-H	307.2273	-0.4
	HMDB0031047	Avocadyne 2-acetate	C19H34O4	M-H2O-H	307.2273	-0.4
	HMDB0031006	1-Acetoxy-2-hydroxy-16-heptadecen-4-one	C19H34O4	M-H2O-H	307.2273	-0.4
	HMDB0031048	Avocadyne 1-acetate	C19H34O4	M-H2O-H	307.2273	-0.4
	HMDB0037519	2-(5,8-Tetradecadienyl)cyclobutanone	C18H30O	M+FA-H	307.2279	-2.2
	HMDB0034495	6,,14-Trimethyl-5,9,13-pentadecatrien-2-one	C18H30O	M+FA-H	307.2279	-2.2
	HMDB0112070	5-Ethyl-3,4-dimethyl-2-furanundecanoic acid	C19H32O3	M-H	307.2279	-2.2
	HMDB0094643	-(3,4-dimethyl-5-propylfuran-2-yl)decanoic acid	C19H32O3	M-H	307.2279	-2.2
	HMDB0112096	8-(3,4-dimethyl-5-pentylfuran-2-yl)-octanoic acid	C19H32O3	M-H	307.2279	-2.2
	HMDB0112090	5-Hexyl-3,4-dimethyl-2-furanheptanoic acid	C19H32O3	M-H	307.2279	-2.2
	HMDB0112100	9-(3,4-dimethyl-5-butylfuran-2-yl)-nonanoic acid	C19H32O3	M-H	307.2279	-2.2
	HMDB0061646	3-Methyl-5-propyl-2-furanundecanoic acid	C19H32O3	M-H	307.2279	-2.2
	HMDB0030960	Isoobtusilactone A	C19H32O3	M-H	307.2279	-2.2
	HMDB0031379	Annosquamosin B	C19H32O3	M-H	307.2279	-2.2
307.2636	HMDB0031091	3-Methyl-5-pentyl-2-furannonanoic acid	C19H32O3	M-H	307.2279	-2.2
	HMDB0172579	(11E)-19-hydroxyicos-11-enoic acid	C20H38O3	M-H2O-H	307.2637	-0.3
	HMDB0172582	SCHEMBL19404	C20H38O3	M-H2O-H	307.2637	-0.3
	HMDB0172581	(11E)--hydroxyicos-11-enoic acid	C20H38O3	M-H2O-H	307.2637	-0.3
	HMDB0172580	11,12-Epoxyicosanoic acid	C20H38O3	M-H2O-H	307.2637	-0.3
	HMDB0172578	(11E)--hydroxyicos-11-enoic acid	C20H38O3	M-H2O-H	307.2637	-0.3
	HMDB0172577	13-hydroxyicos-11-enoic acid	C20H38O3	M-H2O-H	307.2637	-0.3
	HMDB0062432	(8Z,11Z)-icosadienoic acid	C20H36O2	M-H	307.2643	-2.1
	HMDB0005060	Eicosadienoic acid	C20H36O2	M-H	307.2643	-2.1
308.0556	HMDB0036827	Sclareol	C20H36O2	M-H	307.2643	-2.1
	HMDB0173605	2-{9-amino-14,16-dioxatetracyclo-heptadeca-1(0),2,4,6,8,11,13(17)-heptaen-11-yl}-2-oxoacetic acid	C17H11NO5	M-H	308.0564	-2.7
309.1703	HMDB0061935	3,5-Bis(1,1-dimethylethyl)-4-hydroxy-benzoic acid ethyl ester	C16H24O3	M+FA-H	309.1707	-1.4
	HMDB0032090	12-Oxo-2,3-dinor-,15-phytodienoic acid	C16H24O3	M+FA-H	309.1707	-1.4
	HMDB0179990	(4-hydroxy-3-methoxyphenyl)methyl 8-hydroxy-7-methyloctanoate	C17H26O5	M-H	309.1707	-1.4
	HMDB0179989	(4-hydroxy-3-methoxyphenyl)methyl 7-hydroxy-7-methyloctanoate	C17H26O5	M-H	309.1707	-1.4
	HMDB0179993	(3,4-dihydroxy-5-methoxyphenyl)methyl 7-methyloctanoate	C17H26O5	M-H	309.1707	-1.4

	HMDB0179991	(4-hydroxy-3-methoxyphenyl)methyl 2-hydroxy-7-methyloctanoate	C17H26O5	M-H	309.1707	-1.4
	HMDB0040756	3-Hydroxy-6,8-dimethoxy-7(11)-eremophilin-12,8-olide	C17H26O5	M-H	309.1707	-1.4
	HMDB0040980	Valdiate	C17H26O5	M-H	309.1707	-1.4
309.2066	HMDB0061377	2,3-Dinor-8iso prostaglandin F2alpha	C18H32O5	M-H2O-H	309.2066	0.1
	HMDB0038483	Auxin a	C18H32O5	M-H2O-H	309.2066	0.1
	HMDB0040611	(9R,S,12Z)-9,-Dihydroxy-8-oxo-12-octadecenoic acid	C18H32O5	M-H2O-H	309.2066	0.1
	HMDB0035919	Corchorifatty acid F	C18H32O5	M-H2O-H	309.2066	0.1
	HMDB0240268	2-trans-6-trans-farnesyl acetate	C17H28O2	M+FA-H	309.2071	-1.7
	HMDB0037218	Guaiol acetate	C17H28O2	M+FA-H	309.2071	-1.7
	HMDB0039630	Nerolidyl acetate	C17H28O2	M+FA-H	309.2071	-1.7
	HMDB0037273	beta-Caryophyllene alcohol acetate	C17H28O2	M+FA-H	309.2071	-1.7
	HMDB0035910	Cedryl acetate	C17H28O2	M+FA-H	309.2071	-1.7
	HMDB0036153	Shyobunyl acetate	C17H28O2	M+FA-H	309.2071	-1.7
	HMDB0037224	alpha-Caryophyllene alcohol acetate	C17H28O2	M+FA-H	309.2071	-1.7
	HMDB0035337	Sterebin A	C18H30O4	M-H	309.2071	-1.7
	HMDB0033505	(9Z,11R,12S,13S,15Z)-12,13-Epoxy-11-hydroxy-9,15-octadecadienoic acid	C18H30O4	M-H	309.2071	-1.7
	HMDB0038484	Auxin b	C18H30O4	M-H	309.2071	-1.7
	HMDB0013623	12(13)Ep-9-KODE	C18H30O4	M-H	309.2071	-1.7
309.2432	HMDB0011565	MG(16:1(9Z))	C19H36O4	M-H2O-H	309.2430	0.7
	HMDB0031044	Avocadoene 2-acetate	C19H36O4	M-H2O-H	309.2430	0.7
	HMDB0031045	Avocadoene 4-acetate	C19H36O4	M-H2O-H	309.2430	0.7
	HMDB0031043	Avocadoene 1-acetate	C19H36O4	M-H2O-H	309.2430	0.7
	HMDB0011534	MG/16:1(9Z))	C19H36O4	M-H2O-H	309.2430	0.7
	HMDB0037543	(Z)-2-(5-Tetradecenyl)cyclobutanone	C18H32O	M+FA-H	309.2435	-1.0
	HMDB0173880	methyl (9E,12Z)-17-hydroxyoctadeca-9,12-dienoate	C19H34O3	M-H	309.2435	-1.0
	HMDB0173883	methyl (9E,12Z)-18-hydroxyoctadeca-9,12-dienoate	C19H34O3	M-H	309.2435	-1.0
	HMDB0173884	methyl (9E,12Z)-2-hydroxyoctadeca-9,12-dienoate	C19H34O3	M-H	309.2435	-1.0
	HMDB0173876	methyl (9E,12Z)-14-hydroxyoctadeca-9,12-dienoate	C19H34O3	M-H	309.2435	-1.0
	HMDB0173875	methyl (9E,12Z)-8-hydroxyoctadeca-9,12-dienoate	C19H34O3	M-H	309.2435	-1.0
	HMDB0173878	Methyl 13-hydroxy-9,11-octadecadienoate	C19H34O3	M-H	309.2435	-1.0
	HMDB0173879	methyl (12Z)-9-hydroxyoctadeca-,12-dienoate	C19H34O3	M-H	309.2435	-1.0
	HMDB0031060	(R)-2-Hydroxysterculic acid	C19H34O3	M-H	309.2435	-1.0
	HMDB0173881	AC1O2DR2	C19H34O3	M-H	309.2435	-1.0
	HMDB0173882	S1P3	C19H34O3	M-H	309.2435	-1.0
	HMDB0173877	methyl (9E,12Z)-11-hydroxyoctadeca-9,12-dienoate	C19H34O3	M-H	309.2435	-1.0
309.2792	HMDB0158832	7-hydroxy-3,7,11,15-tetramethylhexadecanoic acid	C20H40O3	M-H2O-H	309.2794	-0.5
	HMDB0158834	15-hydroxy-3,7,11,15-tetramethylhexadecanoic acid	C20H40O3	M-H2O-H	309.2794	-0.5
	HMDB0062566	3-hydroxyicosanoic Acid	C20H40O3	M-H2O-H	309.2794	-0.5
	HMDB0158835	3-(hydroxymethyl)-7,11,15-trimethylhexadecanoic acid	C20H40O3	M-H2O-H	309.2794	-0.5
	HMDB0158833	11-hydroxy-3,7,11,15-tetramethylhexadecanoic acid	C20H40O3	M-H2O-H	309.2794	-0.5
	HMDB0158831	3-hydroxy-3,7,11,15-tetramethylhexadecanoic acid	C20H40O3	M-H2O-H	309.2794	-0.5
	HMDB0158838	omega-hydroxyphytanic acid	C20H40O3	M-H2O-H	309.2794	-0.5
	HMDB0061659	2(R)-hydroxyicosanoic acid	C20H40O3	M-H2O-H	309.2794	-0.5
	HMDB0158837	11-(hydroxymethyl)-3,7,15-trimethylhexadecanoic acid	C20H40O3	M-H2O-H	309.2794	-0.5
	HMDB0061666	2-hydroxyphytanic acid	C20H40O3	M-H2O-H	309.2794	-0.5
	HMDB0061664	12-hydroxyicosanoic acid	C20H40O3	M-H2O-H	309.2794	-0.5
	HMDB0061665	15-hydroxyicosanoic acid	C20H40O3	M-H2O-H	309.2794	-0.5
	HMDB0032477	Polyoxyethylene monostearate	C20H40O3	M-H2O-H	309.2794	-0.5
	HMDB0158836	7-(hydroxymethyl)-3,11,15-trimethylhexadecanoic acid	C20H40O3	M-H2O-H	309.2794	-0.5
	HMDB0181951	(11E)--hydroxyicos-11-enal	C20H38O2	M-H	309.2799	-2.3
	HMDB0181953	-(3-octyloxiran-2-yl)decanal	C20H38O2	M-H	309.2799	-2.3
	HMDB0181955	(11E)-2-hydroxyicos-11-enal	C20H38O2	M-H	309.2799	-2.3
	HMDB0181952	(11E)-19-hydroxyicos-11-enal	C20H38O2	M-H	309.2799	-2.3
	HMDB0062436	Gadoleic acid	C20H38O2	M-H	309.2799	-2.3
	HMDB0181956	Trans-gondoic acid	C20H38O2	M-H	309.2799	-2.3
	HMDB0181954	(11E)--hydroxyicos-11-enal	C20H38O2	M-H	309.2799	-2.3
	HMDB0181950	(11E)-13-hydroxyicos-11-enal	C20H38O2	M-H	309.2799	-2.3
	HMDB0002231	11Z-Eicosenoic acid	C20H38O2	M-H	309.2799	-2.3
	HMDB0034296	11Z-Eicosenoic acid	C20H38O2	M-H	309.2799	-2.3
	HMDB0035159	Paullinic acid	C20H38O2	M-H	309.2799	-2.3
	HMDB0037127	Oleyl acetate	C20H38O2	M-H	309.2799	-2.3
	HMDB0034451	Ethyl oleate	C20H38O2	M-H	309.2799	-2.3

	HMDB0035572	6,8-Icosanedione	C20H38O2	M-H	309.2799	-2.3
	HMDB0035574	4,6-Icosanedione	C20H38O2	M-H	309.2799	-2.3
	HMDB0035573	5,7-Icosanedione	C20H38O2	M-H	309.2799	-2.3
311.1864	HMDB0112097	5-Butyl-2-furanheptanoic acid	C16H26O3	M+FA-H	311.1864	0.0
	HMDB0112092	5-Pentyl-2-furanheptanoic acid	C16H26O3	M+FA-H	311.1864	0.0
	HMDB0112088	6-(5-hexylfuran-2-yl)hexanoic acid	C16H26O3	M+FA-H	311.1864	0.0
	HMDB0112085	5-(3,4-dimethyl-5-pentylfuran-2-yl)-pentanoic acid	C16H26O3	M+FA-H	311.1864	0.0
	HMDB0112089	7-(3,4-dimethyl-5-propylfuran-2-yl)heptanoic acid	C16H26O3	M+FA-H	311.1864	0.0
	HMDB0060055	Tetranor 12-HETE	C16H26O3	M+FA-H	311.1864	0.0
	HMDB0033917	4-Hydroxy-3-methoxy-2,-bisaboladien-9-one	C16H26O3	M+FA-H	311.1864	0.0
311.2221	HMDB0004710	9,,13-TriHOME	C18H34O5	M-H2O-H	311.2222	-0.4
	HMDB0004708	9,12,13-TriHOME	C18H34O5	M-H2O-H	311.2222	-0.4
	HMDB0172549	9,-dihydroxy-18-oxooctadecanoic acid	C18H34O5	M-H2O-H	311.2222	-0.4
	HMDB0030936	5,8,12-Trihydroxy-9-octadecenoic acid	C18H34O5	M-H2O-H	311.2222	-0.4
	HMDB0038555	(9S,E,12S,13S)-9,12,13-Trihydroxy--octadecenoic acid	C18H34O5	M-H2O-H	311.2222	-0.4
	HMDB0031050	Methyl 2E,4Z-hexadecadienoate	C17H30O2	M+FA-H	311.2228	-2.2
	HMDB0062281	(11S)-11-hydroperoxylinoleic acid	C18H32O4	M-H	311.2228	-2.2
	HMDB0062434	(9S,E,12Z,15Z)-9-hydroperoxy-,12,15-octadecadienoate	C18H32O4	M-H	311.2228	-2.2
	HMDB0062637	13(S)-HPODE	C18H32O4	M-H	311.2228	-2.2
	HMDB0040900	(E)-13-Hydroxy--oxo-11-octadecenoic acid	C18H32O4	M-H	311.2228	-2.2
	HMDB0010221	9,-DiHODE	C18H32O4	M-H	311.2228	-2.2
	HMDB0010208	15,16-DiHODE	C18H32O4	M-H	311.2228	-2.2
	HMDB0010201	12,13-DiHODE	C18H32O4	M-H	311.2228	-2.2
	HMDB0006940	9(S)-HPODE	C18H32O4	M-H	311.2228	-2.2
	HMDB0003871	13-L-Hydroperoxylinoleic acid	C18H32O4	M-H	311.2228	-2.2
	HMDB0004706	8(R)-Hydroperoxylinoleic acid	C18H32O4	M-H	311.2228	-2.2
311.2948	HMDB0172174	(2E)-3,5-dimethyl-7-(4-methylnonyl)oct-2-ene-1,8-diol	C20H40O2	M-H	311.2956	-2.4
	HMDB0181945	(11E)-icos-11-ene-1,13-diol	C20H40O2	M-H	311.2956	-2.4
	HMDB0181946	(11E)-icos-11-ene-1,-diol	C20H40O2	M-H	311.2956	-2.4
	HMDB0181948	11,12-Epoxyicosan-1-ol	C20H40O2	M-H	311.2956	-2.4
	HMDB0181949	(9E)-icos-9-ene-1,-diol	C20H40O2	M-H	311.2956	-2.4
	HMDB0172172	[3-methyl-3-(2,4,8-trimethyltridecyl)oxiran-2-yl]methanol	C20H40O2	M-H	311.2956	-2.4
	HMDB0172168	(2E)-3,5,7,11-tetramethylhexadec-2-ene-1,11-diol	C20H40O2	M-H	311.2956	-2.4
	HMDB0172170	(2Z)-2-(2,4,8-trimethyltridecyl)but-2-ene-1,4-diol	C20H40O2	M-H	311.2956	-2.4
	HMDB0172171	(2E)-3,5,7,11-tetramethylhexadec-2-ene-1,15-diol	C20H40O2	M-H	311.2956	-2.4
	HMDB0172169	(2E)-3,5,7,11-tetramethylhexadec-2-ene-1,4-diol	C20H40O2	M-H	311.2956	-2.4
	HMDB0172176	(2E)-3,5,7,11-tetramethylhexadec-2-ene-1,16-diol	C20H40O2	M-H	311.2956	-2.4
	HMDB0172173	(2E)-5-(2,6-dimethylundecyl)-3-methylhex-2-ene-1,6-diol	C20H40O2	M-H	311.2956	-2.4
	HMDB0172167	(2E)-3,5,7,11-tetramethylhexadec-2-ene-1,7-diol	C20H40O2	M-H	311.2956	-2.4
	HMDB0172166	(2E)-3,5,7,11-tetramethylhexadec-2-ene-1,5-diol	C20H40O2	M-H	311.2956	-2.4
	HMDB0172175	(2E)-3,5,7-trimethyl-11-pentyldec-2-ene-1,12-diol	C20H40O2	M-H	311.2956	-2.4
	HMDB0181947	(11E)-icos-11-ene-1,19-diol	C20H40O2	M-H	311.2956	-2.4
	HMDB0031318	2,2,6,,14-Pentamethylpentadecanoic acid	C20H40O2	M-H	311.2956	-2.4
	HMDB0035672	5-Hydroxy-7-eicosanone	C20H40O2	M-H	311.2956	-2.4
	HMDB0035673	4-Hydroxy-6-eicosanone	C20H40O2	M-H	311.2956	-2.4
	HMDB0002212	Arachidic acid	C20H40O2	M-H	311.2956	-2.4
	HMDB0000801	Phytanic acid	C20H40O2	M-H	311.2956	-2.4
	HMDB0000553	3L,7D,11D-Phytanic acid	C20H40O2	M-H	311.2956	-2.4
	HMDB0062520	Phytanic acid	C20H40O2	M-H	311.2956	-2.4
	HMDB0034156	Ethyl stearate	C20H40O2	M-H	311.2956	-2.4
	HMDB0000417	3D,7D,11D-Phytanic acid	C20H40O2	M-H	311.2956	-2.4
313.0327	HMDB0172685	7-acetyl-5-hydroxy-3-methoxy-6-methyl-1,2,3,4,8,8a-hexahydronaphthalene-1,2,4,8-tetrone	C14H12O7	M+Na-2H	313.0330	-0.9
	HMDB0164990	2,5,6,7,8-pentahydroxy-2-methyl-2H,3H,4H-naphtho[2,3-b]pyran-4-one	C14H12O7	M+Na-2H	313.0330	-0.9
	HMDB0164989	2,5,6,8-tetrahydroxy-2-(hydroxymethyl)-2H,3H,4H-naphtho[2,3-b]pyran-4-one	C14H12O7	M+Na-2H	313.0330	-0.9
	HMDB0172664	6-acetyl-3,8-dihydroxy-2-methoxy-7-methyl-1,4,4a,5-tetrahydronaphthalene-1,4,5-trione	C14H12O7	M+Na-2H	313.0330	-0.9
	HMDB0172663	2-acetyl-7,8-dihydroxy-6-methoxy-3-methyl-1,4,4a,5-tetrahydronaphthalene-1,4,5-trione	C14H12O7	M+Na-2H	313.0330	-0.9

	HMDB0172665	6-acetyl-4,8-dihydroxy-2-methoxy-7-methyl-1,2,3,5-tetrahydronaphthalene-1,3,5-trione	C14H12O7	M+Na-2H	313.0330	-0.9
	HMDB0172682	6-acetyl-4-hydroxy-2-methoxy-7-methyl-1,2,3,5,8,8a-hexahydronaphthalene-1,3,5,8-tetrone	C14H12O7	M+Na-2H	313.0330	-0.9
	HMDB0172681	2-acetyl-7-hydroxy-6-methoxy-3-methyl-1,4,4a,5,8,8a-hexahydronaphthalene-1,4,5,8-tetrone	C14H12O7	M+Na-2H	313.0330	-0.9
	HMDB0034310	Cordeauxione	C14H12O7	M+Na-2H	313.0330	-0.9
	HMDB0038634	(-)-Dioxibrassinin	C11H12N2O2S2	M+FA-H	313.0322	1.5
313.0779	HMDB0000425	3-Deoxy-D-glycero-D-galacto-2-nonulosonic acid	C9H16O9	M+FA-H	313.0776	0.9
	HMDB0167097	3,4,5-trihydroxy-6-[(2E,6Z)-nona-2,6,8-trien-1-yloxy]oxane-2-carboxylic acid	C15H22O7	M-H	313.1293	0.1
	HMDB0150473	4,5-bis(hydroxymethyl)-6-methoxy-2-(3-methylbut-2-en-1-yl)benzene-1,3-diol	C14H20O5	M+FA-H	313.1293	0.1
	HMDB0061643	3-carboxy-4-methyl-5-pentyl-2-furanpropanoic acid	C14H20O5	M+FA-H	313.1293	0.1
	HMDB0038935	Kamahine C	C14H20O5	M+FA-H	313.1293	0.1
	HMDB0179799	3,4,5-trihydroxy-6-[(5E)-2-oxonon-5-en-1-yl]oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0179791	3,4,5-trihydroxy-6-[(2-oxonon-5-en-4-yl)oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0179793	3,4,5-trihydroxy-6-[(4E)-8-oxonon-4-en-2-yl]oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0179797	3,4,5-trihydroxy-6-[(4E)-8-oxonon-4-en-1-yl]oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0179801	3,4,5-trihydroxy-6-[(2-oxonon-5-en-3-yl)oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0179789	3,4,5-trihydroxy-6-[(4E)-8-oxonon-4-en-3-yl]oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0179760	3,4,5-trihydroxy-6-[(3-oxonon-8-en-1-yl)oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0179757	3,4,5-trihydroxy-6-[(3-oxonon-8-en-2-yl)oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0179755	3,4,5-trihydroxy-6-[(7-oxonon-1-en-3-yl)oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0170954	3,4,5-trihydroxy-6-(non-8-enoyloxy)oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0167135	3,4,5-trihydroxy-6-[(6Z)-non-6-enoyloxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0167111	6-[(2E)-5-(3-ethyloxiran-2-yl)pent-2-en-1-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0179814	3,4,5-trihydroxy-6-[(6Z)-8-oxonon-6-en-2-yl]oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0179812	3,4,5-trihydroxy-6-[(3Z)-2-oxonon-3-en-5-yl]oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0180455	3,4,5-trihydroxy-6-[(2E,4E)-9-hydroxynona-2,4-dien-1-yl]oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0180454	3,4,5-trihydroxy-6-[(5E,7E)-9-hydroxynona-5,7-dien-1-yl]oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0180450	6-[(2E)-3-(3-butyloxiran-2-yl)prop-2-en-1-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0180446	6-(3-[(1E)-hex-1-en-1-yl]oxiran-2-yl)methoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0180443	3,4,5-trihydroxy-6-[(2E,4E)-8-hydroxynona-2,4-dien-1-yl]oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0180442	3,4,5-trihydroxy-6-[(5E,7E)-9-hydroxynona-5,7-dien-2-yl]oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0180439	3,4,5-trihydroxy-6-[(2E,4E)-6-hydroxynona-2,4-dien-1-yl]oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0180438	3,4,5-trihydroxy-6-[(5E,7E)-9-hydroxynona-5,7-dien-4-yl]oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0180042	3,4,5-trihydroxy-6-[(7-methyloct-7-enoyl)oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
313.1293	HMDB0179820	3,4,5-trihydroxy-6-[(3Z)-2-oxonon-3-en-1-yl]oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8

	HMDB0179818	3,4,5-trihydroxy-6-{{(6Z)-8-oxonon-6-en-1-yl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0179762	3,4,5-trihydroxy-6-[(3-oxonon-8-en-4-yl)oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0167107	6-({3-[(3Z)-hex-3-en-1-yl]oxiran-2-yl}methoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0167104	3,4,5-trihydroxy-6-{{(2E,6Z)-5-hydroxynona-2,6-dien-1-yl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0166522	6-[(3,3-dimethyl-2-oxocyclohexyl)methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0163487	3,4,5-trihydroxy-6-{{(6Z)-7-methyl-8-oxooct-6-en-1-yl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0163483	3,4,5-trihydroxy-6-{{(6Z)-7-methyl-8-oxooct-6-en-2-yl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0163477	6-[(2Z)-2-hexylidene-3-oxopropoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0163480	3,4,5-trihydroxy-6-{{(2Z)-2-methyl-1-oxooct-2-en-4-yl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0163476	3,4,5-trihydroxy-6-{{(2Z)-2-methyloct-2-enoyl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0166520	6-[(1,3-dimethyl-2-oxocyclohexyl)methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0166524	3,4,5-trihydroxy-6-[(1,3,3-trimethyl-2-oxocyclohexyl)oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0167081	3,4,5-trihydroxy-6-{{(3Z)-9-oxonon-3-en-5-yl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0167100	3,4,5-trihydroxy-6-{{(2E,6Z)-4-hydroxynona-2,6-dien-1-yl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0167094	3,4,5-trihydroxy-6-{{(2E,6Z)-9-hydroxynona-2,6-dien-1-yl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0167103	3,4,5-trihydroxy-6-{{(6Z)-1-hydroxynona-2,6-dien-5-yl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0167093	3,4,5-trihydroxy-6-{{(3Z,7E)-9-hydroxynona-3,7-dien-1-yl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0167090	3,4,5-trihydroxy-6-{{(2E,6Z)-8-hydroxynona-2,6-dien-1-yl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0167087	3,4,5-trihydroxy-6-{{(6Z)-1-oxonon-6-en-2-yl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0167089	3,4,5-trihydroxy-6-{{(7E)-9-hydroxynona-3,7-dien-2-yl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0167085	3,4,5-trihydroxy-6-{{(3Z)-9-oxonon-3-en-1-yl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0167079	3,4,5-trihydroxy-6-[(9-oxonon-3-en-2-yl)oxy]oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0167099	3,4,5-trihydroxy-6-{{(6Z)-1-hydroxynona-2,6-dien-4-yl}oxy}oxane-2-carboxylic acid	C15H24O8	M-H2O-H	313.1287	1.8
	HMDB0028808	Glutaminytryptophan	C16H20N4O4	M-H2O-H	313.1301	-2.4
	HMDB0029081	Tryptophyl-Glutamine	C16H20N4O4	M-H2O-H	313.1301	-2.4
	HMDB0029097	Tryptophyl-Gamma-glutamate	C16H20N4O4	M-H2O-H	313.1301	-2.4
313.2013	HMDB0159335	(7Z,Z)-6-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M+FA-H	313.2020	-2.4
	HMDB0159337	(7Z,Z)-9-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M+FA-H	313.2020	-2.4
	HMDB0159336	(7Z,Z)-12-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M+FA-H	313.2020	-2.4
	HMDB0159341	6-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}hexanoic acid	C16H28O3	M+FA-H	313.2020	-2.4
	HMDB0159338	(7Z,9E)-11-hydroxyhexadeca-7,9-dienoic acid	C16H28O3	M+FA-H	313.2020	-2.4
	HMDB0159340	(7Z,Z)-15-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M+FA-H	313.2020	-2.4
	HMDB0159339	(Z)-7-hydroxyhexadeca-8,-dienoic acid	C16H28O3	M+FA-H	313.2020	-2.4
	HMDB0159343	(7Z,Z)-16-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M+FA-H	313.2020	-2.4
	HMDB0159342	FA(16:1)(Ep,cyclo)	C16H28O3	M+FA-H	313.2020	-2.4
	HMDB0159345	(7Z,Z)-2-hydroxyhexadeca-7,-dienoic acid	C16H28O3	M+FA-H	313.2020	-2.4
	HMDB0167945	2-(4-hydroxy-5-methoxy-4-methylcyclohex-2-en-1-yl)-6-methylheptan-4-one	C16H28O3	M+FA-H	313.2020	-2.4
	HMDB0034295	Floionolic acid	C18H36O5	M-H2O-H	313.2379	-0.3

313.2378	HMDB0030935	9,,13-Trihydroxystearic acid	C18H36O5	M-H2O-H	313.2379	-0.3
	HMDB0062437	(9Z)-heptadecenoic acid	C17H32O2	M+FA-H	313.2384	-2.0
	HMDB0030997	Cyclohexaneundecanoic acid	C17H32O2	M+FA-H	313.2384	-2.0
	HMDB0031046	9E-Heptadecenoic acid	C17H32O2	M+FA-H	313.2384	-2.0
	HMDB0060038	Z-Heptadecenoic acid	C17H32O2	M+FA-H	313.2384	-2.0
	HMDB0061858	7-Hexadecenoic acid, methyl ester	C17H32O2	M+FA-H	313.2384	-2.0
	HMDB0040888	2,4-Heptadecanedione	C17H32O2	M+FA-H	313.2384	-2.0
	HMDB0004705	12,13-DHOME	C18H34O4	M-H	313.2384	-2.0
	HMDB0004704	9,-DHOME	C18H34O4	M-H	313.2384	-2.0
	HMDB0170230	6-hydroxy-5-oxooctadecanoic acid	C18H34O4	M-H	313.2384	-2.0
	HMDB0170229	4-hydroxy-5-oxooctadecanoic acid	C18H34O4	M-H	313.2384	-2.0
	HMDB0170228	2-hydroxy-5-oxooctadecanoic acid	C18H34O4	M-H	313.2384	-2.0
	HMDB0170226	17-hydroxy-5-oxooctadecanoic acid	C18H34O4	M-H	313.2384	-2.0
	HMDB0170227	18-hydroxy-5-oxooctadecanoic acid	C18H34O4	M-H	313.2384	-2.0
	HMDB0061650	(9R,S)-9,-epoxy-18-hydroxyoctadecanoic acid	C18H34O4	M-H	313.2384	-2.0
	HMDB0000782	Octadecanedioic acid	C18H34O4	M-H	313.2384	-2.0
	HMDB0041220	Dibutyl decanedioate	C18H34O4	M-H	313.2384	-2.0
	HMDB0031679	(9xi,xi,12xi)-9,-Dihydroxy-12-octadecenoic acid	C18H34O4	M-H	313.2384	-2.0
314.0646	HMDB0176556	3-[(1-methoxy-1-oxo-3-phenylpropan-2-yl)carbamoyl]-3-oxopropanoic acid	C14H15NO6	M+Na-2H	314.0646	0.0
314.2458	HMDB0060644	cis-Hydroxy Perhexiline	C19H35NO	M+Na-2H	314.2465	-2.3
	HMDB0061155	Monohydroxyperhexiline	C19H35NO	M+Na-2H	314.2465	-2.3
315.1811	HMDB0040459	Ethylene brassylate	C15H26O4	M+FA-H	315.1813	-0.7
	HMDB0037147	5(6)-Butyl-1,4-dioxan-2-one	C16H28O6	M-H	315.1813	-0.7
	HMDB0060004	Menthol-glucuronide	C16H28O6	M-H	315.1813	-0.7
	HMDB0029856	(S)-alpha-Terpinyl glucoside	C16H28O6	M-H	315.1813	-0.7
	HMDB0040563	Perilloside C	C16H28O6	M-H	315.1813	-0.7
	HMDB0030418	D-Linalool 3-glucoside	C16H28O6	M-H	315.1813	-0.7
	HMDB0029346	Neryl glucoside	C16H28O6	M-H	315.1813	-0.7
	HMDB0034771	3,7-Dimethyl-5-octene-1,7-diol 1-glucoside	C16H30O7	M-H2O-H	315.1808	1.1
	HMDB0033231	trans-p-Menthane-7,8-diol 8-glucoside	C16H30O7	M-H2O-H	315.1808	1.1
	HMDB0033218	2,6-Dimethyl-7-octene-1,6-diol 8-O-glucoside	C16H30O7	M-H2O-H	315.1808	1.1
	HMDB0033230	trans-p-Menthane-7,8-diol 7-glucoside	C16H30O7	M-H2O-H	315.1808	1.1
	HMDB0164511	SCHEMBL93593	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0169430	(2Z,6Z,Z)-4,14-dihydroxy-2,6,,14-tetramethylhexadeca-2,6,,15-tetraenoic acid	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0184817	(5Z)-7-{2-[(1E)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl}hept-5-enoic acid	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0185025	SCHEMBL115281	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0062749	(5S,6E,8Z,11Z,15R)-5,15-dihydroxyicosa-6,8,11,13-tetraenoic acid	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0062409	5,12-dihete	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0062479	(8Z)--hydroxy--[(3S)-3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl]deca-5,8-dienoic acid	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0062615	5(S),11(R)-DiHETE	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0062614	(6E,8E,11E,14E)-5,-dihydroxyicosa-6,8,11,14-tetraenoic acid	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0062619	hepoxilin A3	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0062688	15-HPETE	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0062687	(5Z,11Z,14Z)-8,-dihydroxyicosa-5,9,11,14-tetraenoic acid	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0062684	ACMC-m9i	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0062756	7-[2-(3-hydroxyoct-1-en-1-yl)-5-oxocyclopent-2-en-1-yl]heptanoic acid	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0005087	6-trans-Leukotriene B4	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0010216	5,15-DiHETE	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0011135	5-HPETE	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0010211	17,18-DiHETE	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0005088	6-trans-12-epi-Leukotriene B4	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0005089	12(S)-Leukotriene B4	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0010219	8,15-DiHETE	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0012498	,11-dihydro-12-oxo-LTB4	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0010204	14,15-DiHETE	C20H32O4	M-H2O-H	317.2117	-0.5
	HMDB0039171	9alpha-(3-Methylbutanoyloxy)-4S-hydroxy-(14)-oplopen-3-one	C20H32O4	M-H2O-H	317.2117	-0.5

HMDB0039441	ent-1()-Halimene-15,19-dioic acid	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0034686	(14S)-14,15-Dihydroxy-8(17),13(16)-labdadien-19-oic acid	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0012839	6,7-dihydro-5-oxo-12-epi-LTB4	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0004243	12(S)-HPETE	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0060105	12,-DiHETE	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0060103	9-Deoxy-delta12-PGD2	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0002236	8-iso-PGA1	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0002656	Prostaglandin A1	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0002982	Prostaglandin B1	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0001085	Leukotriene B4	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0001193	5(S)-Hydroperoxyeicosatetraenoic acid	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0060104	Prostaglandin C1	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0004244	15(S)-HPETE	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0004688	Hepoxilin A3	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0004696	11(R)-HPETE	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0004693	11H-14,15-EETA	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0004692	12(R)-HPETE	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0004690	Hepoxilin B3	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0005050	15H-11,12-EETA	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0004699	8(S)-HPETE	C20H32O4	M-H2O-H	317.2117	-0.5
HMDB0006046	5a-Androst-3-en-17-one	C19H28O	M+FA-H	317.2122	-2.3
HMDB0034406	5alpha-androst-16-en-3-one	C19H28O	M+FA-H	317.2122	-2.3
HMDB0156087	(1S,2R,11S,15R)-2,15-dimethyltetracyclo[8.7.,heptadeca-7,13-dien-5-ol	C19H28O	M+FA-H	317.2122	-2.3
HMDB0060053	9-HEPE	C20H30O3	M-H	317.2122	-2.3
HMDB0013633	12-KETE	C20H30O3	M-H	317.2122	-2.3
HMDB0012611	18R-HEPE	C20H30O3	M-H	317.2122	-2.3
HMDB0061114	Atractyligenin	C20H30O3	M-H	317.2122	-2.3
HMDB0012534	11R-HEPE	C20H30O3	M-H	317.2122	-2.3
HMDB0010212	17,18-EpETE	C20H30O3	M-H	317.2122	-2.3
HMDB0010210	15-KETE	C20H30O3	M-H	317.2122	-2.3
HMDB0010209	15-HEPE	C20H30O3	M-H	317.2122	-2.3
HMDB0010205	14,15-EpETE	C20H30O3	M-H	317.2122	-2.3
HMDB0062222	18(R)-HEPE	C20H30O3	M-H	317.2122	-2.3
HMDB0062296	15(S)-HEPE	C20H30O3	M-H	317.2122	-2.3
HMDB0062293	15(R)-HEPE	C20H30O3	M-H	317.2122	-2.3
HMDB0062408	5s-hepe	C20H30O3	M-H	317.2122	-2.3
HMDB0035116	(ent-7alpha)-7-Hydroxy-8(14),15-pimaradien-19-oic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0039716	12alpha-12-Hydroxy-7,13-abietadien-18-oic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0036713	Yucalexin B22	C20H30O3	M-H	317.2122	-2.3
HMDB0036752	Yucalexin P17	C20H30O3	M-H	317.2122	-2.3
HMDB0038521	2-Hydroxy-6-(8-tridecenyl)benzoic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0036712	Yucalexin B	C20H30O3	M-H	317.2122	-2.3
HMDB0041058	Phytocassane C	C20H30O3	M-H	317.2122	-2.3
HMDB0010217	5-KETE	C20H30O3	M-H	317.2122	-2.3
HMDB0010202	12-HEPE	C20H30O3	M-H	317.2122	-2.3
HMDB0006027	Oxymesterone	C20H30O3	M-H	317.2122	-2.3
HMDB0183807	(4E,6Z)-9-[6-(hydroxymethyl)-2,6-dimethylcyclohex-1-en-1-yl]-3,7-dimethylnona-4,6,8-trienoic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0183806	(4E,6Z)-2-hydroxy-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-4,6,8-trienoic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0183808	(4E,6Z)-9-[2-(hydroxymethyl)-6,6-dimethylcyclohex-1-en-1-yl]-3,7-dimethylnona-4,6,8-trienoic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0183809	(4E,6E)-7-(hydroxymethyl)-3-methyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-4,6,8-trienoic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0183810	(4E,6Z)-9-(3-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl)-3,7-dimethylnona-4,6,8-trienoic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0183811	3-{3-[(1Z,3E)-2-methyl-4-(2,6,6-trimethylcyclohex-1-en-1-yl)buta-1,3-dien-1-yl]oxiran-2-yl}butanoic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0183814	(4E,6Z)-3,7-dimethyl-9-{2,2,6-trimethyl-7-oxabicyclo[4.1]heptan-1-yl}nona-4,6,8-trienoic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0183813	(4E,6Z)-3-methyl-7-[3-(2,6,6-trimethylcyclohex-1-en-1-yl)oxiran-2-yl]octa-4,6-dienoic acid	C20H30O3	M-H	317.2122	-2.3

HMDB0183815	(4E,6Z)-9-(5-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl)-3,7-dimethylnona-4,6,8-trienoic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0183812	(4E)-3-methyl-5-{3-methyl-3-[(E)-2-(2,6,6-trimethylcyclohex-1-en-1-yl)ethenyl]oxiran-2-yl}pent-4-enoic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0183816	(4E,6Z)-9-(4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl)-3,7-dimethylnona-4,6,8-trienoic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0001337	Leukotriene A4	C20H30O3	M-H	317.2122	-2.3
HMDB0183804	(4E,6Z)-3-(hydroxymethyl)-7-methyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-4,6,8-trienoic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0183803	(4E,6Z)-3-hydroxy-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-4,6,8-trienoic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0005081	5-HEPE	C20H30O3	M-H	317.2122	-2.3
HMDB0137419	(4E)-1-(3,4-dihydroxyphenyl)tetradec-4-en-3-one	C20H30O3	M-H	317.2122	-2.3
HMDB0137428	(1E)-1-(3,4-dihydroxyphenyl)tetradec-1-en-3-one	C20H30O3	M-H	317.2122	-2.3
HMDB0179594	1-(hydroxymethyl)-4a-methyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carboxylic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0179596	-hydroxy-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carboxylic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0179593	4a-(hydroxymethyl)-1-methyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carboxylic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0179597	2,6-dimethyl-13-(propan-2-yl)-12-oxatetracyclo[8.5.,,]pentadec-9-ene-6-carboxylic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0179598	7-(1-hydroxypropan-2-yl)-1,4a-dimethyl-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carboxylic acid	C20H30O3	M-H	317.2122	-2.3
HMDB00037523	Galanolactone	C20H30O3	M-H	317.2122	-2.3
HMDB00036706	Steviol	C20H30O3	M-H	317.2122	-2.3
HMDB00036698	Ineketone	C20H30O3	M-H	317.2122	-2.3
HMDB00039012	(ent-15beta)-15,19-Dihydroxy-7-trachylobanone	C20H30O3	M-H	317.2122	-2.3
HMDB00035311	Galanal A	C20H30O3	M-H	317.2122	-2.3
HMDB00036724	ent-17-Hydroxy-15-kauren-19-oic acid	C20H30O3	M-H	317.2122	-2.3
HMDB00030101	Methyl [8]-Shogaol	C20H30O3	M-H	317.2122	-2.3
HMDB00036839	(ent-15beta)-15-Hydroxy-19-trachylobanoic acid	C20H30O3	M-H	317.2122	-2.3
HMDB00036776	Yucalexin A19	C20H30O3	M-H	317.2122	-2.3
HMDB00036930	delta-Carotene-1,2-epoxide	C20H30O3	M-H	317.2122	-2.3
HMDB00036806	Aframodial	C20H30O3	M-H	317.2122	-2.3
HMDB0179595	7-(2-hydroxypropan-2-yl)-1,4a-dimethyl-1,2,3,4,4a,4b,5,6,,a-decahydrophenanthrene-1-carboxylic acid	C20H30O3	M-H	317.2122	-2.3
HMDB0180125	(4-hydroxy-3,5-dimethoxyphenyl)methyl 8-methylnonanoate	C19H30O5	M-H20-H	319.1909	-1.0
HMDB0164470	4,5-dihydroxy-1-(4-hydroxy-3-methoxyphenyl)dodecan-3-one	C19H30O5	M-H20-H	319.1909	-1.0
HMDB0164466	5,11-dihydroxy-1-(4-hydroxy-3-methoxyphenyl)dodecan-3-one	C19H30O5	M-H20-H	319.1909	-1.0
HMDB0164469	2,5-dihydroxy-1-(4-hydroxy-3-methoxyphenyl)dodecan-3-one	C19H30O5	M-H20-H	319.1909	-1.0
HMDB0164464	5-hydroxy-1-(4',5'-dihydroxy-3'-methoxyphenyl)-dodecan-3-one	C19H30O5	M-H20-H	319.1909	-1.0
HMDB0164462	1,5-dihydroxy-1-(4-hydroxy-3-methoxyphenyl)dodecan-3-one	C19H30O5	M-H20-H	319.1909	-1.0
HMDB0164467	5,12-dihydroxy-1-(4-hydroxy-3-methoxyphenyl)dodecan-3-one	C19H30O5	M-H20-H	319.1909	-1.0
HMDB00038720	Dodecyl gallate	C19H30O5	M-H20-H	319.1909	-1.0
HMDB00040566	[6]-Gingerdiol 3-acetate	C19H30O5	M-H20-H	319.1909	-1.0
HMDB00040567	[6]-Gingerdiol 5-acetate	C19H30O5	M-H20-H	319.1909	-1.0
HMDB00035579	1-Phenyl-1,3-dodecanedione	C18H26O2	M+FA-H	319.1915	-2.8
HMDB00037191	Rhodinyl phenylacetate	C18H26O2	M+FA-H	319.1915	-2.8
HMDB0184935	4-estren-17-ol-3-one	C18H26O2	M+FA-H	319.1915	-2.8
HMDB00037230	Citronellyl alpha-toluate	C18H26O2	M+FA-H	319.1915	-2.8
HMDB00035963	(Z,14E,16E)-,14,16-Octadecatrien-12-ynoic acid	C18H26O2	M+FA-H	319.1915	-2.8

319.1906	HMDB0002725	Nandrolone	C18H26O2	M+FA-H	319.1915	-2.8
	HMDB0137384	(4E)-1-(3,4-dihydroxy-5-methoxyphenyl)dodec-4-en-3-one	C19H28O4	M-H	319.1915	-2.8
	HMDB0137391	(1Z)-2-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dodec-1-en-3-one	C19H28O4	M-H	319.1915	-2.8
	HMDB0137395	(1E)-1-(2,4-dihydroxy-3-methoxyphenyl)dodec-1-en-3-one	C19H28O4	M-H	319.1915	-2.8
	HMDB0137385	(4E)-11-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dodec-4-en-3-one	C19H28O4	M-H	319.1915	-2.8
	HMDB0137394	(1E)-1-(3,4-dihydroxy-5-methoxyphenyl)dodec-1-en-3-one	C19H28O4	M-H	319.1915	-2.8
	HMDB0137393	(1E)-1-(2,4-dihydroxy-5-methoxyphenyl)dodec-1-en-3-one	C19H28O4	M-H	319.1915	-2.8
	HMDB0137398	(1E)-12-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dodec-1-en-3-one	C19H28O4	M-H	319.1915	-2.8
	HMDB0137396	(1E)-11-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dodec-1-en-3-one	C19H28O4	M-H	319.1915	-2.8
	HMDB0137397	1-[3-(4-hydroxy-3-methoxyphenyl)oxiran-2-yl]decan-1-one	C19H28O4	M-H	319.1915	-2.8
	HMDB0137400	(1E)-4-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dodec-1-en-3-one	C19H28O4	M-H	319.1915	-2.8
	HMDB0137389	(4E)-2-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dodec-4-en-3-one	C19H28O4	M-H	319.1915	-2.8
	HMDB0137386	1-(3-heptyloxiran-2-yl)-3-(4-hydroxy-3-methoxyphenyl)propan-1-one	C19H28O4	M-H	319.1915	-2.8
	HMDB0157552	AC1L48S3	C19H28O4	M-H	319.1915	-2.8
	HMDB0137387	(4E)-12-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dodec-4-en-3-one	C19H28O4	M-H	319.1915	-2.8
	HMDB0039821	-Acetylpanaxytriol	C19H28O4	M-H	319.1915	-2.8
	HMDB0037592	Oryzalide B	C19H28O4	M-H	319.1915	-2.8
	HMDB0037591	Oryzalide A	C19H28O4	M-H	319.1915	-2.8
	HMDB0039276	[8]-Gingerdione	C19H28O4	M-H	319.1915	-2.8
	HMDB0012798	5'-Carboxy-alpha-chromanol	C19H28O4	M-H	319.1915	-2.8
	HMDB0137382	(4E)-1-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dodec-4-en-3-one	C19H28O4	M-H	319.1915	-2.8
	HMDB0137381	(4Z)-4-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dodec-4-en-3-one	C19H28O4	M-H	319.1915	-2.8
	HMDB0137380	(4E)-6-hydroxy-1-(4-hydroxy-3-methoxyphenyl)dodec-4-en-3-one	C19H28O4	M-H	319.1915	-2.8
319.2271	HMDB0184684	PGE1,11-DEOXY	C20H34O4	M-H20-H	319.2273	-0.7
	HMDB0012504	,11-dihydro-leukotriene B4	C20H34O4	M-H20-H	319.2273	-0.7
	HMDB0035379	Sterebin E	C20H34O4	M-H20-H	319.2273	-0.7
	HMDB0002995	12-Keto-tetrahydro-leukotriene B4	C20H34O4	M-H20-H	319.2273	-0.7
	HMDB0002265	14,15-DiHETrE	C20H34O4	M-H20-H	319.2273	-0.7
	HMDB0002311	8,9-DiHETrE	C20H34O4	M-H20-H	319.2273	-0.7
	HMDB0002314	11,12-DiHETrE	C20H34O4	M-H20-H	319.2273	-0.7
	HMDB0002343	5,6-DHET	C20H34O4	M-H20-H	319.2273	-0.7
	HMDB0012838	6,7-dihydro-12-epi-LTB4	C20H34O4	M-H20-H	319.2273	-0.7
	HMDB0060106	15-Hydroperoxyeicosa-8Z,11Z,13E-trienoate	C20H34O4	M-H20-H	319.2273	-0.7
	HMDB0005935	Androstenol	C19H30O	M+FA-H	319.2279	-2.4
	HMDB0062431	(5Z,8Z,14Z)-7-hydroxyicosa-5,8,11,14-tetraenoic acid	C20H32O3	M-H	319.2279	-2.4
	HMDB0062433	8-HETE	C20H32O3	M-H	319.2279	-2.4
	HMDB0112068	(E)-11-(3,4-dimethyl-5-propylfuran-2-yl)undec--enoic acid	C20H32O3	M-H	319.2279	-2.4
	HMDB0112071	11-{3,4-dimethyl-5-[(1E)-prop-1-en-1-yl]furan-2-yl}undecanoic acid	C20H32O3	M-H	319.2279	-2.4
	HMDB0004673	11,12-Epoxyeicosatrienoic acid	C20H32O3	M-H	319.2279	-2.4
	HMDB0062302	18-HETE	C20H32O3	M-H	319.2279	-2.4
	HMDB0062294	15(R)-HETE	C20H32O3	M-H	319.2279	-2.4
	HMDB0062287	(5E,12S,14Z)-12-hydroxyicosa-5,8,,14-tetraenoic acid	C20H32O3	M-H	319.2279	-2.4
	HMDB0002190	5,6-Epoxy-8,11,14-eicosatrienoic acid	C20H32O3	M-H	319.2279	-2.4
	HMDB0011134	5-HETE	C20H32O3	M-H	319.2279	-2.4
	HMDB0011136	19(S)-HETE	C20H32O3	M-H	319.2279	-2.4
	HMDB0036262	Annoglabasin E	C20H32O3	M-H	319.2279	-2.4
	HMDB0036810	8alpha,13R-Epoxy-14-labden-19-oic acid	C20H32O3	M-H	319.2279	-2.4

	HMDB0036705	8-Ocimenyl acetate	C20H32O3	M-H	319.2279	-2.4
	HMDB0038688	(ent-2alpha,3beta,15beta,16beta)-15,16-Epoxy-2,3-kauranediol	C20H32O3	M-H	319.2279	-2.4
	HMDB0038689	(ent-2alpha,3beta,15beta)-16-Kaurene-2,3,15-triol	C20H32O3	M-H	319.2279	-2.4
	HMDB0038520	2-Hydroxy-6-tridecylbenzoic acid	C20H32O3	M-H	319.2279	-2.4
	HMDB0038694	Crispane	C20H32O3	M-H	319.2279	-2.4
	HMDB0010409	11,12-EpETrE	C20H32O3	M-H	319.2279	-2.4
	HMDB0010222	9-HETE	C20H32O3	M-H	319.2279	-2.4
	HMDB0002232	8,9-Epoxyeicosatrienoic acid	C20H32O3	M-H	319.2279	-2.4
	HMDB0002283	14R,15S-EpETrE	C20H32O3	M-H	319.2279	-2.4
	HMDB0003876	15-HETE	C20H32O3	M-H	319.2279	-2.4
	HMDB0004264	14,15-Epoxy-5,8,11-eicosatrienoic acid	C20H32O3	M-H	319.2279	-2.4
	HMDB0004680	16(R)-HETE	C20H32O3	M-H	319.2279	-2.4
	HMDB0004682	11(R)-HETE	C20H32O3	M-H	319.2279	-2.4
	HMDB0004679	8-HETE	C20H32O3	M-H	319.2279	-2.4
	HMDB0005998	-Hydroxyeicosatetraenoic acid	C20H32O3	M-H	319.2279	-2.4
	HMDB0006245	18-Hydroxyarachidonic acid	C20H32O3	M-H	319.2279	-2.4
	HMDB0006111	12-HETE	C20H32O3	M-H	319.2279	-2.4
	HMDB0006118	12-HETE	C20H32O3	M-H	319.2279	-2.4
	HMDB0006119	12(R)-HETE	C20H32O3	M-H	319.2279	-2.4
	HMDB0060101	12 Hydroxy arachidonic acid	C20H32O3	M-H	319.2279	-2.4
	HMDB0012598	17-HETE	C20H32O3	M-H	319.2279	-2.4
	HMDB0012508	-HETE	C20H32O3	M-H	319.2279	-2.4
	HMDB0012567	13-HETE	C20H32O3	M-H	319.2279	-2.4
320.0443	HMDB0166081	{2-[2-(methylamino)benzoyloxy]ethoxy} sulfonic acid	C10H13NO6S	M+FA-H	320.0446	-0.8
	HMDB0144473	(2S)-2-amino-2-methyl-3-[4-(sulfooxy)phenyl]propanoic acid	C10H13NO6S	M+FA-H	320.0446	-0.8
	HMDB0163589	6-[2-(4,5-dihydro-1,3-thiazol-2-yl)-2-oxoethoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C11H15NO8S	M-H	320.0446	-0.8
320.0618	HMDB0013220	Beta-Citryl-L-glutamic acid	C11H15NO10	M-H	320.0623	-1.6
	HMDB0002044	8-Hydroxyguanosine	C10H13N5O6	M+Na-2H	320.0612	1.7
	HMDB0155333	2-[6-hydroxy-2-(hydroxyamino)-9H-purin-9-yl]-5-(hydroxymethyl)oxolane-3,4-diol	C10H13N5O6	M+Na-2H	320.0612	1.7
	HMDB0187538	9-[4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-2-(hydroxyamino)-9H-purine-6,8-diol	C10H13N5O6	M+Na-2H	320.0612	1.7
320.0876	HMDB0029840	Vulgaxanthin I	C14H17N3O7	M-H2O-H	320.0883	-2.1
	HMDB0181271	3,4,5-trihydroxy-6-(1-{3H-imidazo[4,5-c]pyridin-4-yl}ethoxy)oxane-2-carboxylic acid	C14H17N3O7	M-H2O-H	320.0883	-2.1
320.1066	HMDB0014028	6-Hydroxyglyclazide	C15H21N3O4S	M-H2O-H	320.1069	-0.9
	HMDB0014029	Methylhydroxyglyclazide	C15H21N3O4S	M-H2O-H	320.1069	-0.9
	HMDB0014027	7-Hydroxyglyclazide	C15H21N3O4S	M-H2O-H	320.1069	-0.9
320.1379	HMDB0172494	2-hydroxy-1-{7-hydroxy-1,2-dimethyl-1H,2H,3H,4H,9H-2H-pyrido[3,4-b]indol-2-yl}ethan-1-one	C15H19N2O3	M+FA-H	320.1378	0.4
	HMDB0172496	1-{3,7-dihydroxy-1,2-dimethyl-1H,2H,3H,4H,9H-2H-pyrido[3,4-b]indol-2-yl}ethan-1-one	C15H19N2O3	M+FA-H	320.1378	0.4
	HMDB0172493	1-{5,7-dihydroxy-1,2-dimethyl-1H,2H,3H,4H,9H-2H-pyrido[3,4-b]indol-2-yl}ethan-1-one	C15H19N2O3	M+FA-H	320.1378	0.4
	HMDB0172492	1-{7,8-dihydroxy-1,2-dimethyl-1H,2H,3H,4H,9H-2H-pyrido[3,4-b]indol-2-yl}ethan-1-one	C15H19N2O3	M+FA-H	320.1378	0.4
	HMDB0172491	1-{6,7-dihydroxy-1,2-dimethyl-1H,2H,3H,4H,9H-2H-pyrido[3,4-b]indol-2-yl}ethan-1-one	C15H19N2O3	M+FA-H	320.1378	0.4
	HMDB0172490	1-[7-hydroxy-1-(hydroxymethyl)-2-methyl-1H,2H,3H,4H,9H-2H-pyrido[3,4-b]indol-2-yl]ethan-1-one	C15H19N2O3	M+FA-H	320.1378	0.4
	HMDB0172495	1-{1,7-dihydroxy-1,2-dimethyl-1H,2H,3H,4H,9H-2H-pyrido[3,4-b]indol-2-yl}ethan-1-one	C15H19N2O3	M+FA-H	320.1378	0.4

320.1610	HMDB0015116	Physostigmine	C15H21N3O2	M+FA-H	320.1616	-1.8
320.1662	HMDB0061282	(5E)-2,2-dimethyl-7-{methyl[(naphthalen-1-yl)methyl]amino}hept-5-en-3-ynoic acid	C21H23NO2	M-H	320.1656	1.9
	HMDB0015591	Mepenzolate	C21H26NO3	M-H2O-H	320.1656	1.9
	HMDB0015075	Methantheline	C21H26NO3	M-H2O-H	320.1656	1.9
	HMDB0015060	Cyclobenzaprine	C20H21N	M+FA-H	320.1656	1.9
320.1997	HMDB0032996	2-Undecyl-4(1H)-quinolinone	C20H29NO	M+Na-2H	320.1996	0.4
	HMDB0160124	[(2R,15S)-5,13,13-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0160122	[(2R,15S)-5,6,13-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0160125	[(2R,15S)-5,12,13-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0186129	[(2S,15S)-5,8-dihydroxy-2,15-dimethyl-14-oxotetracyclo[8.7.,heptadecan-17-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0186130	[(2S,15S)-5,13-dihydroxy-2,15-dimethyl-14-oxotetracyclo[8.7.,heptadecan-17-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0186131	[(2R,15S)-5-hydroxy-2-(hydroxymethyl)-15-methyl-14-oxotetracyclo[8.7.,heptadecan-17-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0186132	[(2S,15S)-5-hydroxy-15-(hydroxymethyl)-2-methyl-14-oxotetracyclo[8.7.,heptadecan-17-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0160123	[(2R,15S)-5,9,13-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-14-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0160121	[(2R,15S)-5,13-dihydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadec-7-en-14-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0160120	[(2S,15S)-5,13-dihydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadec-7-en-14-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0159854	[(2S,15S)-13,14-dihydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadec-7-en-5-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0159855	[(2R,15S)-13,14-dihydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadec-7-en-5-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0159856	[(2R,15S)-6,13,14-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0159859	[(2R,15S)-13,13,14-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0159860	[(2R,15S)-12,13,14-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0159857	[(2R,15S)-9,13,14-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0159858	[(2R,15S)-13,14,14-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-yl]oxidanyl	C19H29O4	M-H	320.1993	1.2
	HMDB0184955	[(15S)-15-methyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]oxidanyl	C18H27O2	M+FA-H	320.1993	1.2
320.2580	HMDB0062807	sphingosine(1+)	C18H38NO2	M+Na-2H	320.2571	2.8
	HMDB0062571	3-dehydrosphinganine(1+)	C18H38NO2	M+Na-2H	320.2571	2.8
	HMDB0171017	554-87-1	C18H37NO2	M+Na-2H	320.2571	2.8
	HMDB0171016	18-Hydroxystearamide	C18H37NO2	M+Na-2H	320.2571	2.8
	HMDB0001480	3-Dehydrosphinganine	C18H37NO2	M+Na-2H	320.2571	2.8
	HMDB0002100	Palmitoylethanolamide	C18H37NO2	M+Na-2H	320.2571	2.8
	HMDB0000252	Sphingosine	C18H37NO2	M+Na-2H	320.2571	2.8
	HMDB0171015	17-Hydroxystearamide	C18H37NO2	M+Na-2H	320.2571	2.8
	HMDB0013631	Oleoyl glycine	C20H37NO3	M-H2O-H	320.2590	-3.0
320.2957	HMDB0173782	1-(14-methylhexadecanoyl)-3,4-dihydro-2H-pyrrol-1-ium	C21H40NO	M-H	320.2959	-0.6
	HMDB0173784	15-hydroxy-14-methyl-1-(pyrrolidin-1-yl)hexadecan-1-one	C21H41NO2	M-H2O-H	320.2953	1.1
	HMDB0173783	14-hydroxy-14-methyl-1-(pyrrolidin-1-yl)hexadecan-1-one	C21H41NO2	M-H2O-H	320.2953	1.1
	HMDB0173785	14-(hydroxymethyl)-1-(pyrrolidin-1-yl)hexadecan-1-one	C21H41NO2	M-H2O-H	320.2953	1.1
	HMDB0173787	2-hydroxy-14-methyl-1-(pyrrolidin-1-yl)hexadecan-1-one	C21H41NO2	M-H2O-H	320.2953	1.1
	HMDB0173786	16-hydroxy-14-methyl-1-(pyrrolidin-1-yl)hexadecan-1-one	C21H41NO2	M-H2O-H	320.2953	1.1

321.0963	HMDB0013208	{2-[(9Z)-hexadec-9-enoyloxy]ethyl} trimethylazanium	C21H42NO2	M-H2O-H	320.2953	1.1
	HMDB0041405	4-Methoxybenzyl glucoside	C14H20O7	M+Na-2H	321.0956	2.3
	HMDB0038332	2-(3-Hydroxyphenyl)ethanol 1'-glucoside	C14H20O7	M+Na-2H	321.0956	2.3
321.1706	HMDB0137236	Shogaols	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0168366	(8Z)-heptadeca-8,16-dien-11,13-diyne-1,,15-triol	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0015586	Cyclandelate	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0040375	Ginsenoine K	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0041201	Panaquinquecol 7	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0038994	Ginsenoine C	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0038938	Panaquinquecol 2	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0031463	[8]-Shogaol	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0171246	(8E)-heptadeca-8,16-dien-11,13-diyne-1,,15-triol	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0171244	(8E)-heptadeca-8,16-dien-11,13-diyne-2,,15-triol	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0168365	(7Z)-1-(oxiran-2-yl)pentadec-7-en-2,4-diyne-1,6-diol	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0168363	CHEMBL1719	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0137250	4-[(1E,4E)-3-hydroxydeca-1,4-dien-1-yl]-2-methoxyphenol	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0137237	(1E)-1-(4-hydroxy-3-methoxyphenyl)dec-1-en-3-one	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0168944	heptadeca-1,9-dien-4,6-diyne-3,9,-triol	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0168364	(8Z)-heptadeca-8,16-dien-11,13-diyne-2,,15-triol	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0171245	(7E)-1-(oxiran-2-yl)pentadec-7-en-2,4-diyne-1,6-diol	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0171243	(9E)-heptadeca-1,9-dien-4,6-diyne-3,8,11-triol	C17H24O3	M+FA-H	321.1707	-0.5
	HMDB0180045	(4-hydroxy-3-methoxyphenyl)methyl 5-[3-(propan-2-yl)oxiran-2-yl]pentanoate	C18H26O5	M-H	321.1707	-0.5
	HMDB0180044	(4-hydroxy-3-methoxyphenyl)methyl (6E)-5-hydroxy-8-methylnon-6-enoate	C18H26O5	M-H	321.1707	-0.5
	HMDB0180043	(4-hydroxy-3-methoxyphenyl)methyl (6E)-8-hydroxy-8-methylnon-6-enoate	C18H26O5	M-H	321.1707	-0.5
	HMDB0180046	(4-hydroxy-3-methoxyphenyl)methyl (6E)-9-hydroxy-8-methylnon-6-enoate	C18H26O5	M-H	321.1707	-0.5
	HMDB0180047	(4-hydroxy-3-methoxyphenyl)methyl (6E)-2-hydroxy-8-methylnon-6-enoate	C18H26O5	M-H	321.1707	-0.5
	HMDB0180048	(3,4-dihydroxy-5-methoxyphenyl)methyl (6E)-8-methylnon-6-enoate	C18H26O5	M-H	321.1707	-0.5
	HMDB0032702	Zeranol	C18H26O5	M-H	321.1707	-0.5
	HMDB0185600	(3Z)-5-{6-hydroxy-2-[(1E)-3-hydroxyoct-1-en-1-yl]-4-oxooxan-3-yl}pent-3-enoic acid	C18H28O6	M-H2O-H	321.1702	1.2
	HMDB0014876	Pentamidine	C19H24N4O2	M-H2O-H	321.1715	-2.9
321.2063	HMDB0062677	17beta-hydroxy-5beta-estrane-3-one	C18H28O2	M+FA-H	321.2071	-2.6
	HMDB0184936	Estra-4-ene-3,17-diol	C18H28O2	M+FA-H	321.2071	-2.6
	HMDB0184957	(15S)-14-hydroxy-15-methyltetracyclo[8.7,,heptadecan-5-one	C18H28O2	M+FA-H	321.2071	-2.6
	HMDB0186509	(6Z,12Z)-octadeca-6,9,12,17-tetraenoic acid	C18H28O2	M+FA-H	321.2071	-2.6
	HMDB0002697	19-norandrosterone	C18H28O2	M+FA-H	321.2071	-2.6
	HMDB0034382	(E,E)-11,13-Octadecadien-9-ynoic acid	C18H28O2	M+FA-H	321.2071	-2.6
	HMDB0032672	4,8,12,15-Octadecatetraenoic acid	C18H28O2	M+FA-H	321.2071	-2.6
	HMDB0032464	Phenethyl decanoate	C18H28O2	M+FA-H	321.2071	-2.6
	HMDB0005886	19-Noretiocholanolone	C18H28O2	M+FA-H	321.2071	-2.6
	HMDB0006547	Stearidonic acid	C18H28O2	M+FA-H	321.2071	-2.6
	HMDB0004590	19-Nor-5-androstenediol	C18H28O2	M+FA-H	321.2071	-2.6
	HMDB0154830	(2S,15S)-5,9-dihydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7,,heptadecan-14-one	C19H30O4	M-H	321.2071	-2.6
	HMDB0154828	(2S,15S)-5,9,13-trihydroxy-2,15-dimethyltetracyclo[8.7,,heptadecan-14-one	C19H30O4	M-H	321.2071	-2.6
	HMDB0033615	(S)-[8]-Gingerol	C19H30O4	M-H	321.2071	-2.6
	HMDB0154827	(2R,15S)-5,8,9-trihydroxy-2,15-dimethyltetracyclo[8.7,,heptadecan-14-one	C19H30O4	M-H	321.2071	-2.6
	HMDB0154832	(2S,15S)-5,13,17-trihydroxy-2,15-dimethyltetracyclo[8.7,,heptadecan-14-one	C19H30O4	M-H	321.2071	-2.6
	HMDB0185973	(2S,15S)-14,17-dihydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7,,heptadecan-5-one	C19H30O4	M-H	321.2071	-2.6
	HMDB0185971	(2S,15S)-13,14,17-trihydroxy-2,15-dimethyltetracyclo[8.7,,heptadecan-5-one	C19H30O4	M-H	321.2071	-2.6

	HMDB0185972	(2R,15S)-14,17-dihydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-5-one	C19H30O4	M-H	321.2071	-2.6
	HMDB0185970	(2S,15S)-8,14,17-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-one	C19H30O4	M-H	321.2071	-2.6
	HMDB0159845	(1S,2R,S,11S,15S)-2,15-dimethyltetracyclo[8.7.,heptadec-7-ene-5,13,14,17-tetrol	C19H30O4	M-H	321.2071	-2.6
	HMDB0156607	(2S,15R)-5,13-dihydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-3-one	C19H30O4	M-H	321.2071	-2.6
	HMDB0156608	(2S,15S)-5,13-dihydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadecan-3-one	C19H30O4	M-H	321.2071	-2.6
	HMDB0156606	(2R,15R)-5,8,13-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-3-one	C19H30O4	M-H	321.2071	-2.6
	HMDB0154834	(2S,15S)-5,17-dihydroxy-15-(hydroxymethyl)-2-methyltetracyclo[8.7.,heptadecan-14-one	C19H30O4	M-H	321.2071	-2.6
	HMDB0154833	(2R,15S)-5,17-dihydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-14-one	C19H30O4	M-H	321.2071	-2.6
	HMDB0154829	(2R,15S)-5,9-dihydroxy-2-(hydroxymethyl)-15-methyltetracyclo[8.7.,heptadecan-14-one	C19H30O4	M-H	321.2071	-2.6
	HMDB0154831	(2S,15S)-5,8,17-trihydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-14-one	C19H30O4	M-H	321.2071	-2.6
321.2427	HMDB0005830	5a-Androstan-3b-ol	C19H32O	M+FA-H	321.2435	-2.5
	HMDB0185647	(8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-8,11-dienoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0185636	(8Z,14Z)-7-hydroxyicosa-8,11,14-trienoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0062290	12r-hetre	C20H34O3	M-H	321.2435	-2.5
	HMDB0062747	12(S)-HETrE	C20H34O3	M-H	321.2435	-2.5
	HMDB0112091	7-(5-heptyl-3,4-dimethylfuran-2-yl)heptanoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0185648	(8Z,11Z,14Z)--hydroxyicosa-8,11,14-trienoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0185650	(8Z,11Z,14Z)-2-hydroxyicosa-8,11,14-trienoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0185646	CHEMBL132396	C20H34O3	M-H	321.2435	-2.5
	HMDB0185643	(8Z,14Z)-11-hydroxyicosa-8,12,14-trienoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0185645	(11Z,14Z)-8,9-Epoxy-11,14-icosadienoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0185644	(8Z,11Z,14Z)-19-hydroxyicosa-8,11,14-trienoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0185642	15-Hetre	C20H34O3	M-H	321.2435	-2.5
	HMDB0185641	(11Z,14Z)-8-hydroxyicosa-9,11,14-trienoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0185639	(8Z,11Z,14Z)-13-hydroxyicosa-8,11,14-trienoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0185640	(8Z,E,14Z)-12-hydroxyicosa-8,,14-trienoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0185637	(8Z,11Z,14Z)-16-hydroxyicosa-8,11,14-trienoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0185638	(8Z,11Z,14Z)--hydroxyicosa-8,11,14-trienoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0112104	9-(5-hexyl-3-methylfuran-2-yl)nonanoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0061647	3,鈇?-鈇婦imethyl-鈇?-鈇嫗ropyl-2-鈇嫗uranundecanoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0061645	3,4-Dimethyl-5-pentyl-2-furannonanoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0060052	8-HETrE	C20H34O3	M-H	321.2435	-2.5
	HMDB0005045	15(S)-Hydroxyeicosatrienoic acid	C20H34O3	M-H	321.2435	-2.5
	HMDB0036802	Austroinulin	C20H34O3	M-H	321.2435	-2.5
323.0285	HMDB0015380	Olsalazine	C14H10N2O6	M+Na-2H	323.0286	-0.2
	HMDB0156309	286-43-3	C9H13N2O9P	M-H	323.0286	-0.3
	HMDB0060282	Uridine 3'-monophosphate	C9H13N2O9P	M-H	323.0286	-0.3
	HMDB0011641	Uridine 2'-phosphate	C9H13N2O9P	M-H	323.0286	-0.3
	HMDB0001271	Pseudouridine 5'-phosphate	C9H13N2O9P	M-H	323.0286	-0.3
	HMDB0000288	Uridine 5'-monophosphate	C9H13N2O9P	M-H	323.0286	-0.3
	HMDB0015216	Emedastine	C17H26N4O	M+Na-2H	323.1853	0.5
	HMDB0062618	2,3-dinor-6-oxoprostaglandin F1alpha	C18H30O6	M-H20-H	323.1858	-1.1
	HMDB0061154	Monic acid	C18H30O6	M-H20-H	323.1858	-1.1
	HMDB0002277	2,3-Dinor-6-keto-prostaglandin F1 a	C18H30O6	M-H20-H	323.1858	-1.1
	HMDB0038940	(-)-11-Hydroxy-9,15,16-trioxooctadecanoic acid	C18H30O6	M-H20-H	323.1858	-1.1
	HMDB0002904	2,3-Dinor-TXB2	C18H30O6	M-H20-H	323.1858	-1.1

323.1855	HMDB0137260	4-[(4E)-3-hydroxydec-4-en-1-yl]-2-methoxyphenol	C17H26O3	M+FA-H	323.1864	-2.8
	HMDB0137271	4-[(1E)-3-hydroxydec-1-en-1-yl]-2-methoxyphenol	C17H26O3	M+FA-H	323.1864	-2.8
	HMDB0168551	(2E,7E)-1-(oxiran-2-yl)pentadeca-2,7-dien-4-yne-1,6-diol	C17H26O3	M+FA-H	323.1864	-2.8
	HMDB0168550	(8E,13E)-heptadeca-8,13,16-trien-11-yne-2,,15-triol	C17H26O3	M+FA-H	323.1864	-2.8
	HMDB0168549	(4E,9E)-heptadeca-1,4,9-trien-6-yne-3,8,11-triol	C17H26O3	M+FA-H	323.1864	-2.8
	HMDB0168552	(4E)-1-[3-(1-hydroxyprop-2-en-1-yl)oxiran-2-yl]dodec-4-en-1-yn-3-ol	C17H26O3	M+FA-H	323.1864	-2.8
	HMDB0168554	(8E,13E)-heptadeca-8,13,16-trien-11-yne-1,,15-triol	C17H26O3	M+FA-H	323.1864	-2.8
	HMDB0168553	(4E)-1-(3-heptyloxiran-2-yl)octa-4,7-dien-2-yne-1,6-diol	C17H26O3	M+FA-H	323.1864	-2.8
	HMDB0030974	8-Acetoxy-4-acoren-3-one	C17H26O3	M+FA-H	323.1864	-2.8
	HMDB0030801	[6]-Paradol	C17H26O3	M+FA-H	323.1864	-2.8
	HMDB0031928	Panaxytriol	C17H26O3	M+FA-H	323.1864	-2.8
	HMDB0039251	Panaxacol	C17H26O3	M+FA-H	323.1864	-2.8
	HMDB0038580	Cibacic acid	C18H28O5	M-H	323.1864	-2.8
	HMDB0180021	(4-hydroxy-3,5-dimethoxyphenyl)methyl 7-methyloctanoate	C18H28O5	M-H	323.1864	-2.8
	HMDB0180098	(4-hydroxy-3-methoxyphenyl)methyl 8-hydroxy-8-methylnonanoate	C18H28O5	M-H	323.1864	-2.8
	HMDB0180099	(4-hydroxy-3-methoxyphenyl)methyl 9-hydroxy-8-methylnonanoate	C18H28O5	M-H	323.1864	-2.8
	HMDB0180100	(4-hydroxy-3-methoxyphenyl)methyl 2-hydroxy-8-methylnonanoate	C18H28O5	M-H	323.1864	-2.8
	HMDB0180102	(3,4-dihydroxy-5-methoxyphenyl)methyl 8-methylnonanoate	C18H28O5	M-H	323.1864	-2.8
	HMDB0033631	Lactapiperanol D	C18H28O5	M-H	323.1864	-2.8
323.2220	HMDB0040901	13-Hydroxy-9-methoxy--oxo-11-octadecenoic acid	C19H34O5	M-H2O-H	323.2222	-0.7
	HMDB0175409	(5E,9Z)-8-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0175410	(5E,9Z)-12-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0175412	(5E)-6-methyl-8-[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]oct-5-en-2-one	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0175413	(5E,9Z)-12-(3,3-dimethyloxiran-2-yl)-6,-dimethyldodeca-5,9-dien-2-one	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0175415	(5E,9Z)-3-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0175414	(5E,9Z)-1-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0175411	4-{3-[(3Z)-4,8-dimethylnona-3,7-dien-1-yl]-3-methyloxiran-2-yl}butan-2-one	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0175408	(5E,9Z)-4-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0175406	(5E,9Z)-15-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0160594	(z,z)-9,12,17-octadecatrienoic acid	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0173892	(9E,12Z)-octadeca-9,12,17-trienoic acid	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0175403	(5Z,9Z)-6-(hydroxymethyl)-,14-dimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0175402	(5E,9Z)-7-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0175404	(5E,9Z)-11-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0175405	(5E,9E)--(hydroxymethyl)-6,14-dimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0175407	(5E,9Z,13E)-15-hydroxy-6,,14-trimethylpentadeca-5,9,13-trien-2-one	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0001388	alpha-Linolenic acid	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0003073	gamma-Linolenic acid	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0030964	Linolenelaidic acid	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0030962	Calendic acid	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0030963	alpha-Eleostearic acid	C18H30O2	M+FA-H	323.2228	-2.4
	HMDB0031007	1-Acetoxy-2-hydroxy-16-heptadecyn-4-one	C19H32O4	M-H	323.2228	-2.4
	HMDB0164465	1-(4-hydroxy-3-methoxyphenyl)dodecane-3,5-diol	C19H32O4	M-H	323.2228	-2.4

323.2583	HMDB0033609	2-Pentadecylfuran	C19H34O	M+FA-H	323.2592	-2.7
	HMDB0029797	(Z)-15-Oxo-11-eicosenoic acid	C20H36O3	M-H	323.2592	-2.7
	HMDB0034958	(13R,14R)-7-Labdene-13,14,15-triol	C20H36O3	M-H	323.2592	-2.7
	HMDB0034957	(13R,14R)-8-Labdene-13,14,15-triol	C20H36O3	M-H	323.2592	-2.7
325.2743	HMDB0031923	,,-Dihydroxyeicosanoic acid	C20H40O4	M-H2O-H	325.2743	0.1
	HMDB0072846	MG(i-17)	C20H40O4	M-H2O-H	325.2743	0.1
	HMDB0072848	MG(a-17)[rac]	C20H40O4	M-H2O-H	325.2743	0.1
	HMDB0072852	MG(i-17)	C20H40O4	M-H2O-H	325.2743	0.1
	HMDB0072851	MG(a-17)[rac]	C20H40O4	M-H2O-H	325.2743	0.1
	HMDB0240306	Mg(17)[rac]	C20H40O4	M-H2O-H	325.2743	0.1
	HMDB0072856	MG(17)	C20H40O4	M-H2O-H	325.2743	0.1
	HMDB0072875	MG/17)	C20H40O4	M-H2O-H	325.2743	0.1
	HMDB0034496	6,,14-Trimethyl-2-methylenepentadecanal	C19H36O	M+FA-H	325.2748	-1.6
	HMDB0172579	(11E)-19-hydroxyicos-11-enoic acid	C20H38O3	M-H	325.2748	-1.6
	HMDB0172577	13-hydroxyicos-11-enoic acid	C20H38O3	M-H	325.2748	-1.6
	HMDB0172578	(11E)--hydroxyicos-11-enoic acid	C20H38O3	M-H	325.2748	-1.6
	HMDB0172580	11,12-Epoxyicosanoic acid	C20H38O3	M-H	325.2748	-1.6
	HMDB0172582	SCHEMBL19404	C20H38O3	M-H	325.2748	-1.6
	HMDB0172581	(11E)--hydroxyicos-11-enoic acid	C20H38O3	M-H	325.2748	-1.6
326.0653	HMDB0029839	UNII-9F6RS28Y	C15H15NO6	M+Na-2H	326.0646	2.1
326.1008	HMDB0031929	Zanthodioline	C16H19NO5	M+Na-2H	326.1010	-0.6
327.2170	HMDB0029885	Sorbitan laurate	C18H34O6	M-H2O-H	327.2171	-0.5
	HMDB0038483	Auxin a	C18H32O5	M-H	327.2177	-2.1
	HMDB0061377	2,3-Dinor-8iso prostaglandin F2alpha	C18H32O5	M-H	327.2177	-2.1
	HMDB0035919	Corchorifatty acid F	C18H32O5	M-H	327.2177	-2.1
	HMDB0040611	(9R,S,12Z)-9,-Dihydroxy-8-oxo-12-octadecenoic acid	C18H32O5	M-H	327.2177	-2.1
327.2326	HMDB0036722	ent-17-Acetoxy-16b-kauran-19-al	C22H34O3	M-H2O-H	327.2324	0.6
	HMDB0034944	Siderol	C22H34O3	M-H2O-H	327.2324	0.6
	HMDB0041302	(R)-3,4-Dihydro-8-hydroxy-3-tridecyl-1H-2-benzopyran-1-one	C22H34O3	M-H2O-H	327.2324	0.6
	HMDB0041001	Volemolide	C22H34O3	M-H2O-H	327.2324	0.6
	HMDB0033897	Ginkgoic acid	C22H34O3	M-H2O-H	327.2324	0.6
	HMDB0031465	Methyl-[-]-shogaol	C22H34O3	M-H2O-H	327.2324	0.6
	HMDB0035185	Retinol acetate	C22H32O2	M-H	327.2330	-1.1
	HMDB0167219	2-methoxy-4-[(8E,11E)-pentadeca-8,11,14-trien-1-yl]phenol	C22H32O2	M-H	327.2330	-1.1
	HMDB0167215	2-methoxy-3-[(8E,11E)-pentadeca-8,11,14-trien-1-yl]phenol	C22H32O2	M-H	327.2330	-1.1
	HMDB0002183	Docosahexaenoic acid	C22H32O2	M-H	327.2330	-1.1
	HMDB0030446	Grifolin	C22H32O2	M-H	327.2330	-1.1
	HMDB0038908	(Z,Z)-2-Methyl-5-(8,11,14-pentadecatrienyl)-1,3-benzenediol	C22H32O2	M-H	327.2330	-1.1
	HMDB0030053	Neogrifolin	C22H32O2	M-H	327.2330	-1.1
	HMDB0062579	6217-54-5	C22H32O2	M-H	327.2330	-1.1
328.0579	HMDB0000125	Glutathione	C10H17N3O6S	M+Na-2H	328.0585	-1.7
	HMDB0062697	gamma-Glutamylcysteinylglycine	C10H17N3O6S	M+Na-2H	328.0585	-1.7
329.0285	HMDB0000175	Inosinic acid	C10H13N4O8P	M-H2O-H	329.0287	-0.6
	HMDB0011681	Inosine 2'-phosphate	C10H13N4O8P	M-H2O-H	329.0287	-0.6
	HMDB0155745	Disodium inosinate	C10H13N4O8P	M-H2O-H	329.0287	-0.6
	HMDB0014910	Malathion	C10H19O6PS2	M-H	329.0288	-0.9
	HMDB0011680	Coproporphyrinogen I	C10H11N4O7P	M-H	329.0293	-2.3
	HMDB0112073	12,15-epoxy-13,14-dimethyleicosa-12,14,16-trienoic acid	C22H36O3	M-H2O-H	329.2481	-1.1
	HMDB0112069	(E)-11-(3,4-dimethyl-5-pentylfuran-2-yl)undec--enoic acid	C22H36O3	M-H2O-H	329.2481	-1.1
	HMDB0029683	2-Hydroxy-6-pentadecylbenzoic acid	C22H36O3	M-H2O-H	329.2481	-1.1
	HMDB0036801	ent-16b,19-Kauranediol 19-acetate	C22H36O3	M-H2O-H	329.2481	-1.1
	HMDB0035477	Tridecyl phloretate	C22H36O3	M-H2O-H	329.2481	-1.1

329.2477	HMDB0035581	1-Phenyl-1,3-hexadecanedione	C22H34O2	M-H	329.2486	-2.7
	HMDB0039133	4,8,12,15,19-Docosapentaenoic acid	C22H34O2	M-H	329.2486	-2.7
	HMDB0006528	Docosapentaenoic acid (22n-3)	C22H34O2	M-H	329.2486	-2.7
	HMDB0032257	Ethyl abietate	C22H34O2	M-H	329.2486	-2.7
	HMDB0035024	ent-16-Kauren-19-ol acetate	C22H34O2	M-H	329.2486	-2.7
	HMDB0039530	Ethyl icosapentate	C22H34O2	M-H	329.2486	-2.7
	HMDB0038909	2-Methyl-5-(8,11-pentadecadienyl)-1,3-benzenediol	C22H34O2	M-H	329.2486	-2.7
	HMDB0001976	Docosapentaenoic acid (22n-6)	C22H34O2	M-H	329.2486	-2.7
	HMDB0060113	Docosapentaenoic acid (22n-6)	C22H34O2	M-H	329.2486	-2.7
330.9991	HMDB0031781	O-Ethyl S,S-diphenyl phosphorodithioate	C14H15O2PS ₂	M+Na-2H	330.9998	-2.0
331.2641	HMDB0185130	(13Z,16Z,19Z)-docosa-13,16,19,21-tetraenoic acid	C22H36O2	M-H	331.2643	-0.5
	HMDB0062725	ethyl (5Z,8Z,14Z)-icosa-5,8,11,14-tetraenoate	C22H36O2	M-H	331.2643	-0.5
	HMDB0035677	3-Hydroxy-1-phenyl-1-hexadecanone	C22H36O2	M-H	331.2643	-0.5
	HMDB0035676	1-Hydroxy-1-phenyl-3-hexadecanone	C22H36O2	M-H	331.2643	-0.5
	HMDB0002226	Adrenic acid	C22H36O2	M-H	331.2643	-0.5
	HMDB0062580	Adrenic acid	C22H36O2	M-H	331.2643	-0.5
	HMDB0038910	2-Methyl-5-(8-pentadecenyl)-1,3-benzenediol	C22H36O2	M-H	331.2643	-0.5
	HMDB0185119	(13Z,16Z,19Z)-21-hydroxydocosa-13,16,19-trienoic acid	C22H38O3	M-H2O-H	331.2637	1.2
	HMDB0185118	(13Z,16Z,19Z)-12-hydroxydocosa-13,16,19-trienoic acid	C22H38O3	M-H2O-H	331.2637	1.2
	HMDB0185124	(13Z,16Z,18E)--hydroxydocosa-13,16,18-trienoic acid	C22H38O3	M-H2O-H	331.2637	1.2
	HMDB0112078	13-(3,4-dimethyl-5-propylfuran-2-yl)-tridecanoic acid	C22H38O3	M-H2O-H	331.2637	1.2
	HMDB0185121	(13Z,16Z,19Z)-18-hydroxydocosa-13,16,19-trienoic acid	C22H38O3	M-H2O-H	331.2637	1.2
	HMDB0185131	(13Z,16Z,19Z)-2-hydroxydocosa-13,16,19-trienoic acid	C22H38O3	M-H2O-H	331.2637	1.2
	HMDB0185129	(13Z,16Z,19Z)-22-hydroxydocosa-13,16,19-trienoic acid	C22H38O3	M-H2O-H	331.2637	1.2
	HMDB0185125	(13Z,19Z)-16-hydroxydocosa-13,17,19-trienoic acid	C22H38O3	M-H2O-H	331.2637	1.2
	HMDB0185123	(16Z,19Z)-13-hydroxydocosa-14,16,19-trienoic acid	C22H38O3	M-H2O-H	331.2637	1.2
	HMDB0185127	(13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadec-13-enoic acid	C22H38O3	M-H2O-H	331.2637	1.2
	HMDB0185120	(13Z,16Z,19Z)-15-hydroxydocosa-13,16,19-trienoic acid	C22H38O3	M-H2O-H	331.2637	1.2
	HMDB0185122	(13Z,15E,19Z)-17-hydroxydocosa-13,15,19-trienoic acid	C22H38O3	M-H2O-H	331.2637	1.2
	HMDB0185126	12-{3-[(2Z,5Z)-octa-2,5-dien-1-yl]oxiran-2-yl}dodecanoic acid	C22H38O3	M-H2O-H	331.2637	1.2
	HMDB0185128	(13Z,16Z)-18-(3-ethyloxiran-2-yl)octadeca-13,16-dienoic acid	C22H38O3	M-H2O-H	331.2637	1.2
	HMDB0031126	3,4-Dimethyl-5-pentyl-2-furanundecanoic acid	C22H38O3	M-H2O-H	331.2637	1.2
333.0590	HMDB0183406	3,4,5-trihydroxy-6-(2-methylbenzoyloxy)oxane-2-carboxylic acid	C14H16O8	M+Na-2H	333.0592	-0.5
	HMDB0167833	6-(4-acetylphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O8	M+Na-2H	333.0592	-0.5
	HMDB0167831	6-(3-acetylphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O8	M+Na-2H	333.0592	-0.5
	HMDB0140804	3,4,5-trihydroxy-6-[(2-phenylacetyl)oxy]oxane-2-carboxylic acid	C14H16O8	M+Na-2H	333.0592	-0.5
	HMDB0128031	6-(3-ethenyl-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O8	M+Na-2H	333.0592	-0.5
	HMDB0126430	6-(2-ethenyl-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O8	M+Na-2H	333.0592	-0.5
	HMDB0126429	6-(4-ethenyl-3-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O8	M+Na-2H	333.0592	-0.5
	HMDB0124977	6-(5-ethenyl-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O8	M+Na-2H	333.0592	-0.5
	HMDB0124976	6-(4-ethenyl-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H16O8	M+Na-2H	333.0592	-0.5
	HMDB0011649	Glycerophosphoinositol	C9H19O11P	M-H	333.0592	-0.7
	HMDB0060420	7-Hydroxymethyl-12-methylbenz[a]anthracene sulfate	C20H16O4S	M-H2O-H	333.0585	1.4
	HMDB0062291	13,14-dihydro-15-oxolipoxin A4	C20H32O5	M-H2O-H	333.2066	-0.9

HMDB0062798	(6E,8Z,11Z)-5-hydroperoxy-15-hydroxyicosa-6,8,11,13-tetraenoic acid	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0186062	7-{2-[3-(1-hydroxyhexyl)oxiran-2-yl]-5-oxocyclopent-1-en-1-yl}heptanoic acid	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0186065	7-{4-hydroxy-2-[(1E)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopent-1-en-1-yl}heptanoic acid	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0004385	Lipoxin A4	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0186064	7-{2-[(1E)-3,8-dihydroxyoct-1-en-1-yl]-5-oxocyclopent-1-en-1-yl}heptanoic acid	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0004240	15-Keto-prostaglandin F2a	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0186066	2-hydroxy-7-{2-[(1E)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopent-1-en-1-yl}heptanoic acid	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0164486	5-hydroxy-1-(4-hydroxy-3,5-dimethoxyphenyl)dodecan-3-one	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0002776	13,14-Dihydro-15-keto-PGE2	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0062691	7-[3-hydroxy-5-oxo-2-(3-oxooct-1-en-1-yl)cyclopentyl]heptanoic acid	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0062299	(5S,6E,8E,Z,14R,15S)-5,14,15-trihydroxyicosa-6,8,,12-tetraenoic acid	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0002400	Levuglandin D2	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0035338	Sterebin B	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0186060	7-{3-hydroxy-2-[(1E)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopent-1-en-1-yl}heptanoic acid	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0036756	Acorusnol	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0186061	7-{2-[(1E)-3,7-dihydroxyoct-1-en-1-yl]-5-oxocyclopent-1-en-1-yl}heptanoic acid	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0186063	7-{5-[(1E)-3-hydroxyoct-1-en-1-yl]-2-oxo-6-oxabicyclo[3.1]hexan-1-yl}heptanoic acid	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0005844	8-isoprostaglandin E2	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0005082	Lipoxin B4	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0186059	7-hydroxy-7-{2-[(1E)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopent-1-en-1-yl}heptanoic acid	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0005077	8-iso-15-keto-PGF2a	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0035339	Sterebin C	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0002363	Levuglandin E2	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0012481	(5Z)-(15S)-11alpha-Hydroxy-9,15-dioxoprostanoate	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0060041	11b-PGE2	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0034676	Cinnassiol D1	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0035064	Cinnassiol D4	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0001403	Prostaglandin D2	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0001220	Prostaglandin E2	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0060042	13,14-Dihydro-15-keto-PGD2	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0001509	-Hydroxy-leukotriene B4	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0001452	Thromboxane A2	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0002122	Prostaglandin F3a	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0002132	8-iso-PGF3a	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0012564	13,14-Dihydro-15-oxo-lipoxin A4	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0001381	Prostaglandin H2	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0001335	Prostaglandin I2	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0012587	15-Epi-lipoxin A4	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0001320	(13E)-11a-Hydroxy-9,15-dioxoprost-13-enoic acid	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0183411	(5Z)-7-[3-hydroxy-5-oxo-2-(3-oxooctyl)cyclopentyl]hept-5-enoic acid	C20H32O5	M-H2O-H	333.2066	-0.9
HMDB0174394	15-(hydroxymethyl)-2-methyltetracyclo-heptadec-13-en-5-one	C19H28O2	M+FA-H	333.2071	-2.5
HMDB0000628	Epitestosterone	C19H28O2	M+FA-H	333.2071	-2.5
HMDB0036205	alpha-Amylcinnamyl isovalerate	C19H28O2	M+FA-H	333.2071	-2.5
HMDB0000077	Dehydroepiandrosterone	C19H28O2	M+FA-H	333.2071	-2.5
HMDB0000899	Androstenedione	C19H28O2	M+FA-H	333.2071	-2.5
HMDB0006035	4-Dihydroboldenone	C19H28O2	M+FA-H	333.2071	-2.5
HMDB0005962	Dehydroandrosterone	C19H28O2	M+FA-H	333.2071	-2.5
HMDB0003769	Etiocholanedione	C19H28O2	M+FA-H	333.2071	-2.5
HMDB0154975	(+)-testosterone	C19H28O2	M+FA-H	333.2071	-2.5
HMDB0155214	(2S,15S)-2,15-dimethyl-14-oxotetracyclo[8.7,,heptadecan-7-yl]ium-5-olate	C19H28O2	M+FA-H	333.2071	-2.5

	HMDB0154974	AC1L45JX	C19H28O2	M+FA-H	333.2071	-2.5
	HMDB0154835	Androstane-3,17-dione	C19H28O2	M+FA-H	333.2071	-2.5
	HMDB0000234	Testosterone	C19H28O2	M+FA-H	333.2071	-2.5
	HMDB0062298	15-deoxy-delta-12,14-pgd2	C20H30O4	M-H	333.2071	-2.5
	HMDB0062423	(6E,8Z,12S,14Z)-12-hydroxy-5-oxoicosa-6,8,,14-tetraenoic acid	C20H30O4	M-H	333.2071	-2.5
	HMDB0012850	7'-Carboxy-gamma-chromanol	C20H30O4	M-H	333.2071	-2.5
	HMDB0062486	(6E,8E,E,14E,17E)-5,12-dihydroxyicosa-6,8,,14,17-pentaenoic acid	C20H30O4	M-H	333.2071	-2.5
	HMDB0036763	(ent-6alpha,7alpha)-6,7-Dihydroxy-16-kauren-19-oic acid	C20H30O4	M-H	333.2071	-2.5
	HMDB0036828	Dehydronifolic acid	C20H30O4	M-H	333.2071	-2.5
	HMDB0041055	Phytocassane B	C20H30O4	M-H	333.2071	-2.5
	HMDB0035286	Crispanone	C20H30O4	M-H	333.2071	-2.5
	HMDB0036760	Verimol D	C20H30O4	M-H	333.2071	-2.5
	HMDB0001244	15-Keto-13,14-dihydroprostaglandin A2	C20H30O4	M-H	333.2071	-2.5
	HMDB0002710	Prostaglandin J2	C20H30O4	M-H	333.2071	-2.5
	HMDB0004234	12-Keto-leukotriene B4	C20H30O4	M-H	333.2071	-2.5
	HMDB0004236	Prostaglandin B2	C20H30O4	M-H	333.2071	-2.5
	HMDB0004238	Delta-12-Prostaglandin J2	C20H30O4	M-H	333.2071	-2.5
	HMDB0005073	Leukotriene B5	C20H30O4	M-H	333.2071	-2.5
	HMDB0035878	8alpha-8-Hydroxy-12-oxo-13-abieten-18-oic acid	C20H30O4	M-H	333.2071	-2.5
	HMDB0012824	5-Oxo-6-trans-leukotriene B4	C20H30O4	M-H	333.2071	-2.5
	HMDB0002752	Prostaglandin A2	C20H30O4	M-H	333.2071	-2.5
	HMDB0062524	Prostaglandin A2	C20H30O4	M-H	333.2071	-2.5
	HMDB0060046	15d PGD2	C20H30O4	M-H	333.2071	-2.5
	HMDB0060054	bicyclo-PGE2	C20H30O4	M-H	333.2071	-2.5
	HMDB0060095	Prostaglandin-c2	C20H30O4	M-H	333.2071	-2.5
	HMDB0061111	5,6-Epoxytetraene	C20H30O4	M-H	333.2071	-2.5
333.2790	HMDB0040180	Pentadecylbenzene	C21H36	M+FA-H	333.2799	-2.7
	HMDB0005943	5b-Pregnanediol	C21H36	M+FA-H	333.2799	-2.7
	HMDB0167408	2-methoxy-4-pentadecylphenol	C22H38O2	M-H	333.2799	-2.7
	HMDB0002823	Docosatrienoic acid	C22H38O2	M-H	333.2799	-2.7
	HMDB0031099	(all-Z)-7,,13-Docosatrienoic acid	C22H38O2	M-H	333.2799	-2.7
	HMDB0167412	2-methoxy-3-pentadecylphenol	C22H38O2	M-H	333.2799	-2.7
335.1854	HMDB0137392	SCHEMBL19369293	C18H26O3	M+FA-H	335.1864	-3.0
	HMDB0137383	(4E)-1-(3,4-dihydroxyphenyl)dodec-4-en-3-one	C18H26O3	M+FA-H	335.1864	-3.0
	HMDB0031098	(9Z,11E,13E,15Z)-4-Oxo-9,11,13,15-octadecatetraenoic acid	C18H26O3	M+FA-H	335.1864	-3.0
	HMDB0061861	Octyl 4-methoxycinnamic acid	C18H26O3	M+FA-H	335.1864	-3.0
	HMDB0180077	(4-hydroxy-3,5-dimethoxyphenyl)methyl (6E)-8-methylnon-6-enoate	C19H28O5	M-H	335.1864	-3.0
	HMDB0012563	13,14-Dihydro- lipoxin A4	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0013041	Prostaglandin H1	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0060045	15-keto-PGF1alpha	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0060107	(5Z,9E,12S,14Z)-8,11,12-Trihydroxyicosa-5,9,14-trienoate	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0004694	11,14,15-THETA	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0002115	8-isoprostaglandin PGF2b	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0001977	Trioxilin A3	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0005083	8-Isoprostaglandin F2a	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0001442	Prostaglandin E1	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0001965	Troxilin B3	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0004684	11,12,15-THETA	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0004685	13,14-dihydro-15-keto-PGF2alpha	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0062278	(5E,13E)-11,12,15-trihydroxyicosa-5,8,13-trienoic acid	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0004686	8-Isoprostaglandin E1	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0001483	Prostaglandin F2b	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0001139	Prostaglandin F2a	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0183703	(5Z)-8-acetyl-12-hydroxy-9-(hydroxymethyl)heptadeca-5,-dienoic acid	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0184338	(5Z,E)-9-acetyl-12-hydroxy-8-(hydroxymethyl)heptadeca-5,-dienoic acid	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0011137	11-Epi-PGF2a	C20H34O5	M-H2O-H	335.2222	-0.7
	HMDB0035380	Sterebin G	C20H34O5	M-H2O-H	335.2222	-0.7

335.2220

HMDB0010199	11b-PGF2a	C20H34O5	M-H20-H	335.2222	-0.7
HMDB0010170	11,12,15-TriHETE	C20H34O5	M-H20-H	335.2222	-0.7
HMDB0005102	Prostaglandin D1	C20H34O5	M-H20-H	335.2222	-0.7
HMDB0006562	8-iso-13,14-dihydro-15-keto-PGF2a	C20H34O5	M-H20-H	335.2222	-0.7
HMDB0155964	4-Androstene-3,17-diol	C19H30O2	M+FA-H	335.2228	-2.3
HMDB0062608	5beta-Dihydroepitestosterone	C19H30O2	M+FA-H	335.2228	-2.3
HMDB0000546	Epitiocholanolone	C19H30O2	M+FA-H	335.2228	-2.3
HMDB0037711	4-Methylphenyl dodecanoate	C19H30O2	M+FA-H	335.2228	-2.3
HMDB0000031	Androsterone	C19H30O2	M+FA-H	335.2228	-2.3
HMDB0002961	Dihydrotestosterone	C19H30O2	M+FA-H	335.2228	-2.3
HMDB0000365	Epandrosterone	C19H30O2	M+FA-H	335.2228	-2.3
HMDB0003818	5-Androstenediol	C19H30O2	M+FA-H	335.2228	-2.3
HMDB0005849	4-Androstenediol	C19H30O2	M+FA-H	335.2228	-2.3
HMDB0000490	Etiocholanolone	C19H30O2	M+FA-H	335.2228	-2.3
HMDB0006770	5b-Dihydrotestosterone	C19H30O2	M+FA-H	335.2228	-2.3
HMDB0034686	(14S)-14,15-Dihydroxy-8(17),13(16)-labdadien-19-oic acid	C20H32O4	M-H	335.2228	-2.3
HMDB0062756	7-[2-(3-hydroxyoct-1-en-1-yl)-5-oxocyclopent-2-en-1-yl]heptanoic acid	C20H32O4	M-H	335.2228	-2.3
HMDB0010211	17,18-DiHETE	C20H32O4	M-H	335.2228	-2.3
HMDB0010216	5,15-DiHETE	C20H32O4	M-H	335.2228	-2.3
HMDB0010219	8,15-DiHETE	C20H32O4	M-H	335.2228	-2.3
HMDB0011135	5-HPETE	C20H32O4	M-H	335.2228	-2.3
HMDB0004693	11H-14,15-EETA	C20H32O4	M-H	335.2228	-2.3
HMDB0039441	ent-1()-Halimene-15,19-dioic acid	C20H32O4	M-H	335.2228	-2.3
HMDB0039171	9alpha-(3-Methylbutanoyloxy)-4S-hydroxy-(14)-oplopen-3-one	C20H32O4	M-H	335.2228	-2.3
HMDB0062687	(5Z,11Z,14Z)-8,-dihydroxyicosa-5,9,11,14-tetraenoic acid	C20H32O4	M-H	335.2228	-2.3
HMDB0062688	15-HPETE	C20H32O4	M-H	335.2228	-2.3
HMDB0062619	hepoxilin A3	C20H32O4	M-H	335.2228	-2.3
HMDB0062614	(6E,8E,11E,14E)-5,-dihydroxyicosa-6,8,11,14-tetraenoic acid	C20H32O4	M-H	335.2228	-2.3
HMDB0062615	5(S),11(R)-DiHETE	C20H32O4	M-H	335.2228	-2.3
HMDB0062479	(8Z)--hydroxy--[3(S)-3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl]deca-5,8-dienoic acid	C20H32O4	M-H	335.2228	-2.3
HMDB0062409	5,12-dihete	C20H32O4	M-H	335.2228	-2.3
HMDB0002982	Prostaglandin B1	C20H32O4	M-H	335.2228	-2.3
HMDB0004244	15(S)-HPETE	C20H32O4	M-H	335.2228	-2.3
HMDB0062749	(5S,6E,8Z,11Z,15R)-5,15-dihydroxyicosa-6,8,11,13-tetraenoic acid	C20H32O4	M-H	335.2228	-2.3
HMDB0002656	Prostaglandin A1	C20H32O4	M-H	335.2228	-2.3
HMDB0062684	ACMC-mf9i	C20H32O4	M-H	335.2228	-2.3
HMDB0185025	SCHEMBL115281	C20H32O4	M-H	335.2228	-2.3
HMDB0184817	(5Z)-7-{2-[(1E)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl}hept-5-enoic acid	C20H32O4	M-H	335.2228	-2.3
HMDB0169430	(2Z,6Z,Z)-4,14-dihydroxy-2,6,,14-tetramethylhexadeca-2,6,,15-tetraenoic acid	C20H32O4	M-H	335.2228	-2.3
HMDB0164511	SCHEMBL93593	C20H32O4	M-H	335.2228	-2.3
HMDB0001085	Leukotriene B4	C20H32O4	M-H	335.2228	-2.3
HMDB0001193	5(S)-Hydroperoxyeicosatetraenoic acid	C20H32O4	M-H	335.2228	-2.3
HMDB0002236	8-iso-PGA1	C20H32O4	M-H	335.2228	-2.3
HMDB0004243	12(S)-HPETE	C20H32O4	M-H	335.2228	-2.3
HMDB0005089	12(S)-Leukotriene B4	C20H32O4	M-H	335.2228	-2.3
HMDB0005088	6-trans-12-epi-Leukotriene B4	C20H32O4	M-H	335.2228	-2.3
HMDB0005087	6-trans-Leukotriene B4	C20H32O4	M-H	335.2228	-2.3
HMDB0005050	15H-11,12-EETA	C20H32O4	M-H	335.2228	-2.3
HMDB0004690	Hepoxilin B3	C20H32O4	M-H	335.2228	-2.3
HMDB0004688	Hepoxilin A3	C20H32O4	M-H	335.2228	-2.3
HMDB0004696	11(R)-HPETE	C20H32O4	M-H	335.2228	-2.3
HMDB0004692	12(R)-HPETE	C20H32O4	M-H	335.2228	-2.3
HMDB0004699	8(S)-HPETE	C20H32O4	M-H	335.2228	-2.3
HMDB0010204	14,15-DiHETE	C20H32O4	M-H	335.2228	-2.3
HMDB0060103	9-Deoxy-delta12-PGD2	C20H32O4	M-H	335.2228	-2.3
HMDB0060105	12,-DiHETE	C20H32O4	M-H	335.2228	-2.3

	HMDB0060104	Prostaglandin C1	C20H32O4	M-H	335.2228	-2.3
	HMDB0012498	,11-dihydro-12-oxo-LTB4	C20H32O4	M-H	335.2228	-2.3
	HMDB0012839	6,7-dihydro-5-oxo-12-epi-LTB4	C20H32O4	M-H	335.2228	-2.3
336.0503	HMDB0131410	2-({[2-(2H-1,3-benzodioxol-5-yl)-4-hydroxy-1-benzofuran-5-yl](hydroxy)methylidene}amino)acetic acid	C18H13NO7	M-H20-H	336.0508	-1.5
	HMDB0131405	2-({[2-(2H-1,3-benzodioxol-5-yl)-7-hydroxy-1-benzofuran-5-yl](hydroxy)methylidene}amino)acetic acid	C18H13NO7	M-H20-H	336.0508	-1.5
	HMDB0131400	2-({hydroxy[2-(6-hydroxy-2H-1,3-benzodioxol-5-yl)-1-benzofuran-5-yl]methylidene}amino)acetic acid	C18H13NO7	M-H20-H	336.0508	-1.5
	HMDB0131395	2-({[2-(2H-1,3-benzodioxol-5-yl)-6-hydroxy-1-benzofuran-5-yl]formamido}acetic acid	C18H13NO7	M-H20-H	336.0508	-1.5
	HMDB0240559	Sulforaphane-cysteine-glycine	C11H21N3O4S3	M-H20-H	336.0510	-2.2
337.2012	HMDB0041044	5,7-Megastigmadien-9-ol glucoside	C19H32O6	M-H20-H	337.2015	-0.9
	HMDB0173945	(11Z,13E)-2-hydroxyoctadeca-11,13-dien-9-ynoic acid	C18H28O3	M+FA-H	337.2020	-2.5
	HMDB0173944	(11Z,13E)-18-hydroxyoctadeca-11,13-dien-9-ynoic acid	C18H28O3	M+FA-H	337.2020	-2.5
	HMDB0173941	(11Z,13E)-17-hydroxyoctadeca-11,13-dien-9-ynoic acid	C18H28O3	M+FA-H	337.2020	-2.5
	HMDB0173942	-{3-[(1E)-hex-1-en-1-yl]oxiran-2-yl}dec-9-ynoic acid	C18H28O3	M+FA-H	337.2020	-2.5
	HMDB0173940	(11Z,13E)-15-hydroxyoctadeca-11,13-dien-9-ynoic acid	C18H28O3	M+FA-H	337.2020	-2.5
	HMDB0173943	(11Z)-12-(3-butyloxiran-2-yl)dodec-11-en-9-ynoic acid	C18H28O3	M+FA-H	337.2020	-2.5
	HMDB0038035	Panaquinquecol 1	C18H28O3	M+FA-H	337.2020	-2.5
	HMDB0040806	[7]-Paradol	C18H28O3	M+FA-H	337.2020	-2.5
	HMDB0030996	(2'E,4'Z,7'Z,8E)-Colnelenic acid	C18H28O3	M+FA-H	337.2020	-2.5
	HMDB0164470	4,5-dihydroxy-1-(4-hydroxy-3-methoxyphenyl)dodecan-3-one	C19H30O5	M-H	337.2020	-2.5
	HMDB0164466	5,11-dihydroxy-1-(4-hydroxy-3-methoxyphenyl)dodecan-3-one	C19H30O5	M-H	337.2020	-2.5
	HMDB0164469	2,5-dihydroxy-1-(4-hydroxy-3-methoxyphenyl)dodecan-3-one	C19H30O5	M-H	337.2020	-2.5
	HMDB0040567	[6]-Gingerdiol 5-acetate	C19H30O5	M-H	337.2020	-2.5
	HMDB0038720	Dodecyl gallate	C19H30O5	M-H	337.2020	-2.5
	HMDB0040566	[6]-Gingerdiol 3-acetate	C19H30O5	M-H	337.2020	-2.5
	HMDB0180125	(4-hydroxy-3,5-dimethoxyphenyl)methyl 8-methylnonanoate	C19H30O5	M-H	337.2020	-2.5
	HMDB0164467	5,12-dihydroxy-1-(4-hydroxy-3-methoxyphenyl)dodecan-3-one	C19H30O5	M-H	337.2020	-2.5
	HMDB0164462	1,5-dihydroxy-1-(4-hydroxy-3-methoxyphenyl)dodecan-3-one	C19H30O5	M-H	337.2020	-2.5
	HMDB0164464	5-hydroxy-1-(4',5'-dihydroxy-3'-methoxyphenyl)-dodecan-3-one	C19H30O5	M-H	337.2020	-2.5
337.2378	HMDB0002689	13,14-Dihydro PGE1	C20H36O5	M-H20-H	337.2379	-0.2
	HMDB0004239	13,14-Dihydro PGF2a	C20H36O5	M-H20-H	337.2379	-0.2
	HMDB0002685	Prostaglandin F1a	C20H36O5	M-H20-H	337.2379	-0.2
	HMDB0000383	3a,17a-Dihydroxy-5b-androstane	C19H32O2	M+FA-H	337.2384	-1.9
	HMDB0000458	5a-Androstane-3a,17a-diol	C19H32O2	M+FA-H	337.2384	-1.9
	HMDB0158029	HMS3372E	C19H32O2	M+FA-H	337.2384	-1.9
	HMDB0000495	PC(:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C19H32O2	M+FA-H	337.2384	-1.9
	HMDB0060437	Aldophosphamide	C19H32O2	M+FA-H	337.2384	-1.9
	HMDB0000369	3b,17b-Dihydroxyetiocholane	C19H32O2	M+FA-H	337.2384	-1.9
	HMDB0000551	Etiocholanediol	C19H32O2	M+FA-H	337.2384	-1.9
	HMDB0000554	Dihydroandrosterone	C19H32O2	M+FA-H	337.2384	-1.9
	HMDB0000493	5alpha-Androstane-3beta,17beta-diol	C19H32O2	M+FA-H	337.2384	-1.9
	HMDB0000412	3beta,17alpha-Dihydroxy-5alpha-androstane	C19H32O2	M+FA-H	337.2384	-1.9
	HMDB0159493	CHEMBL194858	C19H32O2	M+FA-H	337.2384	-1.9
	HMDB0184684	PGE1,11-DEOXY	C20H34O4	M-H	337.2384	-1.9
	HMDB0002265	14,15-DiHETrE	C20H34O4	M-H	337.2384	-1.9
	HMDB0002311	8,9-DiHETrE	C20H34O4	M-H	337.2384	-1.9
	HMDB0002314	11,12-DiHETrE	C20H34O4	M-H	337.2384	-1.9
	HMDB0002343	5,6-DHET	C20H34O4	M-H	337.2384	-1.9
	HMDB0002995	12-Keto-tetrahydro-leukotriene B4	C20H34O4	M-H	337.2384	-1.9

	HMDB0035379	Sterebin E	C20H34O4	M-H	337.2384	-1.9
	HMDB0012504	,11-dihydro-leukotriene B4	C20H34O4	M-H	337.2384	-1.9
	HMDB0012838	6,7-dihydro-12-epi-LTB4	C20H34O4	M-H	337.2384	-1.9
	HMDB0060106	15-Hydroperoxyeicosa-8Z,11Z,13E-trienoate	C20H34O4	M-H	337.2384	-1.9
337.3104	HMDB0061660	2(R)-hydroxydocosanoic acid	C22H44O3	M-H2O-H	337.3107	-0.8
	HMDB0062659	n-butyl oleate	C22H42O2	M-H	337.3112	-2.4
	HMDB0002068	Erucic acid	C22H42O2	M-H	337.3112	-2.4
	HMDB0002884	Cetoleic acid	C22H42O2	M-H	337.3112	-2.4
	HMDB0031013	Catelaic acid	C22H42O2	M-H	337.3112	-2.4
	HMDB0035569	4,6-Docosanedione	C22H42O2	M-H	337.3112	-2.4
	HMDB0035568	5,7-Docosanedione	C22H42O2	M-H	337.3112	-2.4
	HMDB0035567	6,8-Docosanedione	C22H42O2	M-H	337.3112	-2.4
	HMDB0035566	7,9-Docosanedione	C22H42O2	M-H	337.3112	-2.4
338.9887	HMDB0032470	Phytol acetate	C22H42O2	M-H	337.3112	-2.4
	HMDB0062191	1-phosphatidyl-1D-myo-inositol-3,4-bisphosphate	C6H14O12P2	M-H	338.9888	-0.2
	HMDB0001058	Fructose 1,6-bisphosphate	C6H14O12P2	M-H	338.9888	-0.2
	HMDB0060269	D-Mannose 1,6-bisphosphate	C6H14O12P2	M-H	338.9888	-0.2
	HMDB0006872	D-Tagatose 1,6-bisphosphate	C6H14O12P2	M-H	338.9888	-0.2
	HMDB0006234	D-myo-Inositol 1,3-bisphosphate	C6H14O12P2	M-H	338.9888	-0.2
	HMDB0000968	D-myo-Inositol 1,4-bisphosphate	C6H14O12P2	M-H	338.9888	-0.2
	HMDB0001047	D-Fructose 2,6-bisphosphate	C6H14O12P2	M-H	338.9888	-0.2
	HMDB0006235	D-myo-Inositol 3,4-bisphosphate	C6H14O12P2	M-H	338.9888	-0.2
	HMDB0003514	alpha-D-Glucose 1,6-bisphosphate	C6H14O12P2	M-H	338.9888	-0.2
	HMDB0060444	Fructose 1,6-bisphosphate	C6H14O12P2	M-H	338.9888	-0.2
	HMDB0062568	Inositol 1,4-diphosphate	C6H14O12P2	M-H	338.9888	-0.2
339.2172	HMDB0186497	(6Z,12Z)-5-hydroxyoctadeca-6,9,12-trienoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0186499	(6Z,9Z,12Z)-8-hydroxyoctadeca-6,9,12-trienoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0186501	(6Z,8E,12Z)--hydroxyoctadeca-6,8,12-trienoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0186503	13-hydroxy-6Z,9Z,11E-octadecatrienoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0186500	(6Z,9Z,12Z)-11-hydroxyoctadeca-6,9,12-trienoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0186502	(9Z,12Z)-6-hydroxyoctadeca-7,9,12-trienoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0186504	(6Z,12Z)-9-hydroxyoctadeca-6,,12-trienoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0186507	gamma- 9()-EpODE	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0186506	gamma- 6(7)-EpODE	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0186505	17-hydroxy-linolenic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0186510	(6Z,12Z)-2-hydroxyoctadeca-6,9,12-trienoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0186508	SCHEMBL14956948	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0186498	(6Z,9Z,12Z)-14-hydroxyoctadeca-6,9,12-trienoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0112099	8-(5-hexylfuran-2-yl)octanoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0062288	Gamma- 12(13)-epode	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0112103	9-(5-butyl-3-methylfuran-2-yl)nonanoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0112102	9-(5-pentylfuran-2-yl)-nonanoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0112093	5-heptylfuran-2-yl-heptanoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0004669	9-OxoODE	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0039603	3,4-Dimethyl-5-pentyl-2-furanheptanoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0061644	3,4-Dimethyl-5-propyl-2-furannonoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0030995	(2'E,4'Z,8E)-Colneleic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0031934	(9S,E,12Z,15Z)-9-Hydroxy-,12,15-octadecatrienoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0004668	13-OxoODE	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0010200	A-12(13)-EpODE	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0010203	13-HOTE	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0010206	15(16)-EpODE	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0010220	9()-EpODE	C18H30O3	M+FA-H	339.2177	-1.5

	HMDB0010224	9-HOTE	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0011108	17-Hydroxylinolenic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0030950	15,16-Epoxy-9,12-octadecadienoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0036832	Sterebin D	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0031103	2-Hydroxylinolenic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0029969	Squamostanal A	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0031088	12,13-Epoxy-9,15-octadecadienoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0034586	(9Z,12Z,14E)-16-Hydroxy-9,12,14-octadecatrienoic acid	C18H30O3	M+FA-H	339.2177	-1.5
	HMDB0029786	-Oxo-11-octadecen-13-olide	C18H30O3	M+FA-H	339.2177	-1.5
339.2535	HMDB0005076	13,14-Dihydro PGF-1a	C20H38O5	M-H2O-H	339.2535	-0.1
	HMDB0164373	15-(furan-2-yl)pentadecan-2-ol	C19H34O2	M+FA-H	339.2541	-1.7
	HMDB0164374	15-(furan-2-yl)pentadecan-1-ol	C19H34O2	M+FA-H	339.2541	-1.7
	HMDB0062132	Methyl linolelaidate	C19H34O2	M+FA-H	339.2541	-1.7
	HMDB0034381	Methyl linoleate	C19H34O2	M+FA-H	339.2541	-1.7
339.3262	HMDB0000944	Behenic acid	C22H44O2	M-H	339.3269	-1.9
	HMDB0040290	Butyl octadecanoate	C22H44O2	M-H	339.3269	-1.9
	HMDB0035655	8-Hydroxy-6-docosanone	C22H44O2	M-H	339.3269	-1.9
	HMDB0035667	4-Hydroxy-6-docosanone	C22H44O2	M-H	339.3269	-1.9
	HMDB0035660	5-Hydroxy-7-docosanone	C22H44O2	M-H	339.3269	-1.9
	HMDB0035651	6-Hydroxy-8-docosanone	C22H44O2	M-H	339.3269	-1.9
340.0459	HMDB0177036	(2Z)-2-{4-[(carboxyimino)(hydroxy)methyl]-2-hydroxyphenoxy}-3-(3-hydroxyphenyl)prop-2-enoic acid	C17H13NO8	M-H2O-H	340.0457	0.5
	HMDB0240534	Iberin-cysteine-glycine	C10H19N3O4S3	M-H	340.0465	-1.7
341.2330	HMDB0173890	12,13-epome(9)	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0062652	9-HODE	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0173893	(9E,12Z)-2-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0173887	(9E,12Z)-11-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0173888	alpha-artemismic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0173891	(9E,12Z)-18-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0173889	(9E,12Z)-17-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0173886	(9E,12Z)-14-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0173885	(9E,12Z)-8-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0160595	alpha-Hydroxylinoleic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0160592	17-hydroxylinoleic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0160591	(12Z)-9-hydroxyoctadeca-,12-dienoic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0160593	18-hydroxylinoleic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0160589	(9Z,12Z)-14-hydroxyoctadeca-9,12-dienoic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0160588	8-Hydroxylinoleic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0160590	11-Hode	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0112194	13-HODE	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0029796	(Z)-13-Oxo-9-octadecenoic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0029998	12-Hydroxy-8-,octadecadienoic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0029978	Avenoleic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0010223	9-HODE	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0004702	12,13-EpOME	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0004701	9-,Epoxyoctadecenoic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0004670	alpha-Dimorphecolic acid	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0004667	13-HODE	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0061708	13-HODE	C18H32O3	M+FA-H	341.2333	-1.0
	HMDB0040901	13-Hydroxy-9-methoxy--oxo-11-octadecenoic acid	C19H34O5	M-H	341.2333	-1.0
341.2698	HMDB0175453	15-hydroxy-6,,14-trimethyl-2-methylidenepentadecanal	C19H36O2	M+FA-H	341.2697	0.2
	HMDB0175452	-(hydroxymethyl)-6,14-dimethyl-2-methylidenepentadecanal	C19H36O2	M+FA-H	341.2697	0.2
	HMDB0175451	6-(hydroxymethyl)-,14-dimethyl-2-methylidenepentadecanal	C19H36O2	M+FA-H	341.2697	0.2
	HMDB0175450	2-(4,8,12-trimethyltridecyl)oxirane-2-carbaldehyde	C19H36O2	M+FA-H	341.2697	0.2
	HMDB0175447	-hydroxy-6,,14-trimethyl-2-methylidenepentadecanal	C19H36O2	M+FA-H	341.2697	0.2
	HMDB0175449	3-hydroxy-6,,14-trimethyl-2-methylidenepentadecanal	C19H36O2	M+FA-H	341.2697	0.2
	HMDB0175448	14-hydroxy-6,,14-trimethyl-2-methylidenepentadecanal	C19H36O2	M+FA-H	341.2697	0.2
	HMDB0175446	6-hydroxy-6,,14-trimethyl-2-methylidenepentadecanal	C19H36O2	M+FA-H	341.2697	0.2
	HMDB0175445	SCHEMBL7563427	C19H36O2	M+FA-H	341.2697	0.2
	HMDB0062658	(E)-nonadec--enoate	C19H35O2	M+FA-H	341.2697	0.2

	HMDB0035575	4,6-Nonadecanedione	C19H36O2	M+FA-H	341.2697	0.2
	HMDB0013622	Z-Nonadecenoic acid	C19H36O2	M+FA-H	341.2697	0.2
342.0588	HMDB0172138	3,4,5-trihydroxy-6-(isoquinolin-6-yloxy)oxane-2-carboxylic acid	C15H15NO7	M+Na-2H	342.0595	-2.1
	HMDB0165775	3,4,5-trihydroxy-6-(quinolin-6-yloxy)oxane-2-carboxylic acid	C15H15NO7	M+Na-2H	342.0595	-2.1
	HMDB0165774	3,4,5-trihydroxy-6-(quinolin-7-yloxy)oxane-2-carboxylic acid	C15H15NO7	M+Na-2H	342.0595	-2.1
	HMDB0165776	8-Hydroxyquinoline glucuronide	C15H15NO7	M+Na-2H	342.0595	-2.1
	HMDB0165777	3,4,5-trihydroxy-6-(quinolin-5-yloxy)oxane-2-carboxylic acid	C15H15NO7	M+Na-2H	342.0595	-2.1
	HMDB0172137	3,4,5-trihydroxy-6-(isoquinolin-7-yloxy)oxane-2-carboxylic acid	C15H15NO7	M+Na-2H	342.0595	-2.1
	HMDB0172139	3,4,5-trihydroxy-6-(isoquinolin-8-yloxy)oxane-2-carboxylic acid	C15H15NO7	M+Na-2H	342.0595	-2.1
342.0967	HMDB0032808	Niazirinin	C16H19NO6	M+Na-2H	342.0959	2.3
346.0552	HMDB0059594	2-hydroxy-dAMP	C10H14N5O7P	M-H	346.0558	-1.8
	HMDB0001044	2'-Deoxyguanosine 5'-monophosphate	C10H14N5O7P	M-H	346.0558	-1.8
	HMDB0011617	Adenosine 2'-phosphate	C10H14N5O7P	M-H	346.0558	-1.8
	HMDB0003540	3'-AMP	C10H14N5O7P	M-H	346.0558	-1.8
	HMDB0155033	Adenosine monophosphate	C10H14N5O7P	M-H	346.0558	-1.8
	HMDB0000045	Adenosine monophosphate	C10H14N5O7P	M-H	346.0558	-1.8
	HMDB0155034	Adenosine-3-phosphoric acid	C10H14N5O7P	M-H	346.0558	-1.8
	HMDB0062500	ZINC7257	C8H16NO9P	M+FA-H	346.0545	2.1
	HMDB0059626	N-acetyl-alpha-D-galactosamine 1-phosphate	C8H16NO9P	M+FA-H	346.0545	2.1
	HMDB0001062	N-Acetyl-D-Glucosamine 6-Phosphate	C8H16NO9P	M+FA-H	346.0545	2.1
	HMDB0006480	N-Acetyl-D-galactosamine 1-phosphate	C8H16NO9P	M+FA-H	346.0545	2.1
	HMDB0001121	N-Acetyl-D-mannosamine 6-phosphate	C8H16NO9P	M+FA-H	346.0545	2.1
	HMDB0002817	N-Acetylglucosamine 6-phosphate	C8H16NO9P	M+FA-H	346.0545	2.1
	HMDB0001367	N-Acetyl-glucosamine 1-phosphate	C8H16NO9P	M+FA-H	346.0545	2.1
	HMDB0178044	6-{4-[cyano(hydroxy)methyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C14H15NO8	M+Na-2H	346.0544	2.2
	HMDB0059997	Dihydroxy-1H-indole glucuronide I	C14H15NO8	M+Na-2H	346.0544	2.2
	HMDB0062748	(5S,6R,7E,9E,11Z,15S)-5,6,15,-tetrahydroxyicosa-7,9,11,13-tetraenoic acid	C20H32O6	M-H2O-H	349.2015	-0.6
	HMDB0062683	7-[6-(3,7-dihydroxyoct-1-en-1-yl)-2,3-dioxabicyclo[2.2.1]heptan-5-yl]hept-5-enoic acid	C20H32O6	M-H2O-H	349.2015	-0.6
	HMDB0001908	19-Hydroxy-PGE2	C20H32O6	M-H2O-H	349.2015	-0.6
	HMDB0004242	11-Dehydro-thromboxane B2	C20H32O6	M-H2O-H	349.2015	-0.6
	HMDB0036854	Cinnassiol D3	C20H32O6	M-H2O-H	349.2015	-0.6
	HMDB0004241	6-Ketoprostaglandin E1	C20H32O6	M-H2O-H	349.2015	-0.6
	HMDB0034678	Cinnassiol D2	C20H32O6	M-H2O-H	349.2015	-0.6
	HMDB0001979	6,15-Diketo,13,14-dihydro-PGF1a	C20H32O6	M-H2O-H	349.2015	-0.6
	HMDB0003247	-Hydroxy-PGE2	C20H32O6	M-H2O-H	349.2015	-0.6
	HMDB0184339	(4Z)-2-(6-hydroxy-2-oxoundec-4-en-3-yl)non-4-enedioic acid	C20H32O6	M-H2O-H	349.2015	-0.6
	HMDB0183704	(5Z)-3-acetyl-2-(3-hydroxyoct-1-en-1-yl)dec-5-enedioic acid	C20H32O6	M-H2O-H	349.2015	-0.6
	HMDB0012110	5(6)-Epoxy Prostaglandin E1	C20H32O6	M-H2O-H	349.2015	-0.6
	HMDB0005099	Thromboxane B3	C20H32O6	M-H2O-H	349.2015	-0.6
	HMDB0012635	-dihydroxyleukotriene B4	C20H32O6	M-H2O-H	349.2015	-0.6

349.2013

HMDB0187401	(5Z)-7-[6-hydroxy-2-(3-hydroxyoct-1-en-1-yl)-4-oxooxan-3-yl]hept-5-enoic acid	C20H32O6	M-H2O-H	349.2015	-0.6
HMDB0003235	Prostaglandin G2	C20H32O6	M-H2O-H	349.2015	-0.6
HMDB0012633	-COOH-,11-dihydro-LTB4	C20H32O6	M-H2O-H	349.2015	-0.6
HMDB0169093	3-[(2E)-3,7-dimethylocta-2,6-dien-1-yl]-4-(1-hydroxyethyl)-5-methoxyphenol	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0000324	3a,16a-dihydroxyandrost-4-en-3-one	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0000309	3a,16b-dihydroxyandrost-4-en-3-one	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0137379	4-[(1E,4E)-3-hydroxydodeca-1,4-dien-1-yl]-2-methoxyphenol	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0137366	SCHEMBL668211	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0155962	16,17-Dihydroxyandrost-4-en-3-one	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0155966	4,17-Dihydroxyandrost-4-en-3-one	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0155960	CTK4G5541	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0155961	Androst-4-en-3-one,6,17-dihydroxy-, (6b,17b)-	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0060339	11beta,17beta-Dihydroxy-4-androst-3-one	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0060089	w Hydroxy testosterone	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0012654	SM(d18/24:1(15Z)(OH))	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0012533	11beta-Hydroxytestosterone	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0031464	cis-[8]-Shogaol	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0039589	Ginsenoside G	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0006769	Indole-5,6-quinone	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0004611	7a-Hydroxydehydroepiandrosterone	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0003956	7a-Hydroxytestosterone	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0000388	3a,16-Dihydroxyandrost-4-en-3-one	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0000352	16a-Hydroxydehydroisoandrosterone	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0004624	7b-Hydroxydehydroepiandrosterone	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0006259	DG(O-16/18)	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0039735	-Acetoxy-8-heptadecene-4,6-diyn-3-ol	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0006031	11-Ketoetiocholanolone	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0000322	16-Oxoandrostenediol	C19H28O3	M+FA-H	349.2020	-2.1
HMDB0062797	5-hydroperoxy-18-hydroxyicosa-6,8,11,14,16-pentaenoic acid	C20H30O5	M-H	349.2020	-2.1
HMDB0037593	Oryzolic acid A	C20H30O5	M-H	349.2020	-2.1
HMDB0012552	12-Oxo--hydroxy-leukotriene B4	C20H30O5	M-H	349.2020	-2.1
HMDB0012588	15-Epi-lipoxin B5	C20H30O5	M-H	349.2020	-2.1
HMDB0012590	15-Oxo-lipoxin A4	C20H30O5	M-H	349.2020	-2.1
HMDB0038693	Oryzolic acid B	C20H30O5	M-H	349.2020	-2.1
HMDB0013040	Prostaglandin H3	C20H30O5	M-H	349.2020	-2.1
HMDB0002341	8-iso-15-keto-PGE2	C20H30O5	M-H	349.2020	-2.1
HMDB0002664	Prostaglandin E3	C20H30O5	M-H	349.2020	-2.1
HMDB0177949	3-hydroxy-7,7a-dimethyl-4'-methylidene-2'-oxo-octahydrospiro[indene-2,3'-oxolane]-4-yl 2-methylbutanoate	C20H30O5	M-H	349.2020	-2.1
HMDB0003034	Prostaglandin D3	C20H30O5	M-H	349.2020	-2.1
HMDB0003175	15-Keto-prostaglandin E2	C20H30O5	M-H	349.2020	-2.1
HMDB0168846	3,4,5-trihydroxy-2,4-bis(3-methylbut-2-en-1-yl)-6-(2-methylpropanoyl)cyclohex-2-en-1-one	C20H30O5	M-H	349.2020	-2.1
HMDB0168845	3,4,5-trihydroxy-4,6-bis(3-methylbut-2-en-1-yl)-2-(2-methylpropanoyl)cyclohex-2-en-1-one	C20H30O5	M-H	349.2020	-2.1
HMDB0010410	Resolvin E1	C20H30O5	M-H	349.2020	-2.1
HMDB0036701	(ent-6alpha,7alpha,12alpha)-6,7,12-Trihydroxy-16-kauren-19-oic acid	C20H30O5	M-H	349.2020	-2.1
HMDB0012641	-oxo-leukotriene B4	C20H30O5	M-H	349.2020	-2.1
HMDB0060096	5,12,18R-TriHEPE	C20H30O5	M-H	349.2020	-2.1
HMDB0062297	15-dehydro-prostaglandin D2	C20H30O5	M-H	349.2020	-2.1
HMDB0062300	(5S,6R,7E,9E,11Z)-5,6-dihydroxy-15-oxoicosa-7,9,11,13-tetraenoic acid	C20H30O5	M-H	349.2020	-2.1
HMDB0062616	(5S,6E,8Z,11Z,14Z)-5-hydroperoxy-18-hydroxyicosa-6,8,11,14,16-pentaenoic acid	C20H30O5	M-H	349.2020	-2.1
HMDB0039132	[4]-Gingerdiol 3,5-diacetate	C19H28O6	M-H	351.1813	0.5
HMDB0012799	5'-Carboxy-gamma-chromanol	C18H26O4	M+FA-H	351.1813	0.5
HMDB0180103	(4-hydroxy-3-methoxyphenyl)methyl 8-methylnon-8-enoate	C18H26O4	M+FA-H	351.1813	0.5
HMDB0034780	Capsiate	C18H26O4	M+FA-H	351.1813	0.5

351.1815

	HMDB0036822	(3S,7E,9S)-9-Hydroxy-4,7-megastigmadien-3-one 9-glucoside	C19H30O7	M-H2O-H	351.1808	2.1
	HMDB0032841	5-Megastigmen-7-yne-3,9-diol 9-glucoside	C19H30O7	M-H2O-H	351.1808	2.1
	HMDB0032842	5-Megastigmen-7-yne-3,9-diol 3-glucoside	C19H30O7	M-H2O-H	351.1808	2.1
351.2151	HMDB0004708	9,12,13-TriHOME	C18H34O5	M+Na-2H	351.2153	-0.5
	HMDB0172549	9,-dihydroxy-18-oxooctadecanoic acid	C18H34O5	M+Na-2H	351.2153	-0.5
	HMDB0030936	5,8,12-Trihydroxy-9-octadecenoic acid	C18H34O5	M+Na-2H	351.2153	-0.5
	HMDB0038555	(9S,E,12S,13S)-9,12,13-Trihydroxy--octadecenoic acid	C18H34O5	M+Na-2H	351.2153	-0.5
	HMDB0004710	9,,13-TriHOME	C18H34O5	M+Na-2H	351.2153	-0.5
351.2533	HMDB0174098	(2E)-2-[(3E,7E)-4,8,12-trimethyltrideca-3,7,11-trien-1-yl]but-2-ene-1,4-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174099	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,4-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174096	SCHEMBL116891	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174097	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,8-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174102	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,5-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174103	147-52-2	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174101	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,9-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174100	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,13-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174094	(2Z,6E,Z)-6,-dimethyl-2-(4-methylpent-3-en-1-yl)dodeca-2,6,-triene-1,12-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174093	(6E,E,14Z)-2,6,,14-tetramethylhexadeca-2,6,,14-tetraene-1,16-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174095	(2Z,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,12-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174106	{3-methyl-3-[(3E,7E)-4,8,12-trimethyltrideca-3,7,11-trien-1-yl]oxiran-2-yl}methanol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174104	(2Z,6E)-3,7-dimethyl-9-[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]nona-2,6-dien-1-ol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174157	May-64	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174158	(2E,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,5-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174159	14,15-Epoxygeranylgeraniol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174161	6,7-Epoxygeranylgeraniol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174160	(2E,6E)-3,7-dimethyl-9-[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]nona-2,6-dien-1-ol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174155	(2E,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,4-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174105	(2Z)-3-Methyl-5-[3-methyl-3-(4,8-dimethyl-3,7-nonadienyl)oxiranyl]-2-pentene-1-ol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174149	(6E,E,14E)-2,6,,14-tetramethylhexadeca-2,6,,14-tetraene-1,16-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174150	SCHEMBL8576448	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174152	plaunotol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174151	(2E,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,12-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174153	(2E,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,8-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174154	(2Z)-2-[(3E,7E)-4,8,12-trimethyltrideca-3,7,11-trien-1-yl]but-2-ene-1,4-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0174156	(2E,6E,E)-3,7,11,15-tetramethylhexadeca-2,6,,14-tetraene-1,13-diol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0060039	Dihomo-alpha-linolenic acid	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0036835	Sagittariol	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0031058	Sciadonic acid	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0010378	5,8,11-Eicosatrienoic acid	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0002925	Dihomo-gamma-linolenic acid	C20H34O2	M+FA-H	351.2541	-2.2
	HMDB0011570	MG(18:3(9Z,12Z,15Z))	C21H36O4	M-H	351.2541	-2.2
	HMDB0011569	MG(18:3(6Z,9Z,12Z))	C21H36O4	M-H	351.2541	-2.2
	HMDB0011539	MG/18:3(6Z,9Z,12Z))	C21H36O4	M-H	351.2541	-2.2
	HMDB0164513	[]-Gingerdiol	C21H36O4	M-H	351.2541	-2.2

	HMDB0011540	MG/18:3(9Z,12Z,15Z))	C21H36O4	M-H	351.2541	-2.2
352.0457	HMDB0154719	{[3-hydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-2-yl]methoxy}sulfonic acid	C9H13N3O7S	M+FA-H	352.0456	0.2
	HMDB0154720	[5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)-2-(hydroxymethyl)oxolan-3-yl]oxidanessulfonic acid	C9H13N3O7S	M+FA-H	352.0456	0.2
353.2328	HMDB0184746	2-hydroxy-7-[3-hydroxy-2-(3-hydroxyoctyl)-5-oxocyclopentyl]heptanoic acid	C20H36O6	M-H2O-H	353.2328	0.0
	HMDB0184745	7-[2-(3,8-dihydroxyoctyl)-3-hydroxy-5-oxocyclopentyl]heptanoic acid	C20H36O6	M-H2O-H	353.2328	0.0
	HMDB0184747	7-[1,3-dihydroxy-2-(3-hydroxyoctyl)-5-oxocyclopentyl]heptanoic acid	C20H36O6	M-H2O-H	353.2328	0.0
	HMDB0184748	7-[3,4-dihydroxy-2-(3-hydroxyoctyl)-5-oxocyclopentyl]heptanoic acid	C20H36O6	M-H2O-H	353.2328	0.0
	HMDB0184744	7-[3,3-dihydroxy-2-(3-hydroxyoctyl)-5-oxocyclopentyl]heptanoic acid	C20H36O6	M-H2O-H	353.2328	0.0
	HMDB0184743	7-[2-(3,7-dihydroxyoctyl)-3-hydroxy-5-oxocyclopentyl]heptanoic acid	C20H36O6	M-H2O-H	353.2328	0.0
	HMDB0112100	9-(3,4-dimethyl-5-butylfuran-2-yl)-nonanoic acid	C19H32O3	M+FA-H	353.2333	-1.5
	HMDB0112070	5-Ethyl-3,4-dimethyl-2-furanundecanoic acid	C19H32O3	M+FA-H	353.2333	-1.5
	HMDB0094643	-(3,4-dimethyl-5-propylfuran-2-yl)decanoic acid	C19H32O3	M+FA-H	353.2333	-1.5
	HMDB0112096	8-(3,4-dimethyl-5-pentylfuran-2-yl)-octanoic acid	C19H32O3	M+FA-H	353.2333	-1.5
	HMDB0030960	Isoobtusilactone A	C19H32O3	M+FA-H	353.2333	-1.5
	HMDB0031379	Annosquamosin B	C19H32O3	M+FA-H	353.2333	-1.5
	HMDB0031091	3-Methyl-5-pentyl-2-furannonanoic acid	C19H32O3	M+FA-H	353.2333	-1.5
	HMDB0112090	5-Hexyl-3,4-dimethyl-2-furanheptanoic acid	C19H32O3	M+FA-H	353.2333	-1.5
	HMDB0061646	3-Methyl-5-propyl-2-furanundecanoic acid	C19H32O3	M+FA-H	353.2333	-1.5
	HMDB0183703	(5Z)-8-acetyl-12-hydroxy-9-(hydroxymethyl)heptadeca-5,-dienoic acid	C20H34O5	M-H	353.2333	-1.6
	HMDB0184338	(5Z,E)-9-acetyl-12-hydroxy-8-(hydroxymethyl)heptadeca-5,-dienoic acid	C20H34O5	M-H	353.2333	-1.6
	HMDB0001442	Prostaglandin E1	C20H34O5	M-H	353.2333	-1.6
	HMDB0062278	(5E,13E)-11,12,15-trihydroxyicosa-5,8,13-trienoic acid	C20H34O5	M-H	353.2333	-1.6
	HMDB0012563	13,14-Dihydro- lipoxin A4	C20H34O5	M-H	353.2333	-1.6
	HMDB0035380	Sterebin G	C20H34O5	M-H	353.2333	-1.6
	HMDB0011137	11-Epi-PGF2a	C20H34O5	M-H	353.2333	-1.6
	HMDB0001139	Prostaglandin F2a	C20H34O5	M-H	353.2333	-1.6
	HMDB0001483	Prostaglandin F2b	C20H34O5	M-H	353.2333	-1.6
	HMDB0001965	Troxilin B3	C20H34O5	M-H	353.2333	-1.6
	HMDB0001977	Trioxilin A3	C20H34O5	M-H	353.2333	-1.6
	HMDB0002115	8-isoprostaglandin PGF2b	C20H34O5	M-H	353.2333	-1.6
	HMDB0004684	11,12,15-THETA	C20H34O5	M-H	353.2333	-1.6
	HMDB0004685	13,14-dihydro-15-keto-PGF2alpha	C20H34O5	M-H	353.2333	-1.6
	HMDB0004686	8-Isoprostaglandin E1	C20H34O5	M-H	353.2333	-1.6
	HMDB0004694	11,14,15-THETA	C20H34O5	M-H	353.2333	-1.6
	HMDB0005083	8-Isoprostaglandin F2a	C20H34O5	M-H	353.2333	-1.6
	HMDB0005102	Prostaglandin D1	C20H34O5	M-H	353.2333	-1.6
	HMDB0006562	8-iso-13,14-dihydro-15-keto-PGF2a	C20H34O5	M-H	353.2333	-1.6
	HMDB0010170	11,12,15-TriHETRE	C20H34O5	M-H	353.2333	-1.6
	HMDB0010199	11b-PGF2a	C20H34O5	M-H	353.2333	-1.6
	HMDB0013041	Prostaglandin H1	C20H34O5	M-H	353.2333	-1.6
	HMDB0060045	15-keto-PGF1alpha	C20H34O5	M-H	353.2333	-1.6
	HMDB0060107	(5Z,9E,12S,14Z)-8,11,12-Trihydroxyicosa-5,9,14-trienoate	C20H34O5	M-H	353.2333	-1.6
353.3420	HMDB0062602	1-docosene	C22H44	M+FA-H	353.3425	-1.4
	HMDB0001160	Tricosanoic acid	C23H46O2	M-H	353.3425	-1.4
	HMDB0035638	6-Hydroxy-8-tricosanone	C23H46O2	M-H	353.3425	-1.4
	HMDB0035642	8-Hydroxy-6-tricosanone	C23H46O2	M-H	353.3425	-1.4
	HMDB0035650	6-Hydroxy-4-tricosanone	C23H46O2	M-H	353.3425	-1.4
	HMDB0035649	4-Hydroxy-6-tricosanone	C23H46O2	M-H	353.3425	-1.4
	HMDB0131410	2-([2-(2H-1,3-benzodioxol-5-yl)-4-hydroxy-1-benzofuran-5-yl](hydroxy)methylidene)amino)acetic acid	C18H13NO7	M-H	354.0619	-2.9

354.0609	HMDB0131405	2-([2-(2H-1,3-benzodioxol-5-yl)-7-hydroxy-1-benzofuran-5-yl](hydroxy)methylidene)amino)acetic acid	C18H13NO7	M-H	354.0619	-2.9
	HMDB0131400	2-([hydroxy[2-(6-hydroxy-2H-1,3-benzodioxol-5-yl)-1-benzofuran-5-yl]methylidene]amino)acetic acid	C18H13NO7	M-H	354.0619	-2.9
	HMDB0131395	2-([2-(2H-1,3-benzodioxol-5-yl)-6-hydroxy-1-benzofuran-5-yl]formamido)acetic acid	C18H13NO7	M-H	354.0619	-2.9
354.0962	HMDB0015625	Prasugrel	C20H20FNO3S	M-H20-H	354.0964	-0.6
	HMDB0129292	3,5,7,8-tetrahydroxy-2-(3-hydroxy-4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0132214	2-(3,4-dihydroxyphenyl)-5,6,7-trihydroxy-8-methoxy-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0137865	3-(2,4-dihydroxy-5-methoxyphenyl)-5,7,8-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0138038	5,7-dihydroxy-8-methoxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0138046	2-(3,4-dihydroxy-5-methoxyphenyl)-5,7,8-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0140536	3-(4-hydroxy-3-methoxyphenyl)-1-(2,3,4,5,6-pentahydroxyphenyl)prop-2-en-1-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0140534	5,6,7,8-tetrahydroxy-2-(4-hydroxy-3-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0140550	5,6,7,8-tetrahydroxy-2-(3-hydroxy-5-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0140553	3-(3-hydroxy-5-methoxyphenyl)-1-(2,3,4,5,6-pentahydroxyphenyl)prop-2-en-1-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0151202	5,7,8-trihydroxy-2-(1-hydroxy-4-oxocyclohex-2-en-1-yl)-6-methoxy-4H-chromen-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0132210	3-(3,4-dihydroxyphenyl)-1-(2,3,4,6-tetrahydroxy-5-methoxyphenyl)prop-2-en-1-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0132207	2-(3,4-dihydroxyphenyl)-5,7,8-trihydroxy-6-methoxy-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0132141	3,5,7-trihydroxy-2-(1-hydroxy-4-oxocyclohex-2-en-1-yl)-8-methoxy-4H-chromen-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0130269	3,5,6,7-tetrahydroxy-2-(3-hydroxy-4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0131803	2-(2,4-dihydroxy-5-methoxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0131809	3-(2,4-dihydroxy-5-methoxyphenyl)-1-(2,4,6-trihydroxyphenyl)propane-1,2-dione	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0131890	2-(3,5-dihydroxyphenyl)-3,5,7-trihydroxy-6-methoxy-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0131891	3-(3,5-dihydroxyphenyl)-1-(2,4,6-trihydroxy-3-methoxyphenyl)propane-1,2-dione	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0131933	2-(1,3-dihydroxy-4-oxocyclohex-2-en-1-yl)-5,6-dihydroxy-7-methoxy-4H-chromen-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0131934	2-(1,5-dihydroxy-4-oxocyclohex-2-en-1-yl)-5,6-dihydroxy-7-methoxy-4H-chromen-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0167578	1,3-dimethyl 2-[5-hydroxy-2-(oxiran-2-yl)-4-oxo-4H-chromen-3-yl]propanedioate	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0132079	(2E)-3-(2,5-dihydroxy-4-methoxyphenyl)-1-(2,3,4,6-tetrahydroxyphenyl)prop-2-en-1-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0152022	5,6,7,8-tetrahydroxy-2-(3-hydroxy-4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0152026	2-(2,3-dihydroxy-4-methoxyphenyl)-5,7,8-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0153271	5,7-dihydroxy-6-methoxy-2-(2,3,4-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0153276	1-(2,4,6-trihydroxy-3-methoxyphenyl)-3-(3,4,5-trihydroxyphenyl)prop-2-en-1-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0153281	1-(2,4,6-trihydroxy-3-methoxyphenyl)-3-(2,4,5-trihydroxyphenyl)prop-2-en-1-one	C16H14O8	M+Na-2H	355.0435	-0.4
	HMDB0153280	5,7-dihydroxy-6-methoxy-2-(2,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4

355.0434

HMDB0153284	2-(1,3-dihydroxy-4-oxocyclohex-2-en-1-yl)-5,7-dihydroxy-6-methoxy-4H-chromen-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0153283	2-(1,5-dihydroxy-4-oxocyclohex-2-en-1-yl)-5,7-dihydroxy-6-methoxy-4H-chromen-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0154096	2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-8-methoxy-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0166099	6-[(2E)-dec-2-en-4,6,8-triynoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0167575	1,3-dimethyl 2-(2-ethenyl-5,6-dihydroxy-4-oxo-4H-chromen-3-yl)propanedioate	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0153272	1-(2,4,6-trihydroxy-3-methoxyphenyl)-3-(2,3,4-trihydroxyphenyl)prop-2-en-1-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0153274	5,7-dihydroxy-6-methoxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0152516	2-(1,5-dihydroxy-4-oxocyclohex-2-en-1-yl)-3,7-dihydroxy-5-methoxy-4H-chromen-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0152023	3-(3-hydroxy-4-methoxyphenyl)-1-(2,3,4,5,6-pentahydroxyphenyl)prop-2-en-1-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0152028	3-(2,3-dihydroxy-4-methoxyphenyl)-1-(2,3,4,6-tetrahydroxyphenyl)prop-2-en-1-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0152032	2-(2,5-dihydroxy-4-methoxyphenyl)-5,7,8-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0152034	3-(2,5-dihydroxy-4-methoxyphenyl)-1-(2,3,4,6-tetrahydroxyphenyl)prop-2-en-1-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0152188	2-(3,4-dihydroxyphenyl)-5,6,7-trihydroxy-3-methoxy-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0152194	5,7-dihydroxy-3-methoxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0152200	5,7-dihydroxy-3-methoxy-2-(2,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0152198	5,7-dihydroxy-3-methoxy-2-(2,3,4-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0152515	2-(1,3-dihydroxy-4-oxocyclohex-2-en-1-yl)-3,7-dihydroxy-5-methoxy-4H-chromen-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0167576	1,3-dimethyl 2-(2-ethenyl-5,7-dihydroxy-4-oxo-4H-chromen-3-yl)propanedioate	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0132071	2-(2,5-dihydroxy-4-methoxyphenyl)-5,6,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0128756	2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-6-methoxy-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0033014	Hovenitin I	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0031971	Xanthotoxol arabinoside	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0176940	4-[1-carboxy-2-(3,4-dihydroxyphenyl)ethoxy]-3-hydroxybenzoic acid	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0125082	7-hydroxy-6-methoxy-3-(1,3,6-trihydroxy-4-oxocyclohex-2-en-1-yl)-4H-chromen-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0126502	3,5,6,7-tetrahydroxy-2-(4-hydroxy-3-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0126504	3-(4-hydroxy-3-methoxyphenyl)-1-(2,3,4,6-tetrahydroxyphenyl)propane-1,2-dione	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0126508	3-(3,4-dihydroxy-5-methoxyphenyl)-1-(2,4,6-trihydroxyphenyl)propane-1,2-dione	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0126512	3,5,7-trihydroxy-2-(1-hydroxy-5-methoxy-4-oxocyclohex-2-en-1-yl)-4H-chromen-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0126513	3,5,7-trihydroxy-2-(1-hydroxy-3-methoxy-4-oxocyclohex-2-en-1-yl)-4H-chromen-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0128206	2-(3,4-dihydroxy-5-methoxyphenyl)-5,6,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0128211	3-(3,4-dihydroxy-5-methoxyphenyl)-1-(2,3,4,6-tetrahydroxyphenyl)prop-2-en-1-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0128758	3-(3,4-dihydroxyphenyl)-1-(2,4,6-trihydroxy-3-methoxyphenyl)propane-1,2-dione	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0125081	7-hydroxy-6-methoxy-3-(1,2,5-trihydroxy-4-oxocyclohex-2-en-1-yl)-4H-chromen-4-one	C16H14O8	M+Na-2H	355.0435	-0.4

HMDB0125076	3-(2,5-dihydroxy-4-methoxyphenyl)-5,6,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0125074	5,7-dihydroxy-6-methoxy-3-(2,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0167577	1,3-dimethyl 2-(2-ethenyl-5-hydroxy-4-oxo-4H-chromen-3-yl)-2-hydroxypropanedioate	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0125030	7-hydroxy-6-methoxy-3-(2,3,4,5-tetrahydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0125032	6,7-dihydroxy-3-(2,3,5-trihydroxy-4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0125045	7-hydroxy-6-methoxy-3-(2,3,4,6-tetrahydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0125047	6,7-dihydroxy-3-(2,3,6-trihydroxy-4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0125060	7,8-dihydroxy-6-methoxy-3-(2,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0125062	3-(2,5-dihydroxy-4-methoxyphenyl)-6,7,8-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0129287	3,5,7,8-tetrahydroxy-2-(4-hydroxy-3-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C16H14O8	M+Na-2H	355.0435	-0.4
HMDB0179878	(3Z)-3-({[bis(methylsulfanyl)methylidene]amino}methylidene)-6-hydroxy-1-methoxy-2,3-dihydro-1H-indol-2-one	C13H14N2O3S2	M+FA-H	355.0428	1.7
HMDB0179879	(3Z)-3-({[bis(methylsulfanyl)methylidene]amino}methylidene)-5-hydroxy-1-methoxy-2,3-dihydro-1H-indol-2-one	C13H14N2O3S2	M+FA-H	355.0428	1.7
HMDB0179881	(3Z)-3-({[bis(methylsulfanyl)methylidene]amino}methylidene)-4-hydroxy-1-methoxy-2,3-dihydro-1H-indol-2-one	C13H14N2O3S2	M+FA-H	355.0428	1.7
HMDB0179833	(3E)-3-({[bis(methylsulfanyl)methylidene]amino}methylidene)-4-hydroxy-1-methoxy-2,3-dihydro-1H-indol-2-one	C13H14N2O3S2	M+FA-H	355.0428	1.7
HMDB0179832	(3E)-3-({[bis(methylsulfanyl)methylidene]amino}methylidene)-7-hydroxy-1-methoxy-2,3-dihydro-1H-indol-2-one	C13H14N2O3S2	M+FA-H	355.0428	1.7
HMDB0179831	(3E)-3-({[bis(methylsulfanyl)methylidene]amino}methylidene)-5-hydroxy-1-methoxy-2,3-dihydro-1H-indol-2-one	C13H14N2O3S2	M+FA-H	355.0428	1.7
HMDB0179830	(3E)-3-({[bis(methylsulfanyl)methylidene]amino}methylidene)-6-hydroxy-1-methoxy-2,3-dihydro-1H-indol-2-one	C13H14N2O3S2	M+FA-H	355.0428	1.7
HMDB0172649	{4-hydroxy-1-methoxy-2-oxo-1,2-dihydro-3'H-spiro[indole-3,2'-[1,4]thiazole]-5'-	C13H15N2O3S2	M+FA-H	355.0428	1.7
HMDB0172648	{7-hydroxy-1-methoxy-2-oxo-1,2-dihydro-3'H-spiro[indole-3,2'-[1,4]thiazole]-5'-	C13H15N2O3S2	M+FA-H	355.0428	1.7
HMDB0172646	{5-hydroxy-1-methoxy-2-oxo-1,2-dihydro-3'H-spiro[indole-3,2'-[1,4]thiazole]-5'-	C13H15N2O3S2	M+FA-H	355.0428	1.7
HMDB0172645	{6-hydroxy-1-methoxy-2-oxo-1,2-dihydro-3'H-spiro[indole-3,2'-[1,4]thiazole]-5'-	C13H15N2O3S2	M+FA-H	355.0428	1.7
HMDB0172647	{3'-hydroxy-1-methoxy-2-oxo-1,2-dihydro-3'H-spiro[indole-3,2'-[1,4]thiazole]-5'-	C13H15N2O3S2	M+FA-H	355.0428	1.7
HMDB0179880	(3Z)-3-({[bis(methylsulfanyl)methylidene]amino}methylidene)-7-hydroxy-1-methoxy-2,3-dihydro-1H-indol-2-one	C13H14N2O3S2	M+FA-H	355.0428	1.7
HMDB0168227	(1-hydroxy-9-phenyl-2,3-dihydro-1H-phenalen-2-yl)oxidanesulfonic acid	C19H16O5S	M-H	355.0646	-0.2
HMDB0168226	(2-hydroxy-9-phenyl-2,3-dihydro-1H-phenalen-1-yl)oxidanesulfonic acid	C19H16O5S	M-H	355.0646	-0.2
HMDB0163420	3,4,5-trihydroxy-6-[2-(3-methyl-4,5-dioxoxolan-2-yl)ethoxy]oxane-2-carboxylic acid	C13H18O10	M+Na-2H	355.0647	-0.5
HMDB0163416	3,4,5-trihydroxy-6-[2-(4-hydroxy-3-methyl-5-oxo-2,5-dihydrofuran-2-yl)ethoxy]oxane-2-carboxylic acid	C13H18O10	M+Na-2H	355.0647	-0.5
HMDB0163418	3,4,5-trihydroxy-6-[1-(3-methyl-4,5-dioxoxolan-2-yl)ethoxy]oxane-2-carboxylic acid	C13H18O10	M+Na-2H	355.0647	-0.5

355.0645	HMDB0163414	3,4,5-trihydroxy-6-[1-(4-hydroxy-3-methyl-5-oxo-2,5-dihydrofuran-2-yl)ethoxy]oxane-2-carboxylic acid	C13H18O10	M+Na-2H	355.0647	-0.5
	HMDB0163412	6-[(2-ethyl-4-hydroxy-5-oxo-2,5-dihydrofuran-3-yl)methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H18O10	M+Na-2H	355.0647	-0.5
	HMDB0160742	6-[(4,6-dioxoheptanoyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H18O10	M+Na-2H	355.0647	-0.5
	HMDB0160743	6-(6-carboxy-2,4-dioxohexan-3-yl)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H18O10	M+Na-2H	355.0647	-0.5
	HMDB0147335	{2-methoxy-4-[3-methylidene-5-(prop-1-en-1-yl)-2,3-dihydro-1-benzofuran-2-yl]phenyl}oxidanesulfonic acid	C19H18O6S	M-H2O-H	355.0640	1.4
	HMDB0138962	{4-[(E)-2-(3,5-dihydroxyphenyl)ethenyl]-2-[(1E)-3-methylbuta-1,3-dien-1-yl]phenyl}oxidanesulfonic acid	C19H18O6S	M-H2O-H	355.0640	1.4
	HMDB0138718	[3-(6-hydroxy-1-benzofuran-2-yl)-2-(3-methylbut-2-en-1-yl)phenyl]oxidanesulfonic acid	C19H18O6S	M-H2O-H	355.0640	1.4
	HMDB0129030	{4-[(E)-2-{3,5-dihydroxy-4-[(1E)-3-methylbuta-1,3-dien-1-yl]phenyl}ethenyl]phenyl}oxidanesulfonic acid	C19H18O6S	M-H2O-H	355.0640	1.4
	HMDB0060991	hydroxychlorpromazine	C17H19ClN2OS	M+Na-2H	355.0653	-2.3
	HMDB0060573	Chlorpromazine-N-oxide	C17H19ClN2OS	M+Na-2H	355.0653	-2.3
357.0126	HMDB0164672	{2-[(3,4-dihydroxy-5-oxo-2,5-dihydrofuran-2-yl)methoxy]-4,5-dihydroxyoxan-3-yl}oxidanesulfonic acid	C10H14O12S	M-H	357.0133	-2.0
	HMDB0164698	(4,5-dioxo-2-[(3,4,5-trihydroxyoxan-2-yl)oxy]methyl)oxolan-3-yl}oxidanesulfonic acid	C10H14O12S	M-H	357.0133	-2.0
	HMDB0164696	{3,5-dihydroxy-2-[(3-hydroxy-4,5-dioxooxolan-2-yl)methoxy]oxan-4-yl}oxidanesulfonic acid	C10H14O12S	M-H	357.0133	-2.0
	HMDB0164697	{4,5-dihydroxy-2-[(3-hydroxy-4,5-dioxooxolan-2-yl)methoxy]oxan-3-yl}oxidanesulfonic acid	C10H14O12S	M-H	357.0133	-2.0
	HMDB0164690	(2,4-dioxo-5-[(3,4,5-trihydroxyoxan-2-yl)oxy]methyl)oxolan-3-yl}oxidanesulfonic acid	C10H14O12S	M-H	357.0133	-2.0
	HMDB0164691	{4,5-dihydroxy-6-[(4-hydroxy-3,5-dioxooxolan-2-yl)methoxy]oxan-3-yl}oxidanesulfonic acid	C10H14O12S	M-H	357.0133	-2.0
	HMDB0164689	{4,5-dihydroxy-2-[(4-hydroxy-3,5-dioxooxolan-2-yl)methoxy]oxan-3-yl}oxidanesulfonic acid	C10H14O12S	M-H	357.0133	-2.0
	HMDB0164688	{3,5-dihydroxy-2-[(4-hydroxy-3,5-dioxooxolan-2-yl)methoxy]oxan-4-yl}oxidanesulfonic acid	C10H14O12S	M-H	357.0133	-2.0
	HMDB0164673	{6-[(3,4-dihydroxy-5-oxo-2,5-dihydrofuran-2-yl)methoxy]-4,5-dihydroxyoxan-3-yl}oxidanesulfonic acid	C10H14O12S	M-H	357.0133	-2.0
	HMDB0164671	{2-[(3,4-dihydroxy-5-oxo-2,5-dihydrofuran-2-yl)methoxy]-3,5-dihydroxyoxan-4-yl}oxidanesulfonic acid	C10H14O12S	M-H	357.0133	-2.0
	HMDB0164699	{4,5-dihydroxy-6-[(3-hydroxy-4,5-dioxooxolan-2-yl)methoxy]oxan-3-yl}oxidanesulfonic acid	C10H14O12S	M-H	357.0133	-2.0
	HMDB0137207	7-chloro-5,8-dihydroxy-3,6-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one	C18H15ClO7	M-H2O-H	359.0322	1.3
359.0327	HMDB0137211	7-chloro-3,5-dihydroxy-6,8-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one	C18H15ClO7	M-H2O-H	359.0322	1.3
	HMDB0137209	7-chloro-5,6-dihydroxy-3,8-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one	C18H15ClO7	M-H2O-H	359.0322	1.3
359.0384	HMDB0240564	Umbelliferone glucuronide	C15H14O9	M+Na-2H	359.0384	-0.1
	HMDB0183684	3,4,5-trihydroxy-6-[[3-(4-hydroxyphenyl)prop-2-ynoyl]oxy]oxane-2-carboxylic acid	C15H14O9	M+Na-2H	359.0384	-0.1
	HMDB0183683	6-[4-(2-carboxyeth-1-yn-1-yl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H14O9	M+Na-2H	359.0384	-0.1
	HMDB0183681	3,4,5-trihydroxy-6-[[3-(3-hydroxyphenyl)prop-2-ynoyl]oxy]oxane-2-carboxylic acid	C15H14O9	M+Na-2H	359.0384	-0.1
	HMDB0183680	6-[3-(2-carboxyeth-1-yn-1-yl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H14O9	M+Na-2H	359.0384	-0.1
	HMDB0140950	3,4,5-trihydroxy-6-[(2-oxo-2H-chromen-6-yl)oxy]oxane-2-carboxylic acid	C15H14O9	M+Na-2H	359.0384	-0.1
	HMDB0140952	3,4,5-trihydroxy-6-[(2-oxo-2H-chromen-8-yl)oxy]oxane-2-carboxylic acid	C15H14O9	M+Na-2H	359.0384	-0.1
	HMDB0034621	2-O-Acetyl-trans-coutaric acid	C15H14O9	M+Na-2H	359.0384	-0.1

	HMDB0140951	3,4,5-trihydroxy-6-[(2-oxo-2H-chromen-7-yl)oxy]oxane-2-carboxylic acid	C15H14O9	M+Na-2H	359.0384	-0.1
	HMDB0140953	3,4,5-trihydroxy-6-[(2-oxo-2H-chromen-3-yl)oxy]oxane-2-carboxylic acid	C15H14O9	M+Na-2H	359.0384	-0.1
	HMDB0137928	3,4,5-trihydroxy-6-[(2-oxo-2H-chromen-4-yl)oxy]oxane-2-carboxylic acid	C15H14O9	M+Na-2H	359.0384	-0.1
	HMDB0136745	3,4,5-trihydroxy-6-[(2-oxo-2H-chromen-5-yl)oxy]oxane-2-carboxylic acid	C15H14O9	M+Na-2H	359.0384	-0.1
	HMDB0001517	AICAR	C9H15N4O8P	M+Na-2H	359.0374	2.7
362.0504	HMDB0154952	({3,4-dihydroxy-5-[6-(hydroxyamino)-9H-purin-9-yl]oxolan-2-yl}methoxy)phosphonic acid	C10H14N5O8P	M-H	362.0507	-0.9
	HMDB0240586	Guanosine 2'-monophosphate	C10H14N5O8P	M-H	362.0507	-0.9
	HMDB0001397	Guanosine monophosphate	C10H14N5O8P	M-H	362.0507	-0.9
	HMDB0011670	8-Oxo-dGMP	C10H14N5O8P	M-H	362.0507	-0.9
	HMDB0240587	Guanosine 3'-monophosphate	C10H14N5O8P	M-H	362.0507	-0.9
	HMDB0059639	Cyclic pyranopterin monophosphate	C10H14N5O8P	M-H	362.0507	-0.9
	HMDB0161177	8-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-4-hydroxyquinoline-2-carboxylic acid	C16H15NO10	M-H2O-H	362.0512	-2.2
	HMDB0161178	6-(4,8-dihydroxyquinoline-2-carbonyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H15NO10	M-H2O-H	362.0512	-2.2
	HMDB0161179	5-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-4-oxo-1,4-dihydroquinoline-2-carboxylic acid	C16H15NO10	M-H2O-H	362.0512	-2.2
	HMDB0161180	3,4,5-trihydroxy-6-(5-hydroxy-4-oxo-1,4-dihydroquinoline-2-carbonyloxy)oxane-2-carboxylic acid	C16H15NO10	M-H2O-H	362.0512	-2.2
	HMDB0161174	3,4,5-trihydroxy-6-(7-hydroxy-4-oxo-1,4-dihydroquinoline-2-carbonyloxy)oxane-2-carboxylic acid	C16H15NO10	M-H2O-H	362.0512	-2.2
	HMDB0161173	7-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-4-oxo-1,4-dihydroquinoline-2-carboxylic acid	C16H15NO10	M-H2O-H	362.0512	-2.2
	HMDB0161175	6-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-4-oxo-1,4-dihydroquinoline-2-carboxylic acid	C16H15NO10	M-H2O-H	362.0512	-2.2
	HMDB0161176	3,4,5-trihydroxy-6-(6-hydroxy-4-oxo-1,4-dihydroquinoline-2-carbonyloxy)oxane-2-carboxylic acid	C16H15NO10	M-H2O-H	362.0512	-2.2
	HMDB0240378	HBOA glucuronide	C14H15NO9	M+Na-2H	362.0493	2.9
	HMDB0240438	2-Hydroxy-1,4-benzoxazin-3-one glucuronide	C14H15NO9	M+Na-2H	362.0493	2.9
365.3415	HMDB0039540	Cerebronic acid	C24H48O3	M-H2O-H	365.3420	-1.2
	HMDB0035561	6,8-Tetracosanedione	C24H46O2	M-H	365.3425	-2.8
	HMDB0029799	(E)-2-Tetracosenoic acid	C24H46O2	M-H	365.3425	-2.8
	HMDB0035560	7,9-Tetracosanedione	C24H46O2	M-H	365.3425	-2.8
	HMDB0035562	5,7-Tetracosanedione	C24H46O2	M-H	365.3425	-2.8
	HMDB0035563	4,6-Tetracosanedione	C24H46O2	M-H	365.3425	-2.8
	HMDB0035559	,12-Tetracosanedione	C24H46O2	M-H	365.3425	-2.8
	HMDB0002368	Nervonic acid	C24H46O2	M-H	365.3425	-2.8
367.3571	HMDB0002003	Tetracosanoic acid	C24H48O2	M-H	367.3582	-2.9
	HMDB0035636	4-Hydroxy-6-tetracosanone	C24H48O2	M-H	367.3582	-2.9
	HMDB0035633	5-Hydroxy-7-tetracosanone	C24H48O2	M-H	367.3582	-2.9
	HMDB0040887	-Tetracosene-1,18-diol	C24H48O2	M-H	367.3582	-2.9
368.0404	HMDB0155254	[4-hydroxy-2-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)-5-(hydroxymethyl)oxolan-3-yl]oxidanesulfonic acid	C9H13N3O8S	M+FA-H	368.0405	-0.4
	HMDB0155255	[4-hydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)-2-(hydroxymethyl)oxolan-3-yl]oxidanesulfonic acid	C9H13N3O8S	M+FA-H	368.0405	-0.4
	HMDB0155253	ACMC-9hv8	C9H13N3O8S	M+FA-H	368.0405	-0.4

	HMDB0148115	2-[(4-[(6,7-dihydroxy-2-oxo-2H-chromen-3-yl)oxy]-3-hydroxyphenyl)(hydroxy)methylidene]amino]acetic acid	C18H13NO9	M-H2O-H	368.0406	-0.7
	HMDB0152296	2-[(hydroxy[2-hydroxy-4-(3,5,7-trihydroxy-4-oxo-4H-chromen-2-yl)phenyl]methylidene)amino]acetic acid	C18H13NO9	M-H2O-H	368.0406	-0.7
368.1111	HMDB0136418	2-hydroxy-N-[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-3-(4-hydroxy-3-methoxyphenyl)propanimidic acid	C18H21NO6	M+Na-2H	368.1116	-1.2
	HMDB0136415	3-(3,4-dihydroxy-5-methoxyphenyl)-N-[2-hydroxy-2-(4-hydroxyphenyl)ethyl]propanimidic acid	C18H21NO6	M+Na-2H	368.1116	-1.2
	HMDB0136416	N-[2-(3,4-dihydroxyphenyl)-2-hydroxyethyl]-3-(4-hydroxy-3-methoxyphenyl)propanimidic acid	C18H21NO6	M+Na-2H	368.1116	-1.2
	HMDB0136417	3-hydroxy-N-[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-3-(4-hydroxy-3-methoxyphenyl)propanimidic acid	C18H21NO6	M+Na-2H	368.1116	-1.2
	HMDB0136420	N-[2-hydroxy-2-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)ethyl]-3-(4-hydroxy-3-methoxyphenyl)propanimidic acid	C18H21NO6	M+Na-2H	368.1116	-1.2
	HMDB0136419	N-[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-3-(1-hydroxy-3-methoxy-4-oxocyclohexa-2,5-dien-1-yl)propanimidic acid	C18H21NO6	M+Na-2H	368.1116	-1.2
369.2641	HMDB0029797	(Z)-15-Oxo-11-eicosenoic acid	C20H36O3	M+FA-H	369.2646	-1.5
	HMDB0034958	(13R,14R)-7- Labdene-13,14,15-triol	C20H36O3	M+FA-H	369.2646	-1.5
	HMDB0034957	(13R,14R)-8- Labdene-13,14,15-triol	C20H36O3	M+FA-H	369.2646	-1.5
370.0557	HMDB0006880	Acetyl adenylate	C12H16N5O8P	M-H2O-H	370.0553	1.2
371.0648	HMDB0181366	3,4,5-trihydroxy-6-[(2-hydroxy-4-oxopentan-3-yl)sulfanyl]oxy}oxane-2-carboxylic acid	C11H18O9S	M+FA-H	371.0654	-1.5
	HMDB0181370	3,4,5-trihydroxy-6-[(1-hydroxy-4-oxopentan-3-yl)sulfanyl]oxy}oxane-2-carboxylic acid	C11H18O9S	M+FA-H	371.0654	-1.5
	HMDB0181374	3,4,5-trihydroxy-6-[(1-hydroxy-2-oxopentan-3-yl)sulfanyl]oxy}oxane-2-carboxylic acid	C11H18O9S	M+FA-H	371.0654	-1.5
371.2804	HMDB0092960	DG(8)	C21H40O5	M-H	371.2803	0.3
	HMDB0092902	DG(8/)	C21H40O5	M-H	371.2803	0.3
	HMDB0092959	DG(8)	C21H40O5	M-H	371.2803	0.3
	HMDB0092901	DG(8/)	C21H40O5	M-H	371.2803	0.3
	HMDB0172579	(11E)-19-hydroxyicos-11-enoic acid	C20H38O3	M+FA-H	371.2803	0.3
	HMDB0172577	13-hydroxyicos-11-enoic acid	C20H38O3	M+FA-H	371.2803	0.3
	HMDB0172578	(11E)--hydroxyicos-11-enoic acid	C20H38O3	M+FA-H	371.2803	0.3
	HMDB0172580	11,12-Epoxyicosanoic acid	C20H38O3	M+FA-H	371.2803	0.3
	HMDB0172581	(11E)--hydroxyicos-11-enoic acid	C20H38O3	M+FA-H	371.2803	0.3
	HMDB0172582	SCHEMBL19404	C20H38O3	M+FA-H	371.2803	0.3
373.0442	HMDB0171725	[4-hydroxy-5-(hydroxymethyl)-2-[(3,4,5,6-tetrahydroxyoxan-2-yl)methoxy]oxolan-3-yl]oxidanesulfonic acid	C11H20O13S	M-H2O-H	373.0441	0.3
	HMDB0171726	[4-hydroxy-2-(hydroxymethyl)-5-[(3,4,5,6-tetrahydroxyoxan-2-yl)methoxy]oxolan-3-yl]oxidanesulfonic acid	C11H20O13S	M-H2O-H	373.0441	0.3
	HMDB0171724	({3,4-dihydroxy-5-[(3,4,5,6-tetrahydroxyoxan-2-yl)methoxy]oxolan-2-yl} methoxy)sulfonic acid	C11H20O13S	M-H2O-H	373.0441	0.3
	HMDB0151114	{4,5-dihydroxy-6-[(3,4,5,6-tetrahydroxyoxan-2-yl)methoxy]oxan-3-yl} oxidanesulfonic acid	C11H20O13S	M-H2O-H	373.0441	0.3
	HMDB0151112	{4,5-dihydroxy-2-[(3,4,5,6-tetrahydroxyoxan-2-yl)methoxy]oxan-3-yl} oxidanesulfonic acid	C11H20O13S	M-H2O-H	373.0441	0.3
	HMDB0151113	{3,5-dihydroxy-2-[(3,4,5,6-tetrahydroxyoxan-2-yl)methoxy]oxan-4-yl} oxidanesulfonic acid	C11H20O13S	M-H2O-H	373.0441	0.3
	HMDB0140868	({3,4-dihydroxy-5-[(3,4,5,6-tetrahydroxyoxan-2-yl)methoxy]oxolan-3-yl} methoxy)sulfonic acid	C11H20O13S	M-H2O-H	373.0441	0.3
	HMDB0140869	[4-hydroxy-4-(hydroxymethyl)-2-[(3,4,5,6-tetrahydroxyoxan-2-yl)methoxy]oxolan-3-yl]oxidanesulfonic acid	C11H20O13S	M-H2O-H	373.0441	0.3
	HMDB0182838	3,4,5-trihydroxy-6-[(4-[(4-methoxyphenyl)methoxy]-4-oxobutan-2-yl}oxy)oxane-2-carboxylic acid	C18H24O10	M-H2O-H	381.1186	0.1
	HMDB0125816	3,4,5-trihydroxy-6-[(4-hydroxy-7-methoxy-2,2-dimethyl-3,4-dihydro-2H-1-benzopyran-5-yl)oxy]oxane-2-carboxylic acid	C18H24O10	M-H2O-H	381.1186	0.1

381.1186	HMDB0169503	3,4,5-trihydroxy-6-[2,3,6-trimethoxy-5-(prop-2-en-1-yl)phenoxy]oxane-2-carboxylic acid	C18H24O10	M-H2O-H	381.1186	0.1
	HMDB0169504	3,4,5-trihydroxy-6-[2,3,6-trimethoxy-4-(prop-2-en-1-yl)phenoxy]oxane-2-carboxylic acid	C18H24O10	M-H2O-H	381.1186	0.1
	HMDB0169502	3,4,5-trihydroxy-6-[2,3,4-trimethoxy-6-(prop-2-en-1-yl)phenoxy]oxane-2-carboxylic acid	C18H24O10	M-H2O-H	381.1186	0.1
	HMDB0127783	6-{[4-carboxy-1-(3-methoxyphenyl)butan-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C18H24O10	M-H2O-H	381.1186	0.1
	HMDB0127784	3,4,5-trihydroxy-6-{[4-hydroxy-5-(3-methoxyphenyl)pentanoyl]oxy}oxane-2-carboxylic acid	C18H24O10	M-H2O-H	381.1186	0.1
	HMDB0182842	3,4,5-trihydroxy-6-{4-[(4-methoxyphenyl)methoxy]-4-oxobutoxy}oxane-2-carboxylic acid	C18H24O10	M-H2O-H	381.1186	0.1
	HMDB0127790	6-[4-(4-carboxybutyl)-2-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C18H24O10	M-H2O-H	381.1186	0.1
	HMDB0127791	3,4,5-trihydroxy-6-{[5-(4-hydroxy-3-methoxyphenyl)pentanoyl]oxy}oxane-2-carboxylic acid	C18H24O10	M-H2O-H	381.1186	0.1
	HMDB0169505	3,4,5-trihydroxy-6-[2,3,4-trimethoxy-5-(prop-2-en-1-yl)phenoxy]oxane-2-carboxylic acid	C18H24O10	M-H2O-H	381.1186	0.1
	HMDB0182844	3,4,5-trihydroxy-6-({1-[(4-methoxyphenyl)methoxy]-1-oxobutan-2-yl}oxy)oxane-2-carboxylic acid	C18H24O10	M-H2O-H	381.1186	0.1
	HMDB0146037	2-(2-hydroperoxypropan-2-yl)-4-hydroxy-9-(3-hydroxypropyl)-2H,3H,7H-furo[2,3-f]chromen-7-one	C17H20O7	M+FA-H	381.1191	-1.3
	HMDB0146035	2-(2-hydroperoxypropan-2-yl)-4-hydroxy-9-(2-hydroxypropyl)-2H,3H,7H-furo[2,3-f]chromen-7-one	C17H20O7	M+FA-H	381.1191	-1.3
	HMDB0146034	2-(2-hydroperoxypropan-2-yl)-4-hydroxy-9-(1-hydroxypropyl)-2H,3H,7H-furo[2,3-f]chromen-7-one	C17H20O7	M+FA-H	381.1191	-1.3
	HMDB0146036	2-(2-hydroperoxy-1-hydroxypropan-2-yl)-4-hydroxy-9-propyl-2H,3H,7H-furo[2,3-f]chromen-7-one	C17H20O7	M+FA-H	381.1191	-1.3
	HMDB0178012	3,4,5-trihydroxy-6-[(8-hydroxy-6,7-dimethyl-5-oxo-5,6,7,8-tetrahydronaphthalen-1-yl)oxy]oxane-2-carboxylic acid	C18H22O9	M-H	381.1191	-1.3
	HMDB0140409	3,4,5-trihydroxy-6-[4-hydroxy-3-(3-methylbut-2-en-1-yl)benzoyloxy]oxane-2-carboxylic acid	C18H22O9	M-H	381.1191	-1.3
	HMDB0140408	6-[4-carboxy-2-(3-methylbut-2-en-1-yl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C18H22O9	M-H	381.1191	-1.3
	HMDB0178010	3,4,5-trihydroxy-6-[(5-hydroxy-6,7-dimethyl-8-oxo-5,6,7,8-tetrahydronaphthalen-1-yl)oxy]oxane-2-carboxylic acid	C18H22O9	M-H	381.1191	-1.3
	HMDB0172385	3,4,5-trihydroxy-6-{4-[(1E)-3-oxo-1,3,6,7-tetrahydro-2-benzofuran-1-ylidene]butoxy}oxane-2-carboxylic acid	C18H22O9	M-H	381.1191	-1.3
	HMDB0172381	3,4,5-trihydroxy-6-({4-[(1E)-3-oxo-1,3,6,7-tetrahydro-2-benzofuran-1-ylidene]butan-2-yl}oxy)oxane-2-carboxylic acid	C18H22O9	M-H	381.1191	-1.3
	HMDB0172379	6-{[(3E)-3-butylidene-1-oxo-1,3,4,5-tetrahydro-2-benzofuran-4-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C18H22O9	M-H	381.1191	-1.3
	HMDB0172377	6-{[(3E)-3-butylidene-1-oxo-1,3,4,5-tetrahydro-2-benzofuran-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C18H22O9	M-H	381.1191	-1.3
	HMDB0132995	3,4,5-trihydroxy-6-{[(4E)-5-(4-methoxyphenyl)-3-oxopent-4-en-1-yl]oxy}oxane-2-carboxylic acid	C18H22O9	M-H	381.1191	-1.3
	HMDB0132991	3,4,5-trihydroxy-6-{[(4E)-5-(4-methoxyphenyl)-3-oxopent-4-en-2-yl]oxy}oxane-2-carboxylic acid	C18H22O9	M-H	381.1191	-1.3
	HMDB0132990	3,4,5-trihydroxy-6-{5-methoxy-2-[(1E)-3-oxopent-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C18H22O9	M-H	381.1191	-1.3
	HMDB0015561	Zuclopenthixol	C22H25ClN2OS	M-H2O-H	381.1192	-1.6
381.1674	HMDB0014998	Prednisolone	C21H28O5	M+Na-2H	381.1683	-2.5
	HMDB0000037	Aldosterone	C21H28O5	M+Na-2H	381.1683	-2.5
	HMDB0002802	Cortisone	C21H28O5	M+Na-2H	381.1683	-2.5
	HMDB0035813	7-Methylrosmanol	C21H28O5	M+Na-2H	381.1683	-2.5
	HMDB0030165	Tricyclodehydroisohumulone	C21H28O5	M+Na-2H	381.1683	-2.5
	HMDB0012613	19-Oic-deoxycorticosterone	C21H28O5	M+Na-2H	381.1683	-2.5
	HMDB0167414	[3-(pentadec-14-en-1-yl)phenyl]oxidanesulfonic acid	C21H34O4S	M-H	381.2105	1.0

381.2109	HMDB0240579	ZINC3248	C21H36O5S	M-H2O-H	381.2100	2.5
	HMDB0167411	(2-hydroxy-3-pentadecylphenyl)oxidanesulfonic acid	C21H36O5S	M-H2O-H	381.2100	2.5
	HMDB0167407	(2-hydroxy-5-pentadecylphenyl)oxidanesulfonic acid	C21H36O5S	M-H2O-H	381.2100	2.5
	HMDB0167404	{[15-(3-hydroxyphenyl)pentadecyl]oxy}sulfonic acid	C21H36O5S	M-H2O-H	381.2100	2.5
	HMDB0167401	{[15-(3-hydroxyphenyl)pentadecan-2-yl]oxy}sulfonic acid	C21H36O5S	M-H2O-H	381.2100	2.5
	HMDB0167403	[3-(15-hydroxypentadecyl)phenyl]oxidanesulfonic acid	C21H36O5S	M-H2O-H	381.2100	2.5
	HMDB0167400	[3-(14-hydroxypentadecyl)phenyl]oxidanesulfonic acid	C21H36O5S	M-H2O-H	381.2100	2.5
	HMDB0167398	{[1-(3-hydroxyphenyl)pentadecyl]oxy}sulfonic acid	C21H36O5S	M-H2O-H	381.2100	2.5
	HMDB0167397	[3-(1-hydroxypentadecyl)phenyl]oxidanesulfonic acid	C21H36O5S	M-H2O-H	381.2100	2.5
381.3730	HMDB0240580	[(1R)-1-[(1S,2S,5S,7S,R,11S,14S,15S)-5-hydroxy-2,15-dimethyltetracyclo[8.7.,,]heptadecan-14-yl]ethoxy]sulfonic acid	C21H36O5S	M-H2O-H	381.2100	2.5
	HMDB0002361	Pentacosanoic acid	C25H50O2	M-H	381.3738	-2.1
	HMDB0036843	Lepidiumsesterterpenol	C25H50O2	M-H	381.3738	-2.1
	HMDB0035632	6-Hydroxy-4-pentacosanone	C25H50O2	M-H	381.3738	-2.1
	HMDB0035629	6-Hydroxy-8-pentacosanone	C25H50O2	M-H	381.3738	-2.1
382.0916	HMDB0035630	4-Hydroxy-6-pentacosanone	C25H50O2	M-H	381.3738	-2.1
	HMDB0029297	Avenanthramide A2	C18H19NO7	M+Na-2H	382.0908	2.0
	HMDB0039733	gamma-Glutamylcysteinylserine	C11H19N3O7S	M+FA-H	382.0926	-2.5
382.1287	HMDB0004662	S-(Hydroxymethyl)glutathione	C11H19N3O7S	M+FA-H	382.0926	-2.5
	HMDB0142818	(12aS)-4-(dimethylamino)-5,,12,12a-tetrahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H23NO7	M-H2O-H	382.1291	-0.9
	HMDB0142815	(12aS)-4-(dimethylamino)-3,5,,12,12a-pentahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H23NO7	M-H2O-H	382.1291	-0.9
	HMDB0142707	(12aR)-4-(dimethylamino)-5,,12a-trihydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H23NO7	M-H2O-H	382.1291	-0.9
	HMDB0142702	(12aS)-4-(dimethylamino)-5,,12,12a-tetrahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,3,11-trione	C21H23NO7	M-H2O-H	382.1291	-0.9
	HMDB0142819	(12aR)-4-(dimethylamino)-3,5,,12a-tetrahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H23NO7	M-H2O-H	382.1291	-0.9
	HMDB0142965	(6S,12aS)-4-(dimethylamino)-6,,12,12a-tetrahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,3,11-trione	C21H23NO7	M-H2O-H	382.1291	-0.9
	HMDB0031254	Margrapine A	C21H23NO7	M-H2O-H	382.1291	-0.9
	HMDB0142971	(6S,12aR)-4-(dimethylamino)-6,,12a-trihydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H23NO7	M-H2O-H	382.1291	-0.9
	HMDB0033524	Lambertine	C20H19NO4	M+FA-H	382.1296	-2.4
	HMDB0029827	Junosidine	C20H19NO4	M+FA-H	382.1296	-2.4
	HMDB0029332	5-Methoxynoracronycine	C20H19NO4	M+FA-H	382.1296	-2.4
	HMDB0038554	Gravacridonediolacetate	C21H21NO6	M-H	382.1296	-2.4
	HMDB0032878	13-Oxocryptopine	C21H21NO6	M-H	382.1296	-2.4
384.0700	HMDB0161251	3,4,5-trihydroxy-6- {(2E)-3-(1H-indol-2-yl)prop-2-enoyl]oxy}oxane-2-carboxylic acid	C17H17NO8	M+Na-2H	384.0701	-0.2
	HMDB0006806	Propinol adenylate	C13H18N5O8P	M-H2O-H	384.0709	-2.4
384.1063	HMDB0014291	Phosphatidylserine	C13H24NO10P	M-H	384.1065	-0.5
	HMDB0154103	3,5,7-trihydroxy-2-(1-hydroxy-3-methoxy-4-oxocyclohex-2-en-1-yl)-8-methoxy-4H-chromen-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0132232	2-(1,5-dihydroxy-4-oxocyclohex-2-en-1-yl)-5,7-dihydroxy-6,8-dimethoxy-4H-chromen-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0132231	2-(1,3-dihydroxy-4-oxocyclohex-2-en-1-yl)-5,7-dihydroxy-6,8-dimethoxy-4H-chromen-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0138031	2-(3,4-dihydroxy-5-methoxyphenyl)-5,6,7-trihydroxy-8-methoxy-3,4-dihydro-2H-1-benzopyran-4-one	C17H16O9	M+Na-2H	385.0541	-0.8

385.0538	HMDB0152093	3-(3,4-dihydroxy-5-methoxyphenyl)-1-(2,3,4,6-tetrahydroxy-5-methoxyphenyl)prop-2-en-1-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0152106	5,7-dihydroxy-6,8-dimethoxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0152110	1-(2,4,6-trihydroxy-3,5-dimethoxyphenyl)-3-(3,4,5-trihydroxyphenyl)prop-2-en-1-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0153229	5,7-dihydroxy-3,6-dimethoxy-2-(2,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0153225	5,7-dihydroxy-3,6-dimethoxy-2-(2,3,4-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0153226	5,7-dihydroxy-3,6-dimethoxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0153230	2-(1,5-dihydroxy-4-oxocyclohex-2-en-1-yl)-5,7-dihydroxy-3,6-dimethoxy-4H-chromen-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0153231	2-(1,3-dihydroxy-4-oxocyclohex-2-en-1-yl)-5,7-dihydroxy-3,6-dimethoxy-4H-chromen-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0154090	3,5,6,7-tetrahydroxy-2-(4-hydroxy-3-methoxyphenyl)-8-methoxy-3,4-dihydro-2H-1-benzopyran-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0154092	3-(4-hydroxy-3-methoxyphenyl)-1-(2,3,4,6-tetrahydroxy-5-methoxyphenyl)propane-1,2-dione	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0154102	3,5,7-trihydroxy-2-(1-hydroxy-5-methoxy-4-oxocyclohex-2-en-1-yl)-8-methoxy-4H-chromen-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0154099	2-(3,4-dihydroxy-5-methoxyphenyl)-3,5,7-trihydroxy-8-methoxy-3,4-dihydro-2H-1-benzopyran-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0132230	1-(2,4,6-trihydroxy-3,5-dimethoxyphenyl)-3-(2,4,5-trihydroxyphenyl)prop-2-en-1-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0132227	5,7-dihydroxy-6,8-dimethoxy-2-(2,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0038626	Xanthotoxol glucoside	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0128761	2-(3,4-dihydroxy-5-methoxyphenyl)-3,5,7-trihydroxy-6-methoxy-3,4-dihydro-2H-1-benzopyran-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0128763	3-(3,4-dihydroxy-5-methoxyphenyl)-1-(2,4,6-trihydroxy-3-methoxyphenyl)propane-1,2-dione	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0128767	3,5,7-trihydroxy-2-(1-hydroxy-3-methoxy-4-oxocyclohex-2-en-1-yl)-6-methoxy-4H-chromen-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0128766	3,5,7-trihydroxy-2-(1-hydroxy-5-methoxy-4-oxocyclohex-2-en-1-yl)-6-methoxy-4H-chromen-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0129280	2-(3,4-dimethoxyphenyl)-3,5,6,7,8-pentahydroxy-3,4-dihydro-2H-1-benzopyran-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0130278	2-(2,3-dihydroxy-4-methoxyphenyl)-3,5,7-trihydroxy-6-methoxy-3,4-dihydro-2H-1-benzopyran-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0130282	2-(2,5-dihydroxy-4-methoxyphenyl)-3,5,7-trihydroxy-6-methoxy-3,4-dihydro-2H-1-benzopyran-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0132220	5,7-dihydroxy-6,8-dimethoxy-2-(2,3,4-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	C17H16O9	M+Na-2H	385.0541	-0.8
	HMDB0132223	1-(2,4,6-trihydroxy-3,5-dimethoxyphenyl)-3-(2,3,4-trihydroxyphenyl)prop-2-en-1-one	C17H16O9	M+Na-2H	385.0541	-0.8
386.0508	HMDB0148115	2-[(4-[(6,7-dihydroxy-2-oxo-2H-chromen-3-yl)oxy]-3-hydroxyphenyl}(hydroxy)methylidene)amino]acetic acid	C18H13NO9	M-H	386.0518	-2.5
	HMDB0152296	2-({hydroxy[2-hydroxy-4-(3,5,7-trihydroxy-4-oxo-4H-chromen-2-yl)phenyl]methylidene}amino)acetic acid	C18H13NO9	M-H	386.0518	-2.5
388.2824	HMDB0062335	N-oleoyl gaba	C22H41NO3	M+Na-2H	388.2833	-2.3
390.2979	HMDB0062341	N-stearoyl gaba	C22H43NO3	M+Na-2H	390.2990	-2.7
393.3727	HMDB0183615	26-Hydroxyhexacosanoic acid	C26H52O3	M-H20-H	393.3733	-1.4
	HMDB0183616	2-hydroxyhexacosanoic acid	C26H52O3	M-H20-H	393.3733	-1.4
	HMDB0183614	25-hydroxyhexacosanoic acid	C26H52O3	M-H20-H	393.3733	-1.4
	HMDB0062452	(17Z)-hexacosenoic acid	C26H50O2	M-H	393.3738	-2.8
	HMDB0035554	4,6-Hexacosanedione	C26H50O2	M-H	393.3738	-2.8
	HMDB0035549	11,13-Hexacosanedione	C26H50O2	M-H	393.3738	-2.8
	HMDB0035553	5,7-Hexacosanedione	C26H50O2	M-H	393.3738	-2.8
	HMDB0035552	6,8-Hexacosanedione	C26H50O2	M-H	393.3738	-2.8
	HMDB0035550	,12-Hexacosanedione	C26H50O2	M-H	393.3738	-2.8
	HMDB0035215	Ximenic acid	C26H50O2	M-H	393.3738	-2.8
	HMDB0035551	7,9-Hexacosanedione	C26H50O2	M-H	393.3738	-2.8

395.3883	HMDB0002356	Hexacosanoic acid	C26H52O2	M-H	395.3895	-2.9
	HMDB0035628	6-Hydroxy-8-hexacosanone	C26H52O2	M-H	395.3895	-2.9
396.1080	HMDB0062525	S-(2-hydroxyethyl)glutathione	C12H21N3O7S	M+FA-H	396.1082	-0.6
	HMDB0144747	N-[(4aS)-4a,5,7,12-tetrahydroxy-11-methylidene-2,4,6-trioxo-1,2,3,4,4a,6,11,11a,12,12a-decahydrotetracen-1-yl]-N-methylmethanamine oxide	C21H21NO8	M-H2O-H	396.1083	-0.8
	HMDB0144762	(12aR)-4-(dimethylamino)-5,9,,12a-tetrahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H21NO8	M-H2O-H	396.1083	-0.8
	HMDB0144758	(12aR)-4-(dimethylamino)-4,5,,12a-tetrahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H21NO8	M-H2O-H	396.1083	-0.8
	HMDB0144745	(12aS)-4-(dimethylamino)-5,5a,,12,12a-pentahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,3,11-trione	C21H21NO8	M-H2O-H	396.1083	-0.8
	HMDB0144744	(12aS)-4-(dimethylamino)-2,5,,12,12a-pentahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,3,11-trione	C21H21NO8	M-H2O-H	396.1083	-0.8
	HMDB0144760	(12aR)-4-(dimethylamino)-5,8,,12a-tetrahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H21NO8	M-H2O-H	396.1083	-0.8
	HMDB0144740	(12aS)-4-(dimethylamino)-5,8,,12,12a-pentahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,3,11-trione	C21H21NO8	M-H2O-H	396.1083	-0.8
	HMDB0144741	(12aS)-4-(dimethylamino)-5,9,,12,12a-pentahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,3,11-trione	C21H21NO8	M-H2O-H	396.1083	-0.8
	HMDB0144768	(12aS)-4-(dimethylamino)-2,5,,12a-tetrahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H21NO8	M-H2O-H	396.1083	-0.8
	HMDB0144770	(12aR)-4-(dimethylamino)-5,5a,,12a-tetrahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H21NO8	M-H2O-H	396.1083	-0.8
	HMDB0144774	N-[(4aR)-4a,7,12-trihydroxy-11-methylidene-2,4,5,6-tetraoxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracen-1-yl]-N-methylmethanamine oxide	C21H21NO8	M-H2O-H	396.1083	-0.8
	HMDB0144772	(12aR)-4-(dimethylamino)-4a,5,,12a-tetrahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H21NO8	M-H2O-H	396.1083	-0.8
	HMDB0144777	(12aR)-4-(dimethylamino)-5,,11a,12a-tetrahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H21NO8	M-H2O-H	396.1083	-0.8
	HMDB0144739	(12aS)-4-(dimethylamino)-4,5,,12,12a-pentahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,3,11-trione	C21H21NO8	M-H2O-H	396.1083	-0.8
	HMDB0144746	(12aR)-4-(dimethylamino)-4a,5,,12,12a-pentahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,3,11-trione	C21H21NO8	M-H2O-H	396.1083	-0.8
	HMDB0015042	Tiagabine	C20H25NO2S2	M+Na-2H	396.1073	1.7
	HMDB0187655	CHEMBL3759987	C20H18NO5	M+FA-H	396.1089	-2.2
	HMDB0187658	Berberastine	C20H18NO5	M+FA-H	396.1089	-2.2
	HMDB0187657	12-hydroxy-16,17-dimethoxy-5,7-dioxo-13-azapentacyclo[11.8,,]henicosa-1(13),2,4(8),9,14,16,18,-octaen-13-ylum	C20H18NO5	M+FA-H	396.1089	-2.2
	HMDB0029337	Ceanothine D	C20H17NO5	M+FA-H	396.1089	-2.2
402.0113	HMDB0155219	[([3,4-dihydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-2-yl]methoxy}(hydroxy)phosphoryl)oxy]phosphonic acid	C9H15N3O11P2	M-H	402.0109	1.0
	HMDB0001546	CDP	C9H15N3O11P2	M-H	402.0109	1.0
402.9943	HMDB0000295	Uridine 5'-diphosphate	C9H14N2O12P2	M-H	402.9949	-1.5

402.9949	HMDB0156308	UDP - Na	C9H14N2O12P2	M-H	402.9949	-1.5
410.1232	HMDB0142769	(12aR)-3,5,,12a-tetrahydroxy-6-methyl-4-(methylamino)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C20H23NO7	M+Na-2H	410.1221	2.6
	HMDB0143033	(6S,12aS)-3,6,,12,12a-pentahydroxy-6-methyl-4-(methylamino)-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C20H23NO7	M+Na-2H	410.1221	2.6
	HMDB0142768	(12aS)-5,,12,12a-tetrahydroxy-6-methyl-4-(methylamino)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C20H23NO7	M+Na-2H	410.1221	2.6
	HMDB0143037	(6S,12aR)-3,6,,12a-tetrahydroxy-6-methyl-4-(methylamino)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C20H23NO7	M+Na-2H	410.1221	2.6
	HMDB0143036	(6S,12aS)-6,,12,12a-tetrahydroxy-6-methyl-4-(methylamino)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C20H23NO7	M+Na-2H	410.1221	2.6
	HMDB0142765	(12aS)-3,5,,12,12a-pentahydroxy-6-methyl-4-(methylamino)-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C20H23NO7	M+Na-2H	410.1221	2.6
	HMDB0144971	(4aS)--(dimethylamino)-2,4a,5,7-tetrahydroxy-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,4,6-trione	C20H23NO7	M+Na-2H	410.1221	2.6
412.1019	HMDB0034811	Ribosylzeatin phosphate	C15H22N5O8P	M-H2O-H	412.1022	-0.7
	HMDB0162577	6-({1,4-diamino-4-[(2-sulfoethyl)-C-hydroxycarbonimidoyl]butan-2-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H25N3O11S	M-H2O-H	412.1026	-1.7
	HMDB0162575	6-({1,4-diamino-1-[(2-sulfoethyl)-C-hydroxycarbonimidoyl]butan-2-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C13H25N3O11S	M-H2O-H	412.1026	-1.7
412.1377	HMDB0143038	(6S,12aS)-3,6,,12,12a-pentahydroxy-6-methyl-4-(methylamino)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11-dione	C20H25NO7	M+Na-2H	412.1378	-0.2
	HMDB0142770	(12aS)-3,5,,12,12a-pentahydroxy-6-methyl-4-(methylamino)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11-dione	C20H25NO7	M+Na-2H	412.1378	-0.2
	HMDB0038793	Melleolide G	C24H32O7	M-H2O-H	413.1964	-1.0
	HMDB0038787	Melleolide B	C24H32O7	M-H2O-H	413.1964	-1.0
	HMDB0179891	(2E,4E,6E,8E,E,12E,14E,16E)-18-methoxy-4,8,13,17-tetramethyl-18-oxooctadeca-2,4,6,8,,12,14,16-octaenoic acid	C23H28O4	M+FA-H	413.1970	-2.3
	HMDB0148759	5-hydroxy-8-(hydroxymethyl)-8-methyl-6-(3-methylbutanoyl)-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0147026	5-hydroxy-4-(5-hydroxypentyl)-8,8-dimethyl-6-(2-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0147025	5-hydroxy-6-[2-(hydroxymethyl)butanoyl]-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0147024	5-hydroxy-6-(4-hydroxy-2-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0147022	5-hydroxy-4-(4-hydroxypentyl)-8,8-dimethyl-6-(2-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0147020	5-hydroxy-6-(2-hydroxy-2-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0147021	5-hydroxy-6-(3-hydroxy-2-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0147019	5-hydroxy-4-(1-hydroxypentyl)-8,8-dimethyl-6-(2-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0147018	5-hydroxy-8-(hydroxymethyl)-8-methyl-6-(2-methylbutanoyl)-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0041407	Clausarinol	C24H30O6	M-H	413.1970	-2.3
	HMDB0148762	5-hydroxy-4-(4-hydroxypentyl)-8,8-dimethyl-6-(3-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M-H	413.1970	-2.3

413.1960	HMDB0148761	5-hydroxy-6-(3-hydroxy-3-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0148760	5-hydroxy-4-(1-hydroxypentyl)-8,8-dimethyl-6-(3-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0168750	7-[(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-5-hydroxy-2H-chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0168747	7-[(2E)-5-hydroxy-5-[3-(1-hydroxy-4-methylpent-3-en-1-yl)-3-methyloxiran-2-yl]-3-methylpent-2-en-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0168749	7-[(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-8-hydroxy-2H-chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0168746	7-({3-[(3Z)-2,5-dihydroxy-4,8-dimethylnona-3,7-dien-1-yl]-3-methyloxiran-2-yl}methoxy)-2H-chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0168748	7-[(2E,6Z)-9-(3,3-dimethyloxiran-2-yl)-5,8-dihydroxy-3,7-dimethylnona-2,6-dien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0168743	7-[(2E,6Z)-5,8,12-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0168745	7-[(2E,6Z)-5,8,9-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0168742	7-[(2E,6Z)-5,8-dihydroxy-7-(hydroxymethyl)-3,11-dimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0168744	7-[(2E,6Z,E)-5,8,12-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0168741	7-[(2Z,6Z)-5,8-dihydroxy-3-(hydroxymethyl)-7,11-dimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0168739	7-[(2E,6Z)-5,8-dihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-6-hydroxy-2H-chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0168740	7-[(2E,6Z)-4,5,8-trihydroxy-3,7,11-trimethyldodeca-2,6,-trien-1-yl]oxy}-2H-chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0148765	5-hydroxy-4-(5-hydroxypentyl)-8,8-dimethyl-6-(3-methylbutanoyl)-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0148764	5-hydroxy-6-(4-hydroxy-3-methylbutanoyl)-8,8-dimethyl-4-pentyl-2H,8H-pyrano[2,3-f]chromen-2-one	C24H30O6	M-H	413.1970	-2.3
	HMDB0039380	Armillarin	C24H30O6	M-H	413.1970	-2.3
	HMDB0014838	Eplerenone	C24H30O6	M-H	413.1970	-2.3
414.0811	HMDB0030404	Armillaripin	C24H30O6	M-H	413.1970	-2.3
	HMDB0037039	4-O-Methylmelleolide	C24H30O6	M-H	413.1970	-2.3
414.0811	HMDB0165851	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-(phenyldisulfanyl)ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C16H21N3O6S2	M-H	414.0799	2.9
418.0392	HMDB0162801	6-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-5-hydroxy-4-oxo-1,4-dihydroquinoline-2-carboxylic acid	C16H15NO11	M+Na-2H	418.0392	0.1
	HMDB0162800	5-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-6-hydroxy-4-oxo-1,4-dihydroquinoline-2-carboxylic acid	C16H15NO11	M+Na-2H	418.0392	0.1
	HMDB0162802	6-(5,6-dihydroxy-4-oxo-1,4-dihydroquinoline-2-carbonyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H15NO11	M+Na-2H	418.0392	0.1
	HMDB0162799	3,4,5-trihydroxy-6-(4,6,8-trihydroxyquinoline-2-carbonyloxy)oxane-2-carboxylic acid	C16H15NO11	M+Na-2H	418.0392	0.1
	HMDB0162797	8-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-4,6-dihydroxyquinoline-2-carboxylic acid	C16H15NO11	M+Na-2H	418.0392	0.1
	HMDB0162798	6-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-4,8-dihydroxyquinoline-2-carboxylic acid	C16H15NO11	M+Na-2H	418.0392	0.1
	HMDB0162796	6-(6,7-dihydroxy-4-oxo-1,4-dihydroquinoline-2-carbonyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H15NO11	M+Na-2H	418.0392	0.1
	HMDB0162794	7-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-6-hydroxy-4-oxo-1,4-dihydroquinoline-2-carboxylic acid	C16H15NO11	M+Na-2H	418.0392	0.1
	HMDB0162795	6-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-7-hydroxy-4-oxo-1,4-dihydroquinoline-2-carboxylic acid	C16H15NO11	M+Na-2H	418.0392	0.1

424.1381	HMDB0142709	(12aR)-4-(dimethylamino)-3,5,,12a-tetrahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO7	M+Na-2H	424.1378	0.8
	HMDB0142708	(12aS)-4-(dimethylamino)-5,,12,12a-tetrahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO7	M+Na-2H	424.1378	0.8
	HMDB0142820	(12aS)-4-(dimethylamino)-3,5,,12,12a-pentahydroxy-6-methylidene-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11-dione	C21H25NO7	M+Na-2H	424.1378	0.8
	HMDB0142969	(6S,12aS)-4-(dimethylamino)-3,6,,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO7	M+Na-2H	424.1378	0.8
	HMDB0142972	(6S,12aS)-4-(dimethylamino)-6,,12,12a-tetrahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO7	M+Na-2H	424.1378	0.8
	HMDB0142973	(6S,12aR)-4-(dimethylamino)-3,6,,12a-tetrahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO7	M+Na-2H	424.1378	0.8
	HMDB0142705	(12aS)-4-(dimethylamino)-3,5,,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO7	M+Na-2H	424.1378	0.8
	HMDB0001056	Dihydrofolic acid	C19H21N7O6	M-H2O-H	424.1369	2.7
426.0215	HMDB0000061	Adenosine 3',5'-diphosphate	C10H15N5O10P2	M-H	426.0221	-1.5
	HMDB0000960	dGDP	C10H15N5O10P2	M-H	426.0221	-1.5
	HMDB0001341	ADP	C10H15N5O10P2	M-H	426.0221	-1.5
	HMDB0160059	ADP	C10H15N5O10P2	M-H	426.0221	-1.5
	HMDB0037198	D-Gluconic acid Mn(II) salt	C12H22MnO14	M-H2O-H	426.0206	2.1
426.1168	HMDB0032809	4-Hydroxyphenylacetoneitrile triacetylramnoside	C20H23NO8	M+Na-2H	426.1170	-0.5
	HMDB0144016	(6S,12aR)-5,6,,11,12a-pentahydroxy-6-methyl-4-(methylamino)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,12-trione	C20H23NO8	M+Na-2H	426.1170	-0.5
	HMDB0144017	(6S,12aR)-3,5,6,,12a-pentahydroxy-6-methyl-4-(methylamino)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C20H23NO8	M+Na-2H	426.1170	-0.5
	HMDB0144013	(6S,12aR)-3,5,6,,11,12a-hexahydroxy-6-methyl-4-(methylamino)-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracene-1,12-dione	C20H23NO8	M+Na-2H	426.1170	-0.5
427.0652	HMDB0135169	3,4,5-trihydroxy-6-[2-hydroxy-3-(phenoxycarbonyl)phenoxy]oxane-2-carboxylic acid	C19H18O10	M+Na-2H	427.0647	1.3
	HMDB0135173	3,4,5-trihydroxy-6-[4-hydroxy-3-(phenoxycarbonyl)phenoxy]oxane-2-carboxylic acid	C19H18O10	M+Na-2H	427.0647	1.3
	HMDB0135170	3,4,5-trihydroxy-6-[2-hydroxy-6-(phenoxycarbonyl)phenoxy]oxane-2-carboxylic acid	C19H18O10	M+Na-2H	427.0647	1.3
	HMDB0135175	3,4,5-trihydroxy-6-[2-(2-hydroxybenzoyloxy)phenoxy]oxane-2-carboxylic acid	C19H18O10	M+Na-2H	427.0647	1.3
	HMDB0135174	3,4,5-trihydroxy-6-[4-hydroxy-2-(phenoxycarbonyl)phenoxy]oxane-2-carboxylic acid	C19H18O10	M+Na-2H	427.0647	1.3
	HMDB0135177	3,4,5-trihydroxy-6-[3-(2-hydroxybenzoyloxy)phenoxy]oxane-2-carboxylic acid	C19H18O10	M+Na-2H	427.0647	1.3
	HMDB0135176	3,4,5-trihydroxy-6-{2-[(2-hydroxyphenoxy)carbonyl]phenoxy} oxane-2-carboxylic acid	C19H18O10	M+Na-2H	427.0647	1.3
	HMDB0135180	3,4,5-trihydroxy-6-{2-[(4-hydroxyphenoxy)carbonyl]phenoxy} oxane-2-carboxylic acid	C19H18O10	M+Na-2H	427.0647	1.3
	HMDB0135179	3,4,5-trihydroxy-6-[4-(2-hydroxybenzoyloxy)phenoxy]oxane-2-carboxylic acid	C19H18O10	M+Na-2H	427.0647	1.3

	HMDB0135178	3,4,5-trihydroxy-6-{2-[(3-hydroxyphenoxy)carbonyl]phenoxy}oxane-2-carboxylic acid	C19H18O10	M+Na-2H	427.0647	1.3
	HMDB0137977	6-(2-benzoyl-3,5-dihydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C19H18O10	M+Na-2H	427.0647	1.3
	HMDB0128966	3,4,5-trihydroxy-6-{[2-oxo-6-(3-oxobut-1-en-1-yl)-2H-chromen-7-yl]oxy}oxane-2-carboxylic acid	C19H18O10	M+Na-2H	427.0647	1.3
	HMDB0137978	6-(4-benzoyl-3,5-dihydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C19H18O10	M+Na-2H	427.0647	1.3
428.1337	HMDB0144018	(6S,12aR)-3,5,6,,11,12a-hexahydroxy-6-methyl-4-(methylamino)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,12-dione	C20H25NO8	M+Na-2H	428.1327	2.4
	HMDB0178294	6-(2-{4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]phenyl}-2-oxoethyl)-1-methyl-2,3,4,5-tetrahydropyridin-1-ium	C20H26NO8	M+Na-2H	428.1327	2.4
	HMDB0178296	2-(2-{4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]phenyl}-2-oxoethyl)-1-methyl-2,3,4,5-tetrahydropyridin-1-ium	C20H26NO8	M+Na-2H	428.1327	2.4
436.2831	HMDB0011152	LysoPE(P-16)	C21H44NO6P	M-H	436.2833	-0.6
440.0971	HMDB0161800	3,4,5-trihydroxy-6-{[6-(hydroxymethyl)-8-methoxy-9H-carbazol-2-yl]oxy}oxane-2-carboxylic acid	C20H21NO9	M+Na-2H	440.0963	1.8
	HMDB0142776	(12aS)-3,5,,12,12a-pentahydroxy-6-methyl-1,4,11-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximide acid	C20H21NO9	M+Na-2H	440.0963	1.8
	HMDB0144451	(6S,12aS)-3,6,,12,12a-pentahydroxy-6-methyl-1,4,11-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximide acid	C20H21NO9	M+Na-2H	440.0963	1.8
	HMDB0161798	3,4,5-trihydroxy-6-{[6-(hydroxymethyl)-8-methoxy-9H-carbazol-3-yl]oxy}oxane-2-carboxylic acid	C20H21NO9	M+Na-2H	440.0963	1.8
	HMDB0161808	3,4,5-trihydroxy-6-{[6-(hydroxymethyl)-8-methoxy-9H-carbazol-4-yl]oxy}oxane-2-carboxylic acid	C20H21NO9	M+Na-2H	440.0963	1.8
	HMDB0161802	3,4,5-trihydroxy-6-{[3-(hydroxymethyl)-1-methoxy-9H-carbazol-2-yl]oxy}oxane-2-carboxylic acid	C20H21NO9	M+Na-2H	440.0963	1.8
	HMDB0161806	3,4,5-trihydroxy-6-{[6-(hydroxymethyl)-8-methoxy-9H-carbazol-1-yl]oxy}oxane-2-carboxylic acid	C20H21NO9	M+Na-2H	440.0963	1.8
	HMDB0168837	2-amino-4-({2-[(1-carboxy-2-hydroxyethyl)sulfanyl]-1-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C13H21N3O9S	M+FA-H	440.0981	-2.2
	HMDB0172024	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{[(2Z)-1,2,3-trihydroxyprop-2-en-1-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C13H21N3O9S	M+FA-H	440.0981	-2.2
	HMDB0000121	Folic acid	C19H19N7O6	M-H	440.1324	0.0
	HMDB0143016	(6S,12aS)-4-(dimethylamino)-6,8,,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
	HMDB0143017	(6S,12aR)-4-(dimethylamino)-3,6,8,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
	HMDB0143023	(6S,12aS)-4-(dimethylamino)-3,6,9,,12,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO8	M+Na-2H	440.1327	-0.6
	HMDB0143026	(6S,12aS)-4-(dimethylamino)-6,9,,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
	HMDB0143027	(6S,12aR)-4-(dimethylamino)-3,6,9,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6

HMDB0143013	(6S,12aS)-4-(dimethylamino)-3,6,8,,12,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142993	(6S,12aR)-4-(dimethylamino)-3,6,,12a-tetrahydroxy-6-(hydroxymethyl)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142992	(6S,12aS)-4-(dimethylamino)-6,,12,12a-tetrahydroxy-6-(hydroxymethyl)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142989	(6S,12aS)-4-(dimethylamino)-3,6,,12,12a-pentahydroxy-6-(hydroxymethyl)-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142983	(6S,12aR)-4-(dimethylamino)-3,4,6,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142982	(6S,12aS)-4-(dimethylamino)-4,6,,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142979	(6S,12aS)-4-(dimethylamino)-3,4,6,,12,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142838	(12aR)-4-(dimethylamino)-3,5,,11a,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142834	(12aS)-4-(dimethylamino)-2,5,,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0143067	(6R,12aS)-4-(dimethylamino)-3,5a,6,,12,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0143071	(6R,12aR)-4-(dimethylamino)-3,5a,6,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0143081	(6S,12aR)-4-(dimethylamino)-3,4a,6,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0143964	(6S,12aR)-4-(dimethylamino)-3,5,6,,11,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracene-1,12-dione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0143966	(6S,12aR)-4-(dimethylamino)-5,6,,11,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0143110	(6S,12aR)-4-(dimethylamino)-3,6,,11a,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0143106	(6S,12aS)-4-(dimethylamino)-2,6,,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0143100	(6S,12aS)-4-(dimethylamino)-6,,11a,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0143096	(6S,12aS)-4-(dimethylamino)-2,3,6,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6

HMDB0143094	(6S,12aS)-4-(dimethylamino)-2,3,6,,12,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0143091	N-[(4aR,11S)-2,4a,7,11-tetrahydroxy-11-methyl-4,5,6-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1-yl]-N-methylmethanamine oxide	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0143090	N-[(4aS,11S)-4a,5,7,11-tetrahydroxy-11-methyl-2,4,6-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1-yl]-N-methylmethanamine oxide	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0143087	N-[(4aS,11S)-2,4a,5,7,11-pentahydroxy-11-methyl-4,6-dioxo-1,2,3,4,4a,6,11,11a,12,12a-decahydrotetracene-1-yl]-N-methylmethanamine oxide	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0143080	(6S,12aR)-4-(dimethylamino)-4a,6,,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0143077	(6S,12aR)-4-(dimethylamino)-3,4a,6,,12,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0143070	(6R,12aS)-4-(dimethylamino)-5a,6,,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142828	(12aS)-4-(dimethylamino)-5,,11a,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142822	(12aS)-4-(dimethylamino)-2,3,5,,12,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142824	(12aS)-4-(dimethylamino)-2,3,5,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142745	(12aS)-4-(dimethylamino)-3,5,8,,12,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142738	(12aS)-4-(dimethylamino)-5,6,,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142739	(12aR)-4-(dimethylamino)-3,5,6,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142735	(12aS)-4-(dimethylamino)-3,5,6,,12,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142728	(12aS)-4-(dimethylamino)-5,,12,12a-tetrahydroxy-6-(hydroxymethyl)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142729	(12aR)-4-(dimethylamino)-3,5,,12a-tetrahydroxy-6-(hydroxymethyl)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142725	(12aS)-4-(dimethylamino)-3,5,,12,12a-pentahydroxy-6-(hydroxymethyl)-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142719	(12aR)-4-(dimethylamino)-3,4,5,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142718	(12aS)-4-(dimethylamino)-4,5,,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142715	(12aS)-4-(dimethylamino)-3,4,5,,12,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO8	M+Na-2H	440.1327	-0.6

HMDB0142749	(12aR)-4-(dimethylamino)-3,5,8,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142748	(12aS)-4-(dimethylamino)-5,8,,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142808	N-[(4aS)-4a,5,7,12-tetrahydroxy-11-methyl-2,4,6-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1-yl]-N-methylmethanamine oxide	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142809	N-[(4aR)-2,4a,7,12-tetrahydroxy-11-methyl-4,5,6-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1-yl]-N-methylmethanamine oxide	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142805	N-[(4aS)-2,4a,5,7,12-pentahydroxy-11-methyl-4,6-dioxo-1,2,3,4,4a,6,11,11a,12,12a-decahydrotetracene-1-yl]-N-methylmethanamine oxide	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142799	(12aR)-4-(dimethylamino)-3,5,5a,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142798	(12aS)-4-(dimethylamino)-5,5a,,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142795	(12aS)-4-(dimethylamino)-3,5,5a,,12,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142789	(12aR)-4-(dimethylamino)-3,4a,5,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142788	(12aR)-4-(dimethylamino)-4a,5,,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142785	(12aR)-4-(dimethylamino)-3,4a,5,,12,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142758	(12aS)-4-(dimethylamino)-5,9,,12,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142759	(12aR)-4-(dimethylamino)-3,5,9,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0142755	(12aS)-4-(dimethylamino)-3,5,9,,12,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-1,11-dione	C21H25NO8	M+Na-2H	440.1327	-0.6
HMDB0014349	Dofetilide	C19H27N3O5S2	M-H	440.1319	1.1
HMDB0155306	2-[(4-{[(5-carbamimidamido-6-carboxy-4,5-dihydropyrazin-2-yl)methyl]amino}phenyl)formamido]pentanedioic acid	C19H21N7O7	M-H2O-H	440.1319	1.2
HMDB0059648	8-oxo-dGDP	C10H15N5O11P2	M-H	442.0171	-1.0
HMDB0001201	Guanosine diphosphate	C10H15N5O11P2	M-H	442.0171	-1.0
HMDB0176764	6-[(4-chloro-2-hydroxy-6,7-dimethoxy-1,3-benzoxazol-5-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C15H16ClNO11	M+Na-2H	442.0159	1.7
HMDB0038730	5-O-p-Coumaroylnigrumin	C20H23NO9	M+Na-2H	442.1119	0.6
HMDB0162114	3,4,5-trihydroxy-6-{[6-oxo-1-(3-phenylpropanoyl)-1,2,3,6-tetrahydropyridin-3-yl]oxy}oxane-2-carboxylic acid	C20H23NO9	M+Na-2H	442.1119	0.6
HMDB0144927	(12aS)-4-(dimethylamino)-3,,12,12a-tetrahydroxy-7-(methylamino)-1,11-dioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C22H29N3O7	M-H	446.1933	0.1

446.1933	HMDB0144957	(12aS)-7-(dimethylamino)-3,,12,12a-tetrahydroxy-4-(methylamino)-1,11-dioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C22H29N3O7	M-H	446.1933	0.1
	HMDB0184978	[(15S)-8-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-15-methyl-5-oxotetracyclo[8.7,,heptadec-6-en-14-yl]oxidanyl	C24H33O9	M-H2O-H	446.1941	-1.7
454.1119	HMDB0042044	Tolmetin glucuronide	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0144005	(6S,12aR)-4-(dimethylamino)-5,6,9,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0144030	(6R,12aR)-4-(dimethylamino)-5,5a,6,,11,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracene-1,3,12-trione	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0144034	(6R,12aR)-4-(dimethylamino)-5,5a,6,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0144039	(6S,12aR)-4-(dimethylamino)-4a,5,6,,11,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracene-1,3,12-trione	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0144044	(6S,12aR)-4-(dimethylamino)-4a,5,6,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0144049	N-[(4aR,11S)-4a,6,7,11,12-pentahydroxy-11-methyl-2,4,5-trioxo-1,2,3,4,4a,5,11,11a,12,12a-decahydrotetracen-1-yl]-N-methylmethanamine oxide	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0144054	N-[(4aR,11S)-4a,7,11,12-tetrahydroxy-11-methyl-2,4,5,6-tetraoxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracen-1-yl]-N-methylmethanamine oxide	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0144066	(6S,12aS)-4-(dimethylamino)-2,5,6,,11,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracene-1,3,12-trione	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0144069	(6S,12aR)-4-(dimethylamino)-5,6,,11a,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0144000	(6S,12aR)-4-(dimethylamino)-5,6,9,,11,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracene-1,3,12-trione	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0143995	(6S,12aR)-4-(dimethylamino)-5,6,8,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0143989	(6S,12aR)-4-(dimethylamino)-5,6,8,,11,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracene-1,3,12-trione	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0143984	(6S,12aR)-4-(dimethylamino)-5,6,,12a-tetrahydroxy-6-(hydroxymethyl)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0143979	(6S,12aR)-4-(dimethylamino)-5,6,,11,12a-pentahydroxy-6-(hydroxymethyl)-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracene-1,3,12-trione	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0143974	(6S,12aR)-4-(dimethylamino)-4,5,6,,12a-pentahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,11,12-tetrone	C21H23NO9	M+Na-2H	454.1119	-0.1
	HMDB0143969	(6S,12aR)-4-(dimethylamino)-4,5,6,,11,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracene-1,3,12-trione	C21H23NO9	M+Na-2H	454.1119	-0.1

454.1481	HMDB0062623	5,-methenyltetrahydrofolate mono-L-glutamate	C20H20N7O6	M-H	454.1481	0.1
	HMDB0001354	5,-Methenyltetrahydrofolic acid	C20H21N7O6	M-H	454.1481	0.1
	HMDB0162771	3,4,5-trihydroxy-6- {[(4Z,6E,8Z)-9-(2-methyl-2H-azepin-7-yl)-3-oxonona-4,6,8-trien-1-yl]oxy} oxane-2-carboxylic acid	C22H27NO8	M+Na-2H	454.1483	-0.5
	HMDB0162757	3,4,5-trihydroxy-6- ({7-[(1Z,5Z)-7-oxonona-1,3,5-trien-1-yl]-2H-azepin-2-yl} methoxy)oxane-2-carboxylic acid	C22H27NO8	M+Na-2H	454.1483	-0.5
	HMDB0162713	3,4,5-trihydroxy-6- {[(4Z)-1-oxo-1-(1,2,3,4-tetrahydropyridin-1-yl)undec-4-en-8,-diyn-2-yl]oxy} oxane-2-carboxylic acid	C22H27NO8	M+Na-2H	454.1483	-0.5
	HMDB0162709	3,4,5-trihydroxy-6- {[11-oxo-11-(1,2,3,4-tetrahydropyridin-1-yl)undec-7-en-1,3-diyn-6-yl]oxy} oxane-2-carboxylic acid	C22H27NO8	M+Na-2H	454.1483	-0.5
	HMDB0162707	3,4,5-trihydroxy-6- {[(4Z)-1-oxo-1-(1,2,3,4-tetrahydropyridin-1-yl)undec-4-en-8,-diyn-3-yl]oxy} oxane-2-carboxylic acid	C22H27NO8	M+Na-2H	454.1483	-0.5
	HMDB0162759	3,4,5-trihydroxy-6- {[(4Z,8Z)-9-(2-methyl-2H-azepin-7-yl)-3-oxonona-4,6,8-trien-2-yl]oxy} oxane-2-carboxylic acid	C22H27NO8	M+Na-2H	454.1483	-0.5
	HMDB0014624	Raloxifene	C28H27NO4S	M-H2O-H	454.1477	0.9
	HMDB0002140	Pteroyl-D-glutamic acid	C20H23N7O7	M-H2O-H	454.1475	1.3
	HMDB0000972	-Formyltetrahydrofolate	C20H23N7O7	M-H2O-H	454.1475	1.3
	HMDB0062757	N5-Formyl-THF	C20H23N7O7	M-H2O-H	454.1475	1.3
	HMDB0001562	Folinic acid	C20H23N7O7	M-H2O-H	454.1475	1.3
	HMDB0015108	Ezetimibe	C24H21F2NO ₃	M+FA-H	454.1472	2.1
456.0914	HMDB0144024	(6S,12aS)-3,5,6,,11,12a-hexahydroxy-6-methyl-1,4,12-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximide acid	C20H21NO10	M+Na-2H	456.0912	0.4
	HMDB0144033	(6R,12aR)-4-(dimethylamino)-3,5,5a,6,,11,12a-heptahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracene-1,12-dione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0144007	(6S,12aR)-4-(dimethylamino)-3,5,6,9,,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0144035	(6R,12aR)-4-(dimethylamino)-5,5a,6,,11,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,12-trione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0144036	(6R,12aR)-4-(dimethylamino)-3,5,5a,6,,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0144042	(6S,12aR)-4-(dimethylamino)-3,4a,5,6,,11,12a-heptahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracene-1,12-dione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0144045	(6S,12aR)-4-(dimethylamino)-4a,5,6,,11,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,12-trione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0144046	(6S,12aR)-4-(dimethylamino)-3,4a,5,6,,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0144052	N-[(4aR,11S)-2,4a,6,7,11,12-hexahydroxy-11-methyl-4,5-dioxo-1,2,3,4,4a,5,11,11a,12,12a-decahydrotetracene-1-yl]-N-methylmethanamine oxide	C21H25NO9	M+Na-2H	456.1276	0.9

456.1280	HMDB0144056	N-[(4aR,11S)-2,4a,7,11,12-pentahydroxy-11-methyl-4,5,6-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracen-1-yl]-N-methylmethanamine oxide	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0144055	N-[(4aR,11S)-4a,6,7,11,12-pentahydroxy-11-methyl-2,4,5-trioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracen-1-yl]-N-methylmethanamine oxide	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0144060	(6S,12aS)-4-(dimethylamino)-2,3,5,6,,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0144003	(6S,12aR)-4-(dimethylamino)-3,5,6,9,,11,12a-heptahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracene-1,12-dione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0144006	(6S,12aR)-4-(dimethylamino)-5,6,9,,11,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,12-trione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0144070	(6S,12aR)-4-(dimethylamino)-3,5,6,,11a,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0143972	(6S,12aR)-4-(dimethylamino)-3,4,5,6,,11,12a-heptahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracene-1,12-dione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0143975	(6S,12aR)-4-(dimethylamino)-4,5,6,,11,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,12-trione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0143976	(6S,12aR)-4-(dimethylamino)-3,4,5,6,,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0143982	(6S,12aR)-4-(dimethylamino)-3,5,6,,11,12a-hexahydroxy-6-(hydroxymethyl)-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracene-1,12-dione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0143985	(6S,12aR)-4-(dimethylamino)-5,6,,11,12a-pentahydroxy-6-(hydroxymethyl)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,12-trione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0143986	(6S,12aR)-4-(dimethylamino)-3,5,6,,12a-pentahydroxy-6-(hydroxymethyl)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0143992	(6S,12aR)-4-(dimethylamino)-3,5,6,8,,11,12a-heptahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,12,12a-decahydrotetracene-1,12-dione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0143996	(6S,12aR)-4-(dimethylamino)-5,6,8,,11,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,3,12-trione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0143997	(6S,12aR)-4-(dimethylamino)-3,5,6,8,,12a-hexahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,11,12-trione	C21H25NO9	M+Na-2H	456.1276	0.9
	HMDB0162131	3,4,5-trihydroxy-6-[3-(3-hydroxy-6-oxo-1,2,3,6-tetrahydropyridin-1-yl)-3-oxo-1-phenylpropoxy]oxane-2-carboxylic acid	C20H23NO10	M+Na-2H	458.1069	-2.3
	HMDB0162129	3,4,5-trihydroxy-6-{2-[3-(3-hydroxy-6-oxo-1,2,3,6-tetrahydropyridin-1-yl)-3-oxopropyl]phenoxy}oxane-2-carboxylic acid	C20H23NO10	M+Na-2H	458.1069	-2.3

458.1058	HMDB0162151	3,4,5-trihydroxy-6-({5-[(1-hydroxy-3-phenylpropylidene)amino]-1,5-dioxopent-3-en-2-yl}oxy)oxane-2-carboxylic acid	C20H23NO10	M+Na-2H	458.1069	-2.3
	HMDB0162153	3,4,5-trihydroxy-6-({5-hydroxy-6-oxo-1-(3-phenylpropanoyl)-1,2,3,6-tetrahydropyridin-3-yl}oxy)oxane-2-carboxylic acid	C20H23NO10	M+Na-2H	458.1069	-2.3
	HMDB0162148	3,4,5-trihydroxy-6-({1-(2-hydroxy-3-phenylpropanoyl)-6-oxo-1,2,3,6-tetrahydropyridin-3-yl}oxy)oxane-2-carboxylic acid	C20H23NO10	M+Na-2H	458.1069	-2.3
	HMDB0162147	3,4,5-trihydroxy-6-({1-(3-hydroxy-6-oxo-1,2,3,6-tetrahydropyridin-1-yl)-1-oxo-3-phenylpropan-2-yl}oxy)oxane-2-carboxylic acid	C20H23NO10	M+Na-2H	458.1069	-2.3
	HMDB0162132	3,4,5-trihydroxy-6-({1-(3-hydroxy-3-phenylpropanoyl)-6-oxo-1,2,3,6-tetrahydropyridin-3-yl}oxy)oxane-2-carboxylic acid	C20H23NO10	M+Na-2H	458.1069	-2.3
	HMDB0162141	3,4,5-trihydroxy-6-({2-hydroxy-6-oxo-1-(3-phenylpropanoyl)-1,2,3,6-tetrahydropyridin-3-yl}oxy)oxane-2-carboxylic acid	C20H23NO10	M+Na-2H	458.1069	-2.3
	HMDB0162138	3,4,5-trihydroxy-6-{4-[3-(3-hydroxy-6-oxo-1,2,3,6-tetrahydropyridin-1-yl)-3-oxopropyl]phenoxy}oxane-2-carboxylic acid	C20H23NO10	M+Na-2H	458.1069	-2.3
	HMDB0162135	3,4,5-trihydroxy-6-{3-[3-(3-hydroxy-6-oxo-1,2,3,6-tetrahydropyridin-1-yl)-3-oxopropyl]phenoxy}oxane-2-carboxylic acid	C20H23NO10	M+Na-2H	458.1069	-2.3
	HMDB0162143	3,4,5-trihydroxy-6-({2-oxo-3-(3-phenylpropanoyl)-7-oxa-3-azabicyclo[4.1]heptan-5-yl}oxy)oxane-2-carboxylic acid	C20H23NO10	M+Na-2H	458.1069	-2.3
458.1437	HMDB0144008	(6S,12aR)-4-(dimethylamino)-3,5,6,9,,11,12a-heptahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,12-dione	C21H27NO9	M+Na-2H	458.1432	1.0
	HMDB0144037	(6R,12aR)-4-(dimethylamino)-3,5,5a,6,,11,12a-heptahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,12-dione	C21H27NO9	M+Na-2H	458.1432	1.0
	HMDB0144057	N-[(4aR,11S)-2,4a,6,7,11,12-hexahydroxy-11-methyl-4,5-dioxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracen-1-yl]-N-methylmethanamine oxide	C21H27NO9	M+Na-2H	458.1432	1.0
	HMDB0143998	(6S,12aR)-4-(dimethylamino)-3,5,6,8,,11,12a-heptahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,12-dione	C21H27NO9	M+Na-2H	458.1432	1.0
	HMDB0143987	(6S,12aR)-4-(dimethylamino)-3,5,6,,11,12a-hexahydroxy-6-(hydroxymethyl)-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,12-dione	C21H27NO9	M+Na-2H	458.1432	1.0
	HMDB0143977	(6S,12aR)-4-(dimethylamino)-3,4,5,6,,11,12a-heptahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,12-dione	C21H27NO9	M+Na-2H	458.1432	1.0
	HMDB0144061	(6S,12aS)-4-(dimethylamino)-2,3,5,6,,11,12a-heptahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,12-dione	C21H27NO9	M+Na-2H	458.1432	1.0
	HMDB0144064	(6S,12aR)-4-(dimethylamino)-3,5,6,,11,11a,12a-heptahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,12-dione	C21H27NO9	M+Na-2H	458.1432	1.0
	HMDB0144047	(6S,12aR)-4-(dimethylamino)-3,4a,5,6,,11,12a-heptahydroxy-6-methyl-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1,12-dione	C21H27NO9	M+Na-2H	458.1432	1.0

	HMDB0155306	2-[(4-{[(5-carbamimidamido-6-carboxy-4,5-dihydropyrazin-2-yl)methyl]amino}phenyl)formamido]pentanedioic acid	C19H21N7O7	M-H	458.1430	1.6
465.3037	HMDB0000653	Cholesterol sulfate	C27H46O4S	M-H	465.3044	-1.5
	HMDB0185232	[2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,]heptadec-7-en-5-yl]oxidanesulfonic acid	C27H46O4S	M-H	465.3044	-1.5
466.3069	HMDB0042042	Tiropamide	C28H41N3O3	M-H	466.3075	-1.3
468.1645	HMDB0061144	Hydromorphone-3-glucoside	C23H29NO8	M+Na-2H	468.1640	1.1
	HMDB0176905	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1,2-dihydroxyhexan-3-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C16H29N3O8S	M+FA-H	468.1657	-2.6
	HMDB0176904	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1,3-dihydroxyhexan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C16H29N3O8S	M+FA-H	468.1657	-2.6
	HMDB0163387	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(2,6-dihydroxyhexan-3-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C16H29N3O8S	M+FA-H	468.1657	-2.6
	HMDB0163388	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(3,6-dihydroxyhexan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C16H29N3O8S	M+FA-H	468.1657	-2.6
	HMDB0165624	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1,3-dihydroxy-2-methylpentan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C16H29N3O8S	M+FA-H	468.1657	-2.6
	HMDB0165830	6-{2-[3,4-dimethoxy--(methylamino)phenanthren-1-yl]ethoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H29NO9	M-H2O-H	468.1658	-2.9
	HMDB0149449	3,4,5-trihydroxy-6-[(6-methoxy-1-methyl-2-oxo-4,5-diphenylpiperidin-3-yl)oxy]oxane-2-carboxylic acid	C25H29NO9	M-H2O-H	468.1658	-2.9
470.1067	HMDB0161045	6-{4-[4-(2-amino-2-carboxyethyl)phenoxy]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C21H23NO10	M+Na-2H	470.1069	-0.3
470.1434	HMDB0061170	Norfluoxetine glucuronide	C22H24F3NO7	M-H	470.1432	0.4
	HMDB0006485	-Formyldihydrofolate	C20H21N7O7	M-H	470.1430	0.9
	HMDB0038735	5-O-Feruloylnigrumin	C21H25NO10	M+Na-2H	472.1225	1.5
	HMDB0137058	6-{2,6-dihydroxy-3-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
	HMDB0137057	6-{2,3-dihydroxy-6-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
	HMDB0137052	6-[4-(2-{[(2E)-3-(3,4-dihydroxyphenyl)-1-hydroxyprop-2-en-1-ylidene]amino}ethyl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
	HMDB0137051	6-{4-[(1E)-2-{[2-(3,4-dihydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]-2-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
	HMDB0137050	6-{5-[(1E)-2-{[2-(3,4-dihydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]-2-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5

HMDB0137049	6-[5-(2-{[(2E)-3-(3,4-dihydroxyphenyl)-1-hydroxyprop-2-en-1-ylidene]amino}ethyl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137046	3,4,5-trihydroxy-6-[4-(2-{[(2E)-1-hydroxy-3-(2,4,5-trihydroxyphenyl)prop-2-en-1-ylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137045	6-{2,5-dihydroxy-4-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137044	6-{2,4-dihydroxy-5-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137060	3,4,5-trihydroxy-6-[4-(2-{[(2E)-1-hydroxy-3-(2,3,4-trihydroxyphenyl)prop-2-en-1-ylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137059	6-{2,3-dihydroxy-4-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137075	6-[4-(2-{[(2Z)-3-(3,4-dihydroxyphenyl)-1,2-dihydroxyprop-2-en-1-ylidene]amino}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137074	3,4,5-trihydroxy-6-{2-hydroxy-4-[(1Z)-2-hydroxy-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137070	3,4,5-trihydroxy-6-{2-hydroxy-4-[(1E)-2-{[2-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137073	3,4,5-trihydroxy-6-{2-hydroxy-5-[(1Z)-2-hydroxy-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137069	3,4,5-trihydroxy-6-{2-hydroxy-5-[(1E)-2-{[2-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137067	6-[4-(2-{[(2E)-3-(1,3-dihydroxy-4-oxocyclohexa-2,5-dien-1-yl)-1-hydroxyprop-2-en-1-ylidene]amino}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137062	6-{2,3-dihydroxy-5-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137064	3,4,5-trihydroxy-6-[4-(2-{[(2E)-1-hydroxy-3-(3,4,5-trihydroxyphenyl)prop-2-en-1-ylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137063	6-{2,6-dihydroxy-4-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137043	6-{4,5-dihydroxy-2-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137038	6-{4-[2-(3-(3,4-dihydroxyphenyl)oxiran-2-yl](hydroxy)methylidene]amino}ethyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5

HMDB0137037	3,4,5-trihydroxy-6-[2-hydroxy-4-(3-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}oxiran-2-yl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136353	6-[4-(2-{[(2E)-3-(3,4-dihydroxyphenyl)-1-hydroxyprop-2-en-1-ylidene]amino}-1-hydroxyethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136352	3,4,5-trihydroxy-6-{2-hydroxy-5-[(1E)-2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136349	3,4,5-trihydroxy-6-{3-hydroxy-4-[(1E)-2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136347	3,4,5-trihydroxy-6-{5-hydroxy-2-[(1E)-2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136348	6-[4-(2-{[(2E)-3-(2,4-dihydroxyphenyl)-1-hydroxyprop-2-en-1-ylidene]amino}-1-hydroxyethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136342	3,4,5-trihydroxy-6-[2-hydroxy-4-(1-hydroxy-2-{[(2E)-1-hydroxy-3-(4-hydroxyphenyl)prop-2-en-1-ylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136343	6-{4-[(1E)-2-{[2-(3,4-dihydroxyphenyl)-2-hydroxyethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136341	3,4,5-trihydroxy-6-[2-hydroxy-5-(1-hydroxy-2-{[(2E)-1-hydroxy-3-(4-hydroxyphenyl)prop-2-en-1-ylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136357	3,4,5-trihydroxy-6-{4-[1-hydroxy-2-({hydroxy[3-(4-hydroxyphenyl)oxiran-2-yl]methylidene}amino)ethyl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136354	3,4,5-trihydroxy-6-{2-hydroxy-4-[(1E)-2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136358	3,4,5-trihydroxy-6-[4-(3-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}oxiran-2-yl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0137036	3,4,5-trihydroxy-6-[2-hydroxy-5-(3-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}oxiran-2-yl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136433	3,4,5-trihydroxy-6-[2-hydroxy-5-(2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136431	3,4,5-trihydroxy-6-[2-hydroxy-4-(2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136432	6-[4-(2-{[3-(3,4-dihydroxyphenyl)-1-hydroxyprop-2-en-1-ylidene]amino}-1-hydroxyethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136371	3,4,5-trihydroxy-6-{4-[(1Z)-2-hydroxy-2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
HMDB0136370	6-[4-(2-{[(2Z)-1,2-dihydroxy-3-(4-hydroxyphenyl)prop-2-en-1-ylidene]amino}-1-hydroxyethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5

	HMDB0136367	3,4,5-trihydroxy-6-[4-(1-hydroxy-2-[(2E)-1-hydroxy-3-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)prop-2-en-1-ylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
	HMDB0136364	3,4,5-trihydroxy-6-{4-[(1E)-2-{[2-hydroxy-2-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M-H2O-H	472.1244	-2.5
472.1399	HMDB0180890	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{[1-(3,4-dihydroxyphenyl)-3-hydroxypropan-2-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C19H27N3O9S	M-H	472.1395	0.8
	HMDB0141775	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{[1,3-dihydroxy-1-(4-hydroxyphenyl)propan-2-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C19H27N3O9S	M-H	472.1395	0.8
	HMDB0141774	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{[2,3-dihydroxy-1-(4-hydroxyphenyl)propyl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C19H27N3O9S	M-H	472.1395	0.8
	HMDB0134079	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{[2,3-dihydroxy-1-(2-hydroxyphenyl)propyl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C19H27N3O9S	M-H	472.1395	0.8
	HMDB0134078	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{[1,3-dihydroxy-1-(2-hydroxyphenyl)propan-2-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C19H27N3O9S	M-H	472.1395	0.8
	HMDB0172090	CHEMBL196798	C18H25N3O7S	M+FA-H	472.1395	0.8
	HMDB0161646	(2E,4E,E)-11-(2H-1,3-benzodioxol-5-yl)-N-(2-methylpropyl)-9-(sulfooxy)undeca-2,4,-trienimidic acid	C22H29NO7S	M+Na-2H	472.1411	-2.6
	HMDB0161648	(2E,4E,E)-11-(2H-1,3-benzodioxol-5-yl)-N-(2-methylpropyl)-6-(sulfooxy)undeca-2,4,-trienimidic acid	C22H29NO7S	M+Na-2H	472.1411	-2.6
	HMDB0161657	(2E,4E,E)-11-(2H-1,3-benzodioxol-5-yl)-N-[2-methyl-3-(sulfooxy)propyl]undeca-2,4,-trienimidic acid	C22H29NO7S	M+Na-2H	472.1411	-2.6
482.1430	HMDB0041937	Morphine-6-glucuronide	C23H27NO9	M+Na-2H	482.1432	-0.5
	HMDB0139509	3,4,5-trihydroxy-6-(4-{1-hydroxy-2-[(1-hydroxy-3-phenylpropylidene)amino]ethyl}phenoxy)oxane-2-carboxylic acid	C23H27NO9	M+Na-2H	482.1432	-0.5
	HMDB0060930	N-Desmethyl sildenafil (UK-3,3)	C23H27NO9	M+Na-2H	482.1432	-0.5
	HMDB0060824	Hydromorphone-3-glucuronide	C23H27NO9	M+Na-2H	482.1432	-0.5
	HMDB0041936	Morphine-3-glucuronide	C23H27NO9	M+Na-2H	482.1432	-0.5
	HMDB0142239	6-{4-[2-cyano-2-(diethylcarbamoyl)ethyl]-2-hydroxy-6-nitrophenoxy}-3,4,5-trihydroxyoxane-2-carboxylic	C20H25N3O11	M-H	482.1416	2.8
	HMDB0142238	6-{5-[2-cyano-2-(diethylcarbamoyl)ethyl]-2-hydroxy-3-nitrophenoxy}-3,4,5-trihydroxyoxane-2-carboxylic	C20H25N3O11	M-H	482.1416	2.8
482.1806	HMDB0014856	Adefovir Dipivoxil	C20H32N5O8P	M-H2O-H	482.1805	0.3
	HMDB0166772	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1,3-dihydroxyheptan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C17H31N3O8S	M+FA-H	482.1814	-1.6
	HMDB0166773	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1,2-dihydroxyheptan-3-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C17H31N3O8S	M+FA-H	482.1814	-1.6
484.1588	HMDB0060607	Fluoxetine glucuronide	C23H26F3NO7	M-H	484.1589	-0.1
	HMDB0060821	Dihydromorphone-3-glucuronide	C23H29NO9	M+Na-2H	484.1589	-0.2
	HMDB0061137	Dihydroisomorphine-6-glucuronide	C23H29NO9	M+Na-2H	484.1589	-0.2
	HMDB0060916	Etodolac acyl glucuronide	C23H29NO9	M+Na-2H	484.1589	-0.2
	HMDB0060820	Dihydroisomorphine-3-glucuronide	C23H29NO9	M+Na-2H	484.1589	-0.2
486.1380	HMDB0000121	Folic acid	C19H19N7O6	M+FA-H	486.1379	0.2

489.1399	HMDB0014349	Dofetilide	C19H27N3O5S2	M+FA-H	486.1374	1.2
489.1422	HMDB0061229	2-hydroxydesmethyl clomipramine glucuronide	C24H29ClN2O8	M-H2O-H	489.1429	-1.3
496.1591	HMDB0173741	3,4,5-trihydroxy-6-{2-hydroxy-4-[(1E,3E,5E)-7-oxo-7-(piperidin-1-yl)hepta-1,3,5-trien-1-yl]phenoxy}oxane-2-carboxylic acid	C24H29NO9	M+Na-2H	496.1589	0.4
	HMDB0162045	2-(2-{4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]phenyl}ethyl)-7-hydroxy-4-(hydroxymethyl)-7-methyl-5H,6H,7H-cyclopenta[c]pyridin-2-ium	C24H30NO9	M+Na-2H	496.1589	0.4
	HMDB0162048	2-(2-{4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]phenyl}-2-hydroxyethyl)-4-(hydroxymethyl)-7-methyl-5H,6H,7H-cyclopenta[c]pyridin-2-ium	C24H30NO9	M+Na-2H	496.1589	0.4
	HMDB0162052	2-(2-{3-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-4-hydroxyphenyl}ethyl)-4-(hydroxymethyl)-7-methyl-5H,6H,7H-cyclopenta[c]pyridin-2-ium	C24H30NO9	M+Na-2H	496.1589	0.4
	HMDB0162053	2-(2-{4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-3-hydroxyphenyl}ethyl)-4-(hydroxymethyl)-7-methyl-5H,6H,7H-cyclopenta[c]pyridin-2-ium	C24H30NO9	M+Na-2H	496.1589	0.4
	HMDB0162062	2-(2-{4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]phenyl}ethyl)-5-hydroxy-4-(hydroxymethyl)-7-methyl-5H,6H,7H-cyclopenta[c]pyridin-2-ium	C24H30NO9	M+Na-2H	496.1589	0.4
	HMDB0162066	2-(2-{4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]phenyl}ethyl)-4,7-bis(hydroxymethyl)-5H,6H,7H-cyclopenta[c]pyridin-2-ium	C24H30NO9	M+Na-2H	496.1589	0.4
	HMDB0162071	4-{[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]methyl}-2-[2-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)ethyl]-7-methyl-5H,6H,7H-	C24H30NO9	M+Na-2H	496.1589	0.4
	HMDB0162070	2-(2-{1-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-4-oxocyclohexa-2,5-dien-1-yl}ethyl)-4-(hydroxymethyl)-7-methyl-5H,6H,7H-cyclopenta[c]pyridin-2-ium	C24H30NO9	M+Na-2H	496.1589	0.4
	HMDB0173740	3,4,5-trihydroxy-6-{2-hydroxy-5-[(1E,3E,5E)-7-oxo-7-(piperidin-1-yl)hepta-1,3,5-trien-1-yl]phenoxy}oxane-2-carboxylic acid	C24H29NO9	M+Na-2H	496.1589	0.4
	HMDB0145206	6-({1-amino-3-[2-(3-phenylpropanoyl)phenoxy]propan-2-yl}oxy)-3,4,5-	C24H29NO9	M+Na-2H	496.1589	0.4
	HMDB0139481	3,4,5-trihydroxy-6-{2-[(1-hydroxy-3-phenylpropylidene)amino]-1-(4-methoxyphenyl)ethoxy}oxane-2-carboxylic acid	C24H29NO9	M+Na-2H	496.1589	0.4
	HMDB0060464	Codeine-6-glucuronide	C24H29NO9	M+Na-2H	496.1589	0.4
	HMDB0168548	3,4,5-trihydroxy-6-({1-[(1-hydroxy-4-oxocyclohexyl)methyl]-6-methoxyisoquinolin-7-yl}oxy)oxane-2-carboxylic acid	C23H27NO10	M+Na-2H	498.1382	-0.7
	HMDB0139522	3,4,5-trihydroxy-6-[(1-{1-hydroxy-2-[(1-hydroxy-3-phenylpropylidene)amino]ethyl}-4-oxocyclohexa-2,5-dien-1-yl)oxy]oxane-2-carboxylic acid	C23H27NO10	M+Na-2H	498.1382	-0.7
	HMDB0139523	3,4,5-trihydroxy-6-{2-[(1-hydroxy-3-phenylpropylidene)amino]-1-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)ethoxy}oxane-2-carboxylic acid	C23H27NO10	M+Na-2H	498.1382	-0.7
	HMDB0137034	6-[4-(2-{3-(3,4-dihydroxyphenyl)-1-hydroxypropylidene}amino)ethyl]phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO10	M+Na-2H	498.1382	-0.7
	HMDB0137033	3,4,5-trihydroxy-6-[2-hydroxy-4-(2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO10	M+Na-2H	498.1382	-0.7
	HMDB0137032	3,4,5-trihydroxy-6-[2-hydroxy-5-(2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO10	M+Na-2H	498.1382	-0.7
	HMDB0136336	3,4,5-trihydroxy-6-[4-(1-hydroxy-2-[[1-hydroxy-3-(4-hydroxyphenyl)propylidene]amino]ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO10	M+Na-2H	498.1382	-0.7

498.1378	HMDB0136337	3,4,5-trihydroxy-6-[4-(2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO10	M+Na-2H	498.1382	-0.7
	HMDB0151311	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-({2-[(methylsulfanyl)methyl]-3-oxo-1-phenylpropyl}sulfanyl)ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H29N3O7S2	M-H	498.1374	0.8
	HMDB0151361	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-({1,3-dihydroxy-2-[(methylsulfanyl)methyl]-1-phenylpropan-2-yl}sulfanyl)ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H31N3O8S2	M-H2O-H	498.1369	1.9
	HMDB0151360	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-({2,3-dihydroxy-2-[(methylsulfanyl)methyl]-1-phenylpropyl}sulfanyl)ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H31N3O8S2	M-H2O-H	498.1369	1.9
	HMDB0142267	6-{4-[2-cyano-2-(diethylcarbamoyl)-1-hydroxyethyl]-2-hydroxy-6-nitrophenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H25N3O12	M-H	498.1365	2.5
	HMDB0142266	6-{5-[2-cyano-2-(diethylcarbamoyl)-1-hydroxyethyl]-2-hydroxy-3-nitrophenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H25N3O12	M-H	498.1365	2.5
	HMDB0142271	6-{6-[2-cyano-2-(diethylcarbamoyl)ethyl]-2,3-dihydroxy-4-nitrophenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H25N3O12	M-H	498.1365	2.5
	HMDB0142272	6-{3-[2-cyano-2-(diethylcarbamoyl)ethyl]-2,6-dihydroxy-5-nitrophenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H25N3O12	M-H	498.1365	2.5
	HMDB0142275	6-{5-[2-cyano-2-(diethylcarbamoyl)ethyl]-2,4-dihydroxy-3-nitrophenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H25N3O12	M-H	498.1365	2.5
	HMDB0142273	6-{4-[2-cyano-2-(diethylcarbamoyl)ethyl]-2,3-dihydroxy-6-nitrophenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H25N3O12	M-H	498.1365	2.5
	HMDB0142292	6-({1-[2-cyano-2-(diethylcarbamoyl)ethyl]-3-hydroxy-5-nitro-4-oxocyclohexa-2,5-dien-1-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H25N3O12	M-H	498.1365	2.5
	HMDB0142289	6-{4-[2-cyano-2-(diethylcarbamoyl)-2-hydroxyethyl]-2-hydroxy-6-nitrophenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H25N3O12	M-H	498.1365	2.5
	HMDB0142288	6-{5-[2-cyano-2-(diethylcarbamoyl)-2-hydroxyethyl]-2-hydroxy-3-nitrophenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H25N3O12	M-H	498.1365	2.5
	HMDB0142283	6-(5-{2-cyano-2-[ethyl(2-hydroxyethyl)carbamoyl]ethyl}-2-hydroxy-3-nitrophenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H25N3O12	M-H	498.1365	2.5
	HMDB0142284	6-(4-{2-cyano-2-[ethyl(2-hydroxyethyl)carbamoyl]ethyl}-2-hydroxy-6-nitrophenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H25N3O12	M-H	498.1365	2.5
	HMDB0142276	6-{4-[2-cyano-2-(diethylcarbamoyl)ethyl]-3,6-dihydroxy-2-nitrophenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H25N3O12	M-H	498.1365	2.5
	HMDB0142274	6-{6-[2-cyano-2-(diethylcarbamoyl)ethyl]-3,4-dihydroxy-2-nitrophenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H25N3O12	M-H	498.1365	2.5
	HMDB0142279	6-{2-amino-4-[2-cyano-2-(diethylcarbamoyl)ethyl]-6-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H27N3O9	M+FA-H	498.1729	1.5
	HMDB0142278	6-{3-amino-5-[2-cyano-2-(diethylcarbamoyl)ethyl]-2-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H27N3O9	M+FA-H	498.1729	1.5

498.1737	HMDB0142280	6-({5-[2-cyano-2-(diethylcarbamoyl)ethyl]-2,3-dihydroxyphenyl}amino)-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H27N3O9	M+FA-H	498.1729	1.5
	HMDB0173753	3,4,5-trihydroxy-6-{2-hydroxy-5-[(1E,3E)-7-oxo-7-(piperidin-1-yl)hepta-1,3-dien-1-yl]phenoxy}oxane-2-carboxylic acid	C24H31NO9	M+Na-2H	498.1745	-1.7
	HMDB0173754	3,4,5-trihydroxy-6-{2-hydroxy-4-[(1E,3E)-7-oxo-7-(piperidin-1-yl)hepta-1,3-dien-1-yl]phenoxy}oxane-2-carboxylic acid	C24H31NO9	M+Na-2H	498.1745	-1.7
500.1173	HMDB0162120	6-{3-[3-(acetyloxy)-6-oxo-1,2,3,6-tetrahydropyridin-1-yl]-3-oxo-1-phenylpropoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H25NO11	M+Na-2H	500.1174	-0.3
	HMDB0162128	6-(2-{3-[3-(acetyloxy)-6-oxo-1,2,3,6-tetrahydropyridin-1-yl]-3-oxopropyl}phenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H25NO11	M+Na-2H	500.1174	-0.3
	HMDB0162122	6-(3-{3-[3-(acetyloxy)-6-oxo-1,2,3,6-tetrahydropyridin-1-yl]-3-oxopropyl}phenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H25NO11	M+Na-2H	500.1174	-0.3
	HMDB0162124	6-(4-{3-[3-(acetyloxy)-6-oxo-1,2,3,6-tetrahydropyridin-1-yl]-3-oxopropyl}phenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H25NO11	M+Na-2H	500.1174	-0.3
	HMDB0162116	6-({1-[3-(acetyloxy)-6-oxo-1,2,3,6-tetrahydropyridin-1-yl]-1-oxo-3-phenylpropan-2-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C22H25NO11	M+Na-2H	500.1174	-0.3
	HMDB0162118	3,4,5-trihydroxy-6-(2-oxo-2-{[6-oxo-1-(3-phenylpropanoyl)-1,2,3,6-tetrahydropyridin-3-yl]oxy}ethoxy)oxane-2-carboxylic acid	C22H25NO11	M+Na-2H	500.1174	-0.3
500.1539	HMDB0167460	6-({[(3E)-1-(2H-1,3-benzodioxol-5-yl)-5-oxo-5-(piperidin-1-yl)pent-3-en-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H29NO10	M+Na-2H	500.1538	0.2
	HMDB0167464	3,4,5-trihydroxy-6-({6-[(3E)-5-oxo-5-(piperidin-1-yl)pent-3-en-1-yl]-2H-1,3-benzodioxol-5-yl}oxy)oxane-2-carboxylic acid	C23H29NO10	M+Na-2H	500.1538	0.2
	HMDB0167465	6-({1-[(2E)-5-(2H-1,3-benzodioxol-5-yl)pent-2-enoyl]piperidin-3-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H29NO10	M+Na-2H	500.1538	0.2
	HMDB0167462	6-({[1-(2H-1,3-benzodioxol-5-yl)-5-oxo-5-(piperidin-1-yl)pent-3-en-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H29NO10	M+Na-2H	500.1538	0.2
	HMDB0062623	5,-methenyltetrahydrofolate mono-L-glutamate	C20H20N7O6	M+FA-H	500.1535	0.7
	HMDB0001354	5,-Methenyltetrahydrofolic acid	C20H21N7O6	M+FA-H	500.1535	0.7
504.4766	HMDB0240685	Cer(d17:1/16)	C33H65NO3	M-H2O-H	504.4781	-2.9
505.9879	HMDB0000538	Adenosine triphosphate	C10H16N5O13P3	M-H	505.9885	-1.1
	HMDB0061727	Zidovudine 5'-Triphosphate	C10H16N5O13P3	M-H	505.9885	-1.1
	HMDB0059593	2-hydroxy-dATP	C10H16N5O13P3	M-H	505.9885	-1.1
	HMDB0001440	dGTP	C10H16N5O13P3	M-H	505.9885	-1.1
506.1414	HMDB0060607	Fluoxetine glucuronide	C23H26F3NO7	M+Na-2H	506.1408	1.2
510.9865	HMDB0142303	2-[3,5-dihydroxy-4-(sulfooxy)phenyl]-8-hydroxy-3-(sulfooxy)-3,4-dihydro-2H-1-benzopyran-6-olate	C15H13O13S2	M+FA-H	510.9858	1.4
	HMDB0158427	3-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-4-hydroxyhexanedioic acid	C16H25N3O11S	M+FA-H	512.1192	-1.5
	HMDB0159837	2-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-3-hydroxy-3-methylpentanedioic acid	C16H25N3O11S	M+FA-H	512.1192	-1.5

HMDB0159838	3-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl} sulfanyl)-2-hydroxy-3-methylpentanedioic acid	C16H25N3O11S	M+FA-H	512.1192	-1.5
HMDB0162597	6-{{[1,5-dihydroxy-11-methyl-2-(2-methyloxiran-2-yl)-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin--yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0162594	6-{{[1,5-dihydroxy-11-methyl-2-(2-methyloxiran-2-yl)-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-9-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0162592	6-{{[1,8-dihydroxy-11-methyl-2-(2-methyloxiran-2-yl)-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0162595	6-{{[1,9-dihydroxy-11-methyl-2-(2-methyloxiran-2-yl)-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0162591	6-{{[1,5-dihydroxy-11-methyl-2-(2-methyloxiran-2-yl)-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-8-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0162587	3,4,5-trihydroxy-6-({1-hydroxy-2-[2-(hydroxymethyl)oxiran-2-yl]-11-methyl-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-5-yl}oxy)oxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0145516	3,4,5-trihydroxy-6-({3-[3-hydroxy-1-(4-nitrophenyl)butyl]-2-oxo-2H-chromen-4-yl}oxy)oxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0162598	6-{{[1,5-dihydroxy-11-methyl-2-(2-methyloxiran-2-yl)-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0162600	6-{{[1,5-dihydroxy-11-methyl-2-(2-methyloxiran-2-yl)-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0162620	3,4,5-trihydroxy-6-({7-hydroxy-2-[2-(hydroxymethyl)oxiran-2-yl]-11-methyl-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-5-yl}oxy)oxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0162619	3,4,5-trihydroxy-6-({5-hydroxy-2-[2-(hydroxymethyl)oxiran-2-yl]-11-methyl-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-7-yl}oxy)oxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0162617	3,4,5-trihydroxy-6-({-hydroxy-2-[2-(hydroxymethyl)oxiran-2-yl]-11-methyl-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-5-yl}oxy)oxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0162616	3,4,5-trihydroxy-6-({5-hydroxy-2-[2-(hydroxymethyl)oxiran-2-yl]-11-methyl-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin--yl}oxy)oxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0162613	3,4,5-trihydroxy-6-({5-hydroxy-2-[2-(hydroxymethyl)oxiran-2-yl]-11-methyl-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-9-yl}oxy)oxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0162614	3,4,5-trihydroxy-6-({9-hydroxy-2-[2-(hydroxymethyl)oxiran-2-yl]-11-methyl-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-5-yl}oxy)oxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0162610	3,4,5-trihydroxy-6-({5-hydroxy-2-[2-(hydroxymethyl)oxiran-2-yl]-11-methyl-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-8-yl}oxy)oxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0162611	3,4,5-trihydroxy-6-({8-hydroxy-2-[2-(hydroxymethyl)oxiran-2-yl]-11-methyl-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-5-yl}oxy)oxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7

512.1184

HMDB0162601	6-[[1,7-dihydroxy-11-methyl-2-(2-methyloxiran-2-yl)-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H25NO12	M-H2O-H	512.1193	-1.7
HMDB0137063	6-{2,6-dihydroxy-4-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137064	3,4,5-trihydroxy-6-[4-(2-{[(2E)-1-hydroxy-3-(3,4,5-trihydroxyphenyl)prop-2-en-1-ylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137062	6-{2,3-dihydroxy-5-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137067	6-[4-(2-{[(2E)-3-(1,3-dihydroxy-4-oxocyclohexa-2,5-dien-1-yl)-1-hydroxyprop-2-en-1-ylidene]amino}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137069	3,4,5-trihydroxy-6-{2-hydroxy-5-[(1E)-2-{[2-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137073	3,4,5-trihydroxy-6-{2-hydroxy-5-[(1Z)-2-hydroxy-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137070	3,4,5-trihydroxy-6-{2-hydroxy-4-[(1E)-2-{[2-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137074	3,4,5-trihydroxy-6-{2-hydroxy-4-[(1Z)-2-hydroxy-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137075	6-[4-(2-{[(2Z)-3-(3,4-dihydroxyphenyl)-1,2-dihydroxyprop-2-en-1-ylidene]amino}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136349	3,4,5-trihydroxy-6-{3-hydroxy-4-[(1E)-2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137059	6-{2,3-dihydroxy-4-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137060	3,4,5-trihydroxy-6-[4-(2-{[(2E)-1-hydroxy-3-(2,3,4-trihydroxyphenyl)prop-2-en-1-ylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137058	6-{2,6-dihydroxy-3-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136370	6-[4-(2-{[(2Z)-1,2-dihydroxy-3-(4-hydroxyphenyl)prop-2-en-1-ylidene]amino}-1-hydroxyethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136367	3,4,5-trihydroxy-6-[4-(1-hydroxy-2-{[(2E)-1-hydroxy-3-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)prop-2-en-1-ylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136364	3,4,5-trihydroxy-6-{4-[(1E)-2-{[2-hydroxy-2-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9

HMDB0136358	3,4,5-trihydroxy-6-[4-(3-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}oxiran-2-yl)phenoxy]oxane-2-	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136354	3,4,5-trihydroxy-6-{2-hydroxy-4-[(1E)-2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136357	3,4,5-trihydroxy-6-{4-[1-hydroxy-2-({hydroxy[3-(4-hydroxyphenyl)oxiran-2-yl]methylidene}amino)ethyl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136353	6-[4-(2-{[(2E)-3-(3,4-dihydroxyphenyl)-1-hydroxyprop-2-en-1-ylidene]amino}-1-hydroxyethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136352	3,4,5-trihydroxy-6-{2-hydroxy-5-[(1E)-2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136347	3,4,5-trihydroxy-6-{5-hydroxy-2-[(1E)-2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136348	6-[4-(2-{[(2E)-3-(2,4-dihydroxyphenyl)-1-hydroxyprop-2-en-1-ylidene]amino}-1-hydroxyethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136342	3,4,5-trihydroxy-6-[2-hydroxy-4-(1-hydroxy-2-{[(2E)-1-hydroxy-3-(4-hydroxyphenyl)prop-2-en-1-ylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136343	6-{4-[(1E)-2-{[2-(3,4-dihydroxyphenyl)-2-hydroxyethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136341	3,4,5-trihydroxy-6-[2-hydroxy-5-(1-hydroxy-2-{[(2E)-1-hydroxy-3-(4-hydroxyphenyl)prop-2-en-1-ylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136371	3,4,5-trihydroxy-6-{4-[(1Z)-2-hydroxy-2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136432	6-[4-(2-{[3-(3,4-dihydroxyphenyl)-1-hydroxyprop-2-en-1-ylidene]amino}-1-hydroxyethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137057	6-{2,3-dihydroxy-6-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137052	6-[4-(2-{[(2E)-3-(3,4-dihydroxyphenyl)-1-hydroxyprop-2-en-1-ylidene]amino}ethyl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137051	6-{4-[(1E)-2-{[2-(3,4-dihydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]-2-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137050	6-{5-[(1E)-2-{[2-(3,4-dihydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]-2-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137049	6-[5-(2-{[(2E)-3-(3,4-dihydroxyphenyl)-1-hydroxyprop-2-en-1-ylidene]amino}ethyl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9

HMDB0137046	3,4,5-trihydroxy-6-[4-(2-([2E]-1-hydroxy-3-(2,4,5-trihydroxyphenyl)prop-2-en-1-ylidene)amino)ethyl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137045	6-{2,5-dihydroxy-4-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137044	6-{2,4-dihydroxy-5-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137043	6-{4,5-dihydroxy-2-[(1E)-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137038	6-{4-[2-([3-(3,4-dihydroxyphenyl)oxiran-2-yl](hydroxy)methylidene)amino)ethyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137037	3,4,5-trihydroxy-6-[2-hydroxy-4-(3-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}oxiran-2-yl)phenoxy]oxane-2-	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0137036	3,4,5-trihydroxy-6-[2-hydroxy-5-(3-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}oxiran-2-yl)phenoxy]oxane-2-	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136433	3,4,5-trihydroxy-6-[2-hydroxy-5-(2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0136431	3,4,5-trihydroxy-6-[2-hydroxy-4-(2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl)phenoxy]oxane-2-carboxylic acid	C23H25NO11	M+Na-2H	512.1174	1.9
HMDB0181779	6-[(2-{3,5-dioxo-11-azapentacyclo[7.1,??]icosa-1(0),2(6),7,12,14,16,18-heptaen-13-yl}-2-hydroxyacetyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H23NO11	M-H	512.1198	-2.8
HMDB0181778	6-[carboxy({3,5-dioxo-11-azapentacyclo[7.1,??]icosa-1(0),2(6),7,12,14,16,18-heptaen-13-yl})methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H23NO11	M-H	512.1198	-2.8
HMDB0139515	3,4,5-trihydroxy-6-[4-(2-{[2-hydroxy-2-(4-methoxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C24H29NO10	M+Na-2H	512.1538	0.8
HMDB0139518	3,4,5-trihydroxy-6-(1-{[2-hydroxy-2-(4-methoxyphenyl)ethyl]-C-hydroxycarbonimidoyl}-2-phenylethoxy)oxane-2-carboxylic acid	C24H29NO10	M+Na-2H	512.1538	0.8
HMDB0139519	6-{2-[(1,2-dihydroxy-3-phenylpropylidene)amino]-1-(4-methoxyphenyl)ethoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H29NO10	M+Na-2H	512.1538	0.8
HMDB0139512	3,4,5-trihydroxy-6-[3-(2-{[2-hydroxy-2-(4-methoxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C24H29NO10	M+Na-2H	512.1538	0.8
HMDB0149501	6-[(5-amino-2-hydroxy-5-methoxy-3,4-diphenylpentanoyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H29NO10	M+Na-2H	512.1538	0.8
HMDB0139506	6-{2-[(1,3-dihydroxy-3-phenylpropylidene)amino]-1-(4-methoxyphenyl)ethoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H29NO10	M+Na-2H	512.1538	0.8
HMDB0139505	3,4,5-trihydroxy-6-(2-{[2-hydroxy-2-(4-methoxyphenyl)ethyl]-C-hydroxycarbonimidoyl}-1-phenylethoxy)oxane-2-carboxylic acid	C24H29NO10	M+Na-2H	512.1538	0.8
HMDB0139503	3,4,5-trihydroxy-6-[2-(2-{[2-hydroxy-2-(4-methoxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C24H29NO10	M+Na-2H	512.1538	0.8

	HMDB0149500	6-(4-amino-1-carboxy-4-methoxy-2,3-diphenylbutoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H29NO10	M+Na-2H	512.1538	0.8
	HMDB0029361	Alkaloid RC	C26H29NO11	M-H2O-H	512.1557	-2.9
512.1893	HMDB0145245	6-{[2-benzyl-4-(octahydro-1H-isoindol-2-yl)-4-oxobutanoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H33NO9	M+Na-2H	512.1902	-1.8
	HMDB0161545	3,4,5-trihydroxy-6-{2-hydroxy-5-[(1E,5E,7E)-8-[(2-methylpropyl)-C-hydroxycarbonimidoyl]octa-1,5,7-trien-1-yl]phenoxy}oxane-2-carboxylic acid	C25H33NO9	M+Na-2H	512.1902	-1.8
	HMDB0161546	3,4,5-trihydroxy-6-{2-hydroxy-4-[(1E,5E,7E)-8-[(2-methylpropyl)-C-hydroxycarbonimidoyl]octa-1,5,7-trien-1-yl]phenoxy}oxane-2-carboxylic acid	C25H33NO9	M+Na-2H	512.1902	-1.8
	HMDB0137117	3,4,5-trihydroxy-6-[2-hydroxy-4-(2-{[2-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137087	3,4,5-trihydroxy-6-[4-(2-{[1-hydroxy-3-(2,4,5-trihydroxyphenyl)propylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137090	6-[5-(2-{[3-(3,4-dihydroxyphenyl)-1-hydroxypropylidene]amino}ethyl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137093	6-[4-(2-{[3-(3,4-dihydroxyphenyl)-1-hydroxypropylidene]amino}ethyl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137092	6-[4-(2-{[2-(3,4-dihydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137091	6-[5-(2-{[2-(3,4-dihydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137098	3,4,5-trihydroxy-6-[2-hydroxy-5-(2-hydroxy-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137100	6-[4-(2-{[3-(3,4-dihydroxyphenyl)-1,2-dihydroxypropylidene]amino}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137099	3,4,5-trihydroxy-6-[2-hydroxy-4-(2-hydroxy-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137105	6-[2,6-dihydroxy-3-(2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137104	6-[2,3-dihydroxy-6-(2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137106	6-[2,3-dihydroxy-4-(2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137109	6-[2,3-dihydroxy-5-(2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137107	3,4,5-trihydroxy-6-[4-(2-{[1-hydroxy-3-(2,3,4-trihydroxyphenyl)propylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137110	6-[2,6-dihydroxy-4-(2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137111	3,4,5-trihydroxy-6-[4-(2-{[1-hydroxy-3-(3,4,5-trihydroxyphenyl)propylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0

514.1331

HMDB0137114	6-[4-(2-{[3-(1,3-dihydroxy-4-oxocyclohexa-2,5-dien-1-yl)-1-hydroxypropylidene]amino}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0137116	3,4,5-trihydroxy-6-[2-hydroxy-5-(2-{[2-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0137086	6-[2,5-dihydroxy-4-(2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0137084	6-[4,5-dihydroxy-2-(2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0137085	6-[2,4-dihydroxy-5-(2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0136387	3,4,5-trihydroxy-6-[2-hydroxy-5-(2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0136375	6-[4-(2-{[1,3-dihydroxy-3-(4-hydroxyphenyl)propylidene]amino}-1-hydroxyethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0136376	3,4,5-trihydroxy-6-[4-(1-hydroxy-2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0136381	3,4,5-trihydroxy-6-[2-hydroxy-5-(1-hydroxy-2-{[1-hydroxy-3-(4-hydroxyphenyl)propylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0136382	3,4,5-trihydroxy-6-[2-hydroxy-4-(1-hydroxy-2-{[1-hydroxy-3-(4-hydroxyphenyl)propylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0136383	6-[4-(2-{[2-(3,4-dihydroxyphenyl)-2-hydroxyethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0136388	6-[4-(2-{[3-(3,4-dihydroxyphenyl)-1-hydroxypropylidene]amino}-1-hydroxyethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0136389	3,4,5-trihydroxy-6-[2-hydroxy-4-(2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0137078	3,4,5-trihydroxy-6-[2-hydroxy-5-(1-hydroxy-2-{[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0136393	6-[4-(2-{[1,2-dihydroxy-3-(4-hydroxyphenyl)propylidene]amino}-1-hydroxyethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0136394	3,4,5-trihydroxy-6-[4-(2-hydroxy-2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
HMDB0136399	3,4,5-trihydroxy-6-[4-(2-{[2-hydroxy-2-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0

	HMDB0136402	3,4,5-trihydroxy-6-[4-(1-hydroxy-2-[[1-hydroxy-3-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)propylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137079	3,4,5-trihydroxy-6-[2-hydroxy-4-(1-hydroxy-2-[[2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)phenoxy]oxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0137080	6-[4-(2-[[3-(3,4-dihydroxyphenyl)-1,3-dihydroxypropylidene]amino}ethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H27NO11	M+Na-2H	514.1331	0.0
	HMDB0151323	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{1-(4-hydroxyphenyl)-2-[(methylsulfanyl)methyl]-3-oxopropyl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H29N3O8 S2	M-H	514.1323	1.5
	HMDB0151320	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{1-(2-hydroxyphenyl)-2-[(methylsulfanyl)methyl]-3-oxopropyl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H29N3O8 S2	M-H	514.1323	1.5
	HMDB0151330	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{2-(methanesulfinylmethyl)-3-oxo-1-phenylpropyl}sulfanyl}ethyl}-C-	C21H29N3O8 S2	M-H	514.1323	1.5
	HMDB0151332	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-({1-hydroxy-2-[(methylsulfanyl)methyl]-3-oxo-1-phenylpropan-2-yl}sulfanyl)ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H29N3O8 S2	M-H	514.1323	1.5
	HMDB0151331	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-({2-hydroxy-2-[(methylsulfanyl)methyl]-3-oxo-1-phenylpropyl}sulfanyl)ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H29N3O8 S2	M-H	514.1323	1.5
	HMDB0151327	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{1-(3-hydroxyphenyl)-2-[(methylsulfanyl)methyl]-3-oxopropyl}sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C21H29N3O8 S2	M-H	514.1323	1.5
516.4775	HMDB0035480	N-[(4E,8E)-1,3-dihydroxyoctadeca-4,8-dien-2-yl]hexadecanamide	C34H65NO3	M-H20-H	516.4781	-1.1
	HMDB0240686	Cer(d18:2(4E,14Z)/16)	C34H65NO3	M-H20-H	516.4781	-1.1
518.4932	HMDB0004949	Cer(d18:1/16)	C34H67NO3	M-H20-H	518.4937	-1.0
	HMDB0000790	N-Palmitoylsphingosine	C34H67NO3	M-H20-H	518.4937	-1.0
526.1346	HMDB0161504	3,4,5-trihydroxy-6-{{9-hydroxy-2-(hydroxymethyl)--methoxy-2,11-dimethyl-6-oxo-6,11-dihydro-2H-1-oxa-11-azatetracen-5-yl}oxy}oxane-2-carboxylic acid	C26H27NO12	M-H20-H	526.1349	-0.6
	HMDB0161505	3,4,5-trihydroxy-6-{{5-hydroxy-2-(hydroxymethyl)--methoxy-2,11-dimethyl-6-oxo-6,11-dihydro-2H-1-oxa-11-azatetracen-9-yl}oxy}oxane-2-carboxylic acid	C26H27NO12	M-H20-H	526.1349	-0.6
	HMDB0161496	6-[(5,9-dihydroxy--methoxy-2,2,11-trimethyl-6-oxo-6,11-dihydro-2H-1-oxa-11-azatetracen-8-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H27NO12	M-H20-H	526.1349	-0.6
	HMDB0161498	6-[(5,8-dihydroxy--methoxy-2,2,11-trimethyl-6-oxo-6,11-dihydro-2H-1-oxa-11-azatetracen-9-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H27NO12	M-H20-H	526.1349	-0.6
	HMDB0161497	6-[(8,9-dihydroxy--methoxy-2,2,11-trimethyl-6-oxo-6,11-dihydro-2H-1-oxa-11-azatetracen-5-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H27NO12	M-H20-H	526.1349	-0.6
	HMDB0136421	3,4,5-trihydroxy-6-[4-(2-{{2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl)-2-methoxyphenoxy]oxane-2-carboxylic acid	C24H27NO11	M+Na-2H	526.1331	2.9
	HMDB0136422	3,4,5-trihydroxy-6-[4-(1-hydroxy-2-{{1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)prop-2-en-1-ylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C24H27NO11	M+Na-2H	526.1331	2.9

526.1693	HMDB0173757	6-([(6E)-7-(2H-1,3-benzodioxol-5-yl)-1-oxo-1-(piperidin-1-yl)hepta-4,6-dien-2-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO10	M+Na-2H	526.1695	-0.3
	HMDB0177137	6-([1-[(3,4-dimethoxyphenyl)methyl]-6-hydroxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO10	M+Na-2H	526.1695	-0.3
	HMDB0177138	6-([1-[(3,4-dimethoxyphenyl)methyl]-7-hydroxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-6-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO10	M+Na-2H	526.1695	-0.3
	HMDB0177135	3,4,5-trihydroxy-6-{4-[(7-hydroxy-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl]-2-methoxyphenoxy}oxane-2-carboxylic acid	C25H31NO10	M+Na-2H	526.1695	-0.3
	HMDB0177134	3,4,5-trihydroxy-6-([1-[(4-hydroxy-3-methoxyphenyl)methyl]-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-yl]oxy)oxane-2-carboxylic acid	C25H31NO10	M+Na-2H	526.1695	-0.3
	HMDB0177132	3,4,5-trihydroxy-6-{5-[(7-hydroxy-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl]-2-methoxyphenoxy}oxane-2-carboxylic acid	C25H31NO10	M+Na-2H	526.1695	-0.3
	HMDB0177131	3,4,5-trihydroxy-6-([1-[(3-hydroxy-4-methoxyphenyl)methyl]-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-yl]oxy)oxane-2-carboxylic acid	C25H31NO10	M+Na-2H	526.1695	-0.3
	HMDB0177122	6-([1-[(3,4-dimethoxyphenyl)methyl]-6-methoxy-1,2,3,4-tetrahydroisoquinolin-7-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO10	M+Na-2H	526.1695	-0.3
	HMDB0173746	3,4,5-trihydroxy-6-([6-[(1E,3E)-7-oxo-7-(piperidin-1-yl)hepta-1,3-dien-1-yl]-2H-1,3-benzodioxol-5-yl]oxy)oxane-2-carboxylic acid	C25H31NO10	M+Na-2H	526.1695	-0.3
	HMDB0173747	6-([1-[(4E,6E)-7-(2H-1,3-benzodioxol-5-yl)hepta-4,6-dienyl]piperidin-3-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO10	M+Na-2H	526.1695	-0.3
	HMDB0173744	6-([(4E)-7-(2H-1,3-benzodioxol-5-yl)-1-oxo-1-(piperidin-1-yl)hepta-4,6-dien-3-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO10	M+Na-2H	526.1695	-0.3
	HMDB0149451	6-[1-carboxy-4-methoxy-4-(methylamino)-2,3-diphenylbutoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO10	M+Na-2H	526.1695	-0.3
	HMDB0149452	3,4,5-trihydroxy-6-{[2-hydroxy-5-methoxy-5-(methylamino)-3,4-diphenylpentanoyl]oxy}oxane-2-carboxylic acid	C25H31NO10	M+Na-2H	526.1695	-0.3
527.3029	HMDB0168871	[(2S,15S)-14-(3,4-dihydroxy-5,6-dimethylheptan-2-yl)-4,17-dihydroxy-2,15-dimethyltetraacyclo-heptadecan-5-yl]oxidanesulfonic acid	C28H50O8S	M-H2O-H	527.3043	-2.6
	HMDB0168869	[(2S,15S)-4-hydroxy-2,15-dimethyl-14-(1,3,4-trihydroxy-5,6-dimethylheptan-2-yl)tetraacycloheptadecan-5-yl]oxidanesulfonic acid	C28H50O8S	M-H2O-H	527.3043	-2.6
528.1485	HMDB0136426	3,4,5-trihydroxy-6-[4-(2-{[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}ethyl)-2-methoxyphenoxy]oxane-2-carboxylic acid	C24H29NO11	M+Na-2H	528.1487	-0.4
	HMDB0136427	3,4,5-trihydroxy-6-[4-(1-hydroxy-2-{[1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)propylidene]amino}ethyl)phenoxy]oxane-2-carboxylic acid	C24H29NO11	M+Na-2H	528.1487	-0.4
	HMDB0142239	6-{4-[2-cyano-2-(diethylcarbamoyl)ethyl]-2-hydroxy-6-nitrophenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H25N3O11	M+FA-H	528.1471	2.6
	HMDB0142238	6-{5-[2-cyano-2-(diethylcarbamoyl)ethyl]-2-hydroxy-3-nitrophenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H25N3O11	M+FA-H	528.1471	2.6
530.1265	HMDB0151377	2-amino-4-{[2-([2-carboxy-2-hydroxy-2-[(methylsulfanyl)methyl]-1-phenylethyl]sulfanyl)-1-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl]-C-hydroxycarbonimidoyl}butanoic acid	C21H29N3O9S2	M-H	530.1272	-1.4
	HMDB0151378	2-amino-4-{[2-([1-carboxy-2-hydroxy-1-[(methylsulfanyl)methyl]-2-phenylethyl]sulfanyl)-1-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl]-C-hydroxycarbonimidoyl}butanoic acid	C21H29N3O9S2	M-H	530.1272	-1.4
532.4725	HMDB0011759	Cer(d18/14)	C32H65NO3	M+Na-2H	532.4711	2.6

533.2980	HMDB0175529	3,4,5-trihydroxy-6-[(3-hydroxy-6,,14-trimethyl-2-methylidenepentadecanoyl)oxy]oxane-2-carboxylic acid	C25H44O9	M+FA-H	533.2967	2.4
	HMDB0175534	3,4,5-trihydroxy-6-[[6-(hydroxymethyl)-,14-dimethyl-2-methylidenepentadecanoyl]oxy]oxane-2-carboxylic acid	C25H44O9	M+FA-H	533.2967	2.4
	HMDB0175533	6-[[6-carboxy-2-(4,8-dimethylnonyl)-6-methylidenehexyl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H44O9	M+FA-H	533.2967	2.4
	HMDB0175539	6-[(14-carboxy-2,6,-trimethyl-14-methylidenetetradecyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H44O9	M+FA-H	533.2967	2.4
	HMDB0175536	6-[-carboxy-6-methyl--methylidene-2-(4-methylpentyl)decyl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H44O9	M+FA-H	533.2967	2.4
	HMDB0175537	3,4,5-trihydroxy-6-[-(hydroxymethyl)-6,14-dimethyl-2-methylidenepentadecanoyl]oxy]oxane-2-carboxylic acid	C25H44O9	M+FA-H	533.2967	2.4
	HMDB0175531	3,4,5-trihydroxy-6-[2-(4,8,12-trimethyltridecyl)oxirane-2-carbonyloxy]oxane-2-carboxylic acid	C25H44O9	M+FA-H	533.2967	2.4
	HMDB0175528	6-[(1-carboxy-5,9,13-trimethyl-1-methylidenetetradecan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H44O9	M+FA-H	533.2967	2.4
	HMDB0175525	3,4,5-trihydroxy-6-[(hydroxy-6,,14-trimethyl-2-methylidenepentadecanoyl)oxy]oxane-2-carboxylic acid	C25H44O9	M+FA-H	533.2967	2.4
	HMDB0175527	3,4,5-trihydroxy-6-[(14-hydroxy-6,,14-trimethyl-2-methylidenepentadecanoyl)oxy]oxane-2-carboxylic acid	C25H44O9	M+FA-H	533.2967	2.4
	HMDB0175524	6-[(14-carboxy-2,6,-trimethyl-14-methylidenetetradecan-6-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H44O9	M+FA-H	533.2967	2.4
	HMDB0175526	6-[(14-carboxy-2,6,-trimethyl-14-methylidenetetradecan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H44O9	M+FA-H	533.2967	2.4
	HMDB0175522	6-[(1-carboxy-5,9,13-trimethyl-1-methylidenetetradecan-5-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H44O9	M+FA-H	533.2967	2.4
	HMDB0175523	3,4,5-trihydroxy-6-[(6-hydroxy-6,,14-trimethyl-2-methylidenepentadecanoyl)oxy]oxane-2-carboxylic acid	C25H44O9	M+FA-H	533.2967	2.4
	HMDB0175540	3,4,5-trihydroxy-6-[(15-hydroxy-6,,14-trimethyl-2-methylidenepentadecanoyl)oxy]oxane-2-carboxylic acid	C25H44O9	M+FA-H	533.2967	2.4
534.4888	HMDB0035480	N-[(4E,8E)-1,3-dihydroxyoctadeca-4,8-dien-2-yl]hexadecanamide	C34H65NO3	M-H	534.4892	-0.7
	HMDB0240686	Cer(d18:2(4E,14Z)/16)	C34H65NO3	M-H	534.4892	-0.7
536.5032	HMDB0010697	Cer(t18/16)	C34H69NO4	M-H20-H	536.5043	-2.0
	HMDB0037105	Armillaramide	C34H69NO4	M-H20-H	536.5043	-2.0
	HMDB0038010	Malvidin 3-galactoside	C23H25O12	M+FA-H	537.1255	1.4
	HMDB0030777	Malvidin 3-glucoside	C23H25O12	M+FA-H	537.1255	1.4
	HMDB0138007	6-{3,5-dihydroxy-2,6-dimethoxy-4-[3-(4-methoxyphenyl)-2-oxopropanoyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H26O14	M-H	537.1250	2.5
	HMDB0151607	6-{4-[(5,8-dihydroxy-6,7-dimethoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-3-yl)(hydroxy)methyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H26O14	M-H	537.1250	2.5
	HMDB0152114	3,4,5-trihydroxy-6-{2-methoxy-4-[3-oxo-3-(2,4,6-trihydroxy-3,5-dimethoxyphenyl)prop-1-en-1-yl]phenoxy}oxane-2-carboxylic acid	C24H26O14	M-H	537.1250	2.5
	HMDB0151608	3,4,5-trihydroxy-6-({5-hydroxy-3-[hydroxy(4-hydroxyphenyl)methyl]-6,7-dimethoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-8-yl}oxy)oxane-2-carboxylic acid	C24H26O14	M-H	537.1250	2.5
	HMDB0151606	3,4,5-trihydroxy-6-({8-hydroxy-3-[hydroxy(4-hydroxyphenyl)methyl]-6,7-dimethoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-5-yl}oxy)oxane-2-carboxylic acid	C24H26O14	M-H	537.1250	2.5

HMDB0151611	6-{5-[(5,8-dihydroxy-6,7-dimethoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-3-yl)methyl]-2-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H26O14	M-H	537.1250	2.5
HMDB0151612	6-({3-[(3,4-dihydroxyphenyl)methyl]-8-hydroxy-6,7-dimethoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-5-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H26O14	M-H	537.1250	2.5
HMDB0151613	6-{4-[(5,8-dihydroxy-6,7-dimethoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-3-yl)methyl]-2-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H26O14	M-H	537.1250	2.5
HMDB0151614	6-({3-[(3,4-dihydroxyphenyl)methyl]-5-hydroxy-6,7-dimethoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-8-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H26O14	M-H	537.1250	2.5
HMDB0138006	6-{3,5-dihydroxy-2,4-dimethoxy-6-[3-(4-methoxyphenyl)-2-oxopropanoyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H26O14	M-H	537.1250	2.5
HMDB0177013	6-(4-{2-carboxy-2-[4-(2-carboxyethyl)-2-hydroxyphenoxy]ethyl}-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H26O14	M-H	537.1250	2.5
HMDB0177015	6-{2-[1-carboxy-2-(3,4-dihydroxyphenyl)ethoxy]-5-(2-carboxyethyl)phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H26O14	M-H	537.1250	2.5
HMDB0177016	6-[(3-{4-[1-carboxy-2-(3,4-dihydroxyphenyl)ethoxy]-3-hydroxyphenyl}propanoyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H26O14	M-H	537.1250	2.5
HMDB0038757	Isolimocitrol 3-glucoside	C24H26O14	M-H	537.1250	2.5
HMDB0037690	Limocitrol 3-glucoside	C24H26O14	M-H	537.1250	2.5
HMDB0177014	6-(5-{2-carboxy-2-[4-(2-carboxyethyl)-2-hydroxyphenoxy]ethyl}-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H26O14	M-H	537.1250	2.5
HMDB0152113	6-{3,5-dihydroxy-4-[3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]-2,6-dimethoxyphenoxy}-3,4,5-trihydroxyoxane-2-	C24H26O14	M-H	537.1250	2.5
HMDB0152112	6-{3,5-dihydroxy-2-[3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]-4,6-dimethoxyphenoxy}-3,4,5-trihydroxyoxane-2-	C24H26O14	M-H	537.1250	2.5
HMDB0177017	6-{2-[4-(2-carboxyethyl)-2-hydroxyphenoxy]-3-(3,4-dihydroxyphenyl)propanoyl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C24H26O14	M-H	537.1250	2.5
HMDB0132096	5,7-dihydroxy-2-(3-hydroxy-4,5-dimethoxyphenyl)-3-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-1H-chromen-1-ylum	C23H25O12	M+FA-H	537.1250	2.5
HMDB0132100	3,7-dihydroxy-2-(3-hydroxy-4,5-dimethoxyphenyl)-5-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-1H-chromen-1-ylum	C23H25O12	M+FA-H	537.1250	2.5
HMDB0138476	6-{5-[(5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-3-yl)methyl]-2-methoxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0138456	3,4,5-trihydroxy-6-{2-hydroxy-4-[(7-hydroxy-5-methoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-3-yl)methyl]phenoxy}oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0138474	3,4,5-trihydroxy-6-({7-hydroxy-3-[(3-hydroxy-4-methoxyphenyl)methyl]-4-oxo-3,4-dihydro-2H-1-benzopyran-5-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0138475	3,4,5-trihydroxy-6-({5-hydroxy-3-[(3-hydroxy-4-methoxyphenyl)methyl]-4-oxo-3,4-dihydro-2H-1-benzopyran-7-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0138457	3,4,5-trihydroxy-6-{2-hydroxy-5-[(7-hydroxy-5-methoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-3-yl)methyl]phenoxy}oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0138455	6-({3-[(3,4-dihydroxyphenyl)methyl]-5-methoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-7-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5

HMDB0151656	6-[(3-benzyl-6,8-dihydroxy-7-methoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-5-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0151655	6-[(3-benzyl-5,8-dihydroxy-7-methoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-6-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0151661	6-{3-[(5,8-dihydroxy-7-methoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-3-yl)methyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0151658	3,4,5-trihydroxy-6-({8-hydroxy-3-[hydroxy(phenyl)methyl]-7-methoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-5-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0151659	3,4,5-trihydroxy-6-({5-hydroxy-3-[hydroxy(phenyl)methyl]-7-methoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-8-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0151662	3,4,5-trihydroxy-6-({8-hydroxy-3-[(3-hydroxyphenyl)methyl]-7-methoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-5-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0151663	3,4,5-trihydroxy-6-({5-hydroxy-3-[(3-hydroxyphenyl)methyl]-7-methoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-8-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0151840	6-{2-[3-(2,4-dimethoxyphenyl)prop-2-enoyl]-3,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0151841	6-{4-[3-(2,4-dimethoxyphenyl)prop-2-enoyl]-3,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0152005	6-{3,5-dihydroxy-2-methoxy-4-[3-(2-methoxyphenyl)prop-2-enoyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0152007	6-{3,5-dihydroxy-4-methoxy-2-[3-(2-methoxyphenyl)prop-2-enoyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0152006	6-{3,5-dihydroxy-2-methoxy-6-[3-(2-methoxyphenyl)prop-2-enoyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0153145	5,6-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-7-methoxy-8-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-4H-chromen-4-one	C23H24O12	M+FA-H	537.1250	2.5
HMDB0153154	2-(2,5-dihydroxy-4-methoxyphenyl)-5-hydroxy-7-methoxy-8-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-4H-chromen-4-one	C23H24O12	M+FA-H	537.1250	2.5
HMDB0153286	6-{2-[3-(3,5-dimethoxyphenyl)prop-2-enoyl]-3,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0151657	6-[(3-benzyl-5,6-dihydroxy-7-methoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-8-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0151635	3,4,5-trihydroxy-6-({5-hydroxy-3-[(4-hydroxyphenyl)methyl]-7-methoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-8-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0151634	3,4,5-trihydroxy-6-({8-hydroxy-3-[(4-hydroxyphenyl)methyl]-7-methoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-5-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0150290	3,4,5-trihydroxy-6-{[7-hydroxy-6-(hydroxymethyl)-2-(4-methoxyphenyl)-4-oxo-3,4-dihydro-2H-1-benzopyran-5-yl]oxy}oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0150291	3,4,5-trihydroxy-6-{[5-hydroxy-6-(hydroxymethyl)-2-(4-methoxyphenyl)-4-oxo-3,4-dihydro-2H-1-benzopyran-7-yl]oxy}oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0150297	6-[3,5-dihydroxy-2-(hydroxymethyl)-6-[3-(4-methoxyphenyl)prop-2-enoyl]phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5

HMDB0150298	6-[3,5-dihydroxy-2-(hydroxymethyl)-4-[3-(4-methoxyphenyl)prop-2-enoyl]phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0150299	6-[3,5-dihydroxy-4-(hydroxymethyl)-2-[3-(4-methoxyphenyl)prop-2-enoyl]phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0151469	6-[(6,7-dihydroxy-3-methoxy-8-methyl-4-oxo-2-phenyl-3,4-dihydro-2H-1-benzopyran-5-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0151467	6-[(5,6-dihydroxy-3-methoxy-8-methyl-4-oxo-2-phenyl-3,4-dihydro-2H-1-benzopyran-7-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0151468	6-[(5,7-dihydroxy-3-methoxy-8-methyl-4-oxo-2-phenyl-3,4-dihydro-2H-1-benzopyran-6-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0151633	6-{4-[(5,8-dihydroxy-7-methoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-3-yl)methyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0153287	6-{4-[3-(3,5-dimethoxyphenyl)prop-2-enoyl]-3,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0030553	Tricin 7-glucoside	C23H24O12	M+FA-H	537.1250	2.5
HMDB0153371	Rhamnazin 3-glucoside	C23H24O12	M+FA-H	537.1250	2.5
HMDB0037578	Limocitrin 3-rhamnoside	C23H24O12	M+FA-H	537.1250	2.5
HMDB0039336	3',4',5-Trihydroxy-3,7-dimethoxyflavone 5-glucoside	C23H24O12	M+FA-H	537.1250	2.5
HMDB0035448	Licoagroside A	C23H24O12	M+FA-H	537.1250	2.5
HMDB0038825	3',8-Dimethoxyapigenin 7-glucoside	C23H24O12	M+FA-H	537.1250	2.5
HMDB0040479	3',7-Dimethoxy-4',5,8-trihydroxyflavone 8-glucoside	C23H24O12	M+FA-H	537.1250	2.5
HMDB0138121	3,4,5-trihydroxy-6-({13-hydroxy-5,14-dimethoxy-8,17-dioxatetracyclo[8.7.,heptadeca-2(7),3,5,11,13,15-hexaen-3-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0137451	3,4,5-trihydroxy-6-({6-hydroxy-5,14-dimethoxy-8,17-dioxatetracyclo[8.7.,heptadeca-2(7),3,5,11(16),12,14-hexaen-12-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0137445	3,4,5-trihydroxy-6-({6-hydroxy-5,14-dimethoxy-8,17-dioxatetracyclo[8.7.,heptadeca-2,4,6,11(16),12,14-hexaen-4-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0137446	3,4,5-trihydroxy-6-({4-hydroxy-5,14-dimethoxy-8,17-dioxatetracyclo[8.7.,heptadeca-2,4,6,11(16),12,14-hexaen-6-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0137447	3,4,5-trihydroxy-6-({6-hydroxy-5,14-dimethoxy-8,17-dioxatetracyclo[8.7.,heptadeca-2(7),3,5,11,13,15-hexaen-13-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0136836	2-(2,5-dihydroxy-4-methoxyphenyl)-6-[3,4-dihydroxy-6-(hydroxymethyl)-5-methoxyoxan-2-yl]-5,7-dihydroxy-4H-chromen-4-one	C23H24O12	M+FA-H	537.1250	2.5
HMDB0130702	6-[3,5-dihydroxy-2,6-dimethoxy-4-(3-phenylprop-2-enoyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0130701	6-[3,5-dihydroxy-2,4-dimethoxy-6-(3-phenylprop-2-enoyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0128614	6-{3,5-dihydroxy-2-methoxy-6-[3-(4-methoxyphenyl)prop-2-enoyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0137448	3,4,5-trihydroxy-6-({13-hydroxy-5,14-dimethoxy-8,17-dioxatetracyclo[8.7.,heptadeca-2(7),3,5,11,13,15-hexaen-6-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0137450	3,4,5-trihydroxy-6-({15-hydroxy-5,14-dimethoxy-8,17-dioxatetracyclo[8.7.,heptadeca-2(7),3,5,11(16),12,14-hexaen-6-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0137449	3,4,5-trihydroxy-6-({6-hydroxy-5,14-dimethoxy-8,17-dioxatetracyclo[8.7.,heptadeca-2(7),3,5,11(16),12,14-hexaen-15-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5

HMDB0138119	3,4,5-trihydroxy-6-({13-hydroxy-5,14-dimethoxy-8,17-dioxatetracyclo[8.7.,heptadeca-2(7),3,5,11,13,15-hexaen-12-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0138120	3,4,5-trihydroxy-6-({12-hydroxy-5,14-dimethoxy-8,17-dioxatetracyclo[8.7.,heptadeca-2(7),3,5,11,13,15-hexaen-13-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0138117	3,4,5-trihydroxy-6-({13-hydroxy-5,14-dimethoxy-8,17-dioxatetracyclo[8.7.,heptadeca-2(7),3,5,11,13,15-hexaen-15-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0138116	3,4,5-trihydroxy-6-({4-hydroxy-5,14-dimethoxy-8,17-dioxatetracyclo[8.7.,heptadeca-2,4,6,11,13,15-hexaen-13-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0138115	3,4,5-trihydroxy-6-({13-hydroxy-5,14-dimethoxy-8,17-dioxatetracyclo[8.7.,heptadeca-2,4,6,11,13,15-hexaen-4-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0138118	3,4,5-trihydroxy-6-({15-hydroxy-5,14-dimethoxy-8,17-dioxatetracyclo[8.7.,heptadeca-2(7),3,5,11,13,15-hexaen-13-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0137452	3,4,5-trihydroxy-6-({12-hydroxy-5,14-dimethoxy-8,17-dioxatetracyclo[8.7.,heptadeca-2(7),3,5,11,13,15-hexaen-6-yl}oxy)oxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0128612	6-{3,5-dihydroxy-4-methoxy-2-[3-(4-methoxyphenyl)prop-2-enoyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0128613	6-{3,5-dihydroxy-2-methoxy-4-[3-(4-methoxyphenyl)prop-2-enoyl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C23H24O12	M+FA-H	537.1250	2.5
HMDB0128567	2-(2,5-dihydroxy-4-methoxyphenyl)-5-hydroxy-7-methoxy-6-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-4H-chromen-4-one	C23H24O12	M+FA-H	537.1250	2.5
HMDB0186331	6-{2-[(1E,3E,5E,7Z)-8-carboxy-3,7-dimethylocta-1,3,5,7-tetraen-1-yl]-5-methoxy-3,4-dimethylphenyl}methoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
HMDB0186326	3,4,5-trihydroxy-6-{{(2Z,4E,6Z,8E)-7-(hydroxymethyl)-9-(4-methoxy-2,3,6-trimethylphenyl)-3-methylnona-2,4,6,8-tetraenoyl}oxy}oxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
HMDB0186328	3,4,5-trihydroxy-6-{{(2E,4E,6E,8E)-2-hydroxy-9-(4-methoxy-2,3,6-trimethylphenyl)-3,7-dimethylnona-2,4,6,8-tetraenoyl}oxy}oxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
HMDB0186325	6-{{(2Z,4E,6Z)-7-carboxy-2-[(E)-2-(4-methoxy-2,3,6-trimethylphenyl)ethenyl]-6-methylhepta-2,4,6-trien-1-yl}oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
HMDB0186322	6-{{(2E)-3-carboxy-2-[(3E,5E)-6-(4-methoxy-2,3,6-trimethylphenyl)-4-methylhexa-1,3,5-trien-1-yl]prop-2-en-1-yl}oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
HMDB0186323	3,4,5-trihydroxy-6-{{(2E,4E,6E,8E)-3-(hydroxymethyl)-9-(4-methoxy-2,3,6-trimethylphenyl)-7-methylnona-2,4,6,8-tetraenoyl}oxy}oxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
HMDB0131873	3,4,5-trihydroxy-6-({9-hydroxy-16,17-dimethoxytricyclo[12.3.1.1,nonadeca-1(17),2,4,6(19),14(18),15-hexaen-3-yl}oxy)oxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
HMDB0186332	3,4,5-trihydroxy-6-{{(2Z,4E,6E)-9-[6-(hydroxymethyl)-4-methoxy-2,3-dimethylphenyl]-3,7-dimethylnona-2,4,6,8-tetraenoyl}oxy}oxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
HMDB0186337	6-({3-[(1E,3E,5E,7Z)-8-carboxy-3,7-dimethylocta-1,3,5,7-tetraen-1-yl]-6-methoxy-2,4-dimethylphenyl}methoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0

	HMDB0186351	3,4,5-trihydroxy-6-{{(2Z,4E,6E)-7-[3-(4-methoxy-2,3,6-trimethylphenyl)oxiran-2-yl]-3-methylocta-2,4,6-trienoyl}oxy}oxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
	HMDB0186348	3,4,5-trihydroxy-6-{{(2Z,4E)-5-{3-[(E)-2-(4-methoxy-2,3,6-trimethylphenyl)ethenyl]-3-methyloxiran-2-yl}-3-methylpenta-2,4-dienoyl}oxy}oxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
	HMDB0186345	3,4,5-trihydroxy-6-{{(2Z)-3-{3-[(1E,3E)-4-(4-methoxy-2,3,6-trimethylphenyl)-2-methylbuta-1,3-dien-1-yl]oxiran-2-yl}but-2-enoyl}oxy}oxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
	HMDB0186342	3,4,5-trihydroxy-6-{3-[(1E,3E,5E)-6-(4-methoxy-2,3,6-trimethylphenyl)-4-methylhexa-1,3,5-trien-1-yl]-3-methyloxirane-2-carbonyloxy}oxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
	HMDB0186338	3,4,5-trihydroxy-6-{{(2Z,4E,6E,8E)-9-[3-(hydroxymethyl)-4-methoxy-2,6-dimethylphenyl]-3,7-dimethylnona-2,4,6,8-tetraenoyl}oxy}oxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
	HMDB0186340	6-{3-[(1E,3E,5E,7Z)-8-carboxy-3,7-dimethylocta-1,3,5,7-tetraen-1-yl]-6-methoxy-2,4,5-trimethylphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
	HMDB0186341	3,4,5-trihydroxy-6-{{(2Z,4E,6E,8E)-9-(3-hydroxy-4-methoxy-2,5,6-trimethylphenyl)-3,7-dimethylnona-2,4,6,8-tetraenoyl}oxy}oxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
	HMDB0186334	6-({2-[(1E,3E,5E,7Z)-8-carboxy-3,7-dimethylocta-1,3,5,7-tetraen-1-yl]-5-methoxy-3,6-dimethylphenyl}methoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
	HMDB0186335	3,4,5-trihydroxy-6-{{(2Z,4E,6E)-9-[2-(hydroxymethyl)-4-methoxy-3,6-dimethylphenyl]-3,7-dimethylnona-2,4,6,8-tetraenoyl}oxy}oxane-2-carboxylic acid	C27H34O10	M+Na-2H	539.1899	-2.0
540.0541	HMDB0001178	Adenosine diphosphate ribose	C15H23N5O14P2	M-H2O-H	540.0533	1.5
	HMDB0012276	1-(5-phosphoribosyl)-5'-AMP	C15H23N5O14P2	M-H2O-H	540.0533	1.5
540.1484	HMDB0029331	Gravacridonetriol glucoside	C25H29NO11	M+Na-2H	540.1487	-0.6
540.1851	HMDB0161543	6-(3-{[(2E,4E,8E)-9-(2H-1,3-benzodioxol-5-yl)-1-hydroxynona-2,4,8-trien-1-ylidene]amino}-2-methylpropoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO10	M+Na-2H	540.1851	0.0
	HMDB0177118	6-({1-[(3,4-dimethoxyphenyl)methyl]-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO10	M+Na-2H	540.1851	0.0
	HMDB0161532	6-({[(1E,5E,7E)-1-(2H-1,3-benzodioxol-5-yl)-8-[(2-methylpropyl)-C-hydroxycarbonimidoyl]octa-1,5,7-trien-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO10	M+Na-2H	540.1851	0.0
	HMDB0161534	6-({[(1E,7E)-1-(2H-1,3-benzodioxol-5-yl)-8-[(2-methylpropyl)-C-hydroxycarbonimidoyl]octa-1,5,7-trien-4-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO10	M+Na-2H	540.1851	0.0
	HMDB0161536	3,4,5-trihydroxy-6-({6-[(1E,5E,7E)-8-[(2-methylpropyl)-C-hydroxycarbonimidoyl]octa-1,5,7-trien-1-yl]-2H-1,3-benzodioxol-5-yl}oxy)oxane-2-carboxylic acid	C26H33NO10	M+Na-2H	540.1851	0.0
	HMDB0161549	6-([1-[(2E,4E,8E)-9-(2H-1,3-benzodioxol-5-yl)-1-hydroxynona-2,4,8-trien-1-ylidene]amino}-2-methylpropan-2-yl)oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO10	M+Na-2H	540.1851	0.0
	HMDB0176839	1-({4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-3-hydroxyphenyl}methyl)-7,8-dimethoxy-2,2-dimethyl-1,2,3,4-tetrahydroisoquinolin-2-ium	C26H34NO10	M+Na-2H	540.1851	0.0

	HMDB0176850	1-({1-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-4-oxocyclohexa-2,5-dien-1-yl} methyl)-7,8-dimethoxy-2,2-dimethyl-1,2,3,4-tetrahydroisoquinolin-2-ium	C26H34NO10	M+Na-2H	540.1851	0.0
	HMDB0176848	1-({4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]phenyl} methyl)-3-hydroxy-7,8-dimethoxy-2,2-dimethyl-1,2,3,4-tetrahydroisoquinolin-2-ium	C26H34NO10	M+Na-2H	540.1851	0.0
	HMDB0177130	2-[(6-carboxy-3,4-dihydroxyoxan-2-yl)oxy]-1-[(3,4-dimethoxyphenyl)methyl]-7-hydroxy-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-2-ium	C26H34NO10	M+Na-2H	540.1851	0.0
	HMDB0176838	1-({3-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-4-hydroxyphenyl} methyl)-7,8-dimethoxy-2,2-dimethyl-1,2,3,4-tetrahydroisoquinolin-2-ium	C26H34NO10	M+Na-2H	540.1851	0.0
	HMDB0176832	1-({4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]phenyl} methyl)-4-hydroxy-7,8-dimethoxy-2,2-dimethyl-1,2,3,4-tetrahydroisoquinolin-2-ium	C26H34NO10	M+Na-2H	540.1851	0.0
	HMDB0176835	1-({4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]phenyl} (hydroxy)methyl)-7,8-dimethoxy-2,2-dimethyl-1,2,3,4-tetrahydroisoquinolin-2-ium	C26H34NO10	M+Na-2H	540.1851	0.0
	HMDB0176829	6-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1-[(4-hydroxyphenyl)methyl]-7,8-dimethoxy-2,2-dimethyl-1,2,3,4-tetrahydroisoquinolin-2-ium	C26H34NO10	M+Na-2H	540.1851	0.0
	HMDB0176830	1-({4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]phenyl} methyl)-6-hydroxy-7,8-dimethoxy-2,2-dimethyl-1,2,3,4-tetrahydroisoquinolin-2-ium	C26H34NO10	M+Na-2H	540.1851	0.0
542.1298	HMDB0187660	16-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-17-methoxy-5,7-dioxo-13位?azapentacyclo[11.8,??]癸henicosa-1(13),2,4(8),9,14,16,18,-octaen-13-ylum	C25H24NO10	M+FA-H	542.1304	-1.1
	HMDB0187661	17-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-16-methoxy-5,7-dioxo-13位?azapentacyclo[11.8,??]癸henicosa-1(13),2,4(8),9,14,16,18,-octaen-13-ylum	C25H24NO10	M+FA-H	542.1304	-1.1
	HMDB0162630	3,4,5-trihydroxy-6-({4,5,14,16-tetramethoxy-8-oxo--azatetracyclo[7.7.1,,heptadeca-1(16),2,4,6,9,11,13(17),14-octaen-15-yl} oxy)oxane-2-carboxylic acid	C26H25NO12	M-H	542.1304	-1.1
	HMDB0162632	3,4,5-trihydroxy-6-({5,14,15,16-tetramethoxy-8-oxo--azatetracyclo[7.7.1,,heptadeca-1(16),2,4,6,9,11,13(17),14-octaen-4-yl} oxy)oxane-2-carboxylic acid	C26H25NO12	M-H	542.1304	-1.1
	HMDB0162631	3,4,5-trihydroxy-6-({4,5,14,15-tetramethoxy-8-oxo--azatetracyclo[7.7.1,,heptadeca-1(16),2,4,6,9,11,13(17),14-octaen-16-yl} oxy)oxane-2-carboxylic acid	C26H25NO12	M-H	542.1304	-1.1
	HMDB0162629	3,4,5-trihydroxy-6-({4,5,15,16-tetramethoxy-8-oxo--azatetracyclo[7.7.1,,heptadeca-1(16),2,4,6,9,11,13(17),14-octaen-14-yl} oxy)oxane-2-carboxylic acid	C26H25NO12	M-H	542.1304	-1.1
	HMDB0162633	3,4,5-trihydroxy-6-({4,14,15,16-tetramethoxy-8-oxo--azatetracyclo[7.7.1,,heptadeca-1(16),2,4,6,9,11,13(17),14-octaen-5-yl} oxy)oxane-2-carboxylic acid	C26H25NO12	M-H	542.1304	-1.1
	HMDB0149480	6-{[2,4-dihydroxy-5-methoxy-5-(methylamino)-3,4-diphenylpentanoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149510	3,4,5-trihydroxy-6-{[2-hydroxy-3-(2-hydroxyphenyl)-5-methoxy-5-(methylamino)-4-phenylpentanoyl]oxy} oxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149509	6-{2-[1-carboxy-1-hydroxy-4-methoxy-4-(methylamino)-3-phenylbutan-2-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149506	6-{2-[4-carboxy-4-hydroxy-1-methoxy-1-(methylamino)-3-phenylbutan-2-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149507	3,4,5-trihydroxy-6-{[2-hydroxy-4-(2-hydroxyphenyl)-5-methoxy-5-(methylamino)-3-phenylpentanoyl]oxy} oxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7

542.1640	HMDB0149498	3,4,5-trihydroxy-6-{{2-hydroxy-3-(4-hydroxyphenyl)-5-methoxy-5-(methylamino)-4-phenylpentanoyl}oxy}oxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149497	6-{4-[1-carboxy-1-hydroxy-4-methoxy-4-(methylamino)-3-phenylbutan-2-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149494	3,4,5-trihydroxy-6-{{2-hydroxy-4-(4-hydroxyphenyl)-5-methoxy-5-(methylamino)-3-phenylpentanoyl}oxy}oxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149493	6-{4-[4-carboxy-4-hydroxy-1-methoxy-1-(methylamino)-3-phenylbutan-2-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149490	6-{3-[1-carboxy-1-hydroxy-4-methoxy-4-(methylamino)-3-phenylbutan-2-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149491	3,4,5-trihydroxy-6-{{2-hydroxy-3-(3-hydroxyphenyl)-5-methoxy-5-(methylamino)-4-phenylpentanoyl}oxy}oxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149486	6-{3-[4-carboxy-4-hydroxy-1-methoxy-1-(methylamino)-3-phenylbutan-2-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149487	3,4,5-trihydroxy-6-{{2-hydroxy-4-(3-hydroxyphenyl)-5-methoxy-5-(methylamino)-3-phenylpentanoyl}oxy}oxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149484	6-{{2,3-dihydroxy-5-methoxy-5-(methylamino)-3,4-diphenylpentanoyl}oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149483	6-[1-carboxy-2-hydroxy-4-methoxy-4-(methylamino)-2,3-diphenylbutoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149482	6-{{1-carboxy-1-hydroxy-4-methoxy-4-(methylamino)-2,3-diphenylbutan-2-yl}oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149478	6-{{4-carboxy-4-hydroxy-1-methoxy-1-(methylamino)-2,3-diphenylbutan-2-yl}oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0149479	6-[1-carboxy-3-hydroxy-4-methoxy-4-(methylamino)-2,3-diphenylbutoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0177139	3,4,5-trihydroxy-6-({1-[(1-hydroxy-3-methoxy-4-oxocyclohexa-2,5-dien-1-yl)methyl]-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-yl}oxy)oxane-2-carboxylic acid	C25H31NO11	M+Na-2H	542.1644	-0.7
	HMDB0060709	17-Desacetyl Rocuronium	C30H51BrN2O3	M-H2O-H	547.2899	0.7
	HMDB0156576	6-{{(2R,15R)-14-(4-carboxybutan-2-yl)-9-hydroxy-2,15-dimethyltetraacyclo[8.7,,heptadec-7-en-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
	HMDB0156574	6-{{(2R,15R)-14-(4-carboxybutan-2-yl)-6-hydroxy-2,15-dimethyltetraacyclo[8.7,,heptadec-7-en-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
	HMDB0156572	6-{{(2R,15S)-14-(4-carboxy-2-hydroxybutan-2-yl)-2,15-dimethyltetraacyclo[8.7,,heptadec-7-en-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
	HMDB0156568	6-{{(2S,15R)-14-(4-carboxybutan-2-yl)-2-(hydroxymethyl)-15-methyltetraacyclo[8.7,,heptadec-7-en-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
	HMDB0156570	6-{{(2R,15S)-14-(4-carboxybutan-2-yl)-15-(hydroxymethyl)-2-methyltetraacyclo[8.7,,heptadec-7-en-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
	HMDB0156566	6-{{(2R,15S)-14-(4-carboxybutan-2-yl)-13-hydroxy-2,15-dimethyltetraacyclo[8.7,,heptadec-7-en-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7

547.2903

HMDB0156562	6-{[(2R,15S)-14-(4-carboxy-1-hydroxybutan-2-yl)-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
HMDB0156564	6-{[(2R,15R)-14-(4-carboxybutan-2-yl)-17-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
HMDB0156577	6-{[(2R,15R)-14-(4-carboxybutan-2-yl)-5-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadec-7-en-9-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
HMDB0184418	3,4,5-trihydroxy-6-({4-[(2S,15R)-16-hydroxy-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoyl}oxy)oxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
HMDB0159728	6-{[(1S,2S,7R,R,11S,15R)-14-(4-carboxybutan-2-yl)-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-9-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
HMDB0159240	6-{[(1S,2S,7S,R,11S,15R)-14-(4-carboxybutan-2-yl)-2,15-dimethyl-9-oxotetracyclo[8.7.,heptadecan-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
HMDB0159183	6-{[(2S,15R)-14-(4-carboxybutan-2-yl)-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-9-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
HMDB0159180	6-{[(1S,2S,7S,R,11S,15R)-14-(4-carboxybutan-2-yl)-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-9-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
HMDB0157499	6-{[(2S,15S)-14-(4-carboxybut-1-en-2-yl)-16-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
HMDB0157475	3,4,5-trihydroxy-6-({4-[(2S,15R)-16-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadecan-14-yl]pentanoyl}oxy)oxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
HMDB0157089	6-{[(1S,2S,7R,R,11S,14R,15R)-14-(4-carboxybutan-2-yl)-2,15-dimethyl-16-oxotetracyclo[8.7.,heptadecan-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H46O10	M-H2O-H	547.2907	-0.7
HMDB0165566	3-hydroxy-6-{[11-hydroxy-2,15-dimethyl-14-(5-oxo-2,5-dihydrofuran-3-yl)tetracyclo[8.7.,heptadecan-5-yl]oxy}-2-methyloxan-4-one	C29H42O7	M+FA-H	547.2913	-1.7
HMDB0159330	6-({4-[(2S,15R)-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadec-8-en-14-yl]pentanoyl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H44O9	M-H	547.2913	-1.7
HMDB0156560	6-({4-[(2R,15R)-2,15-dimethyl-5-oxotetracyclo[8.7.,heptadec-7-en-14-yl]pentanoyl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H44O9	M-H	547.2913	-1.7
HMDB0185166	6-{[(3Z,6Z,9Z)-21-carboxyhenicosa-3,6,9-trien-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
HMDB0185145	6-{[(3Z,9Z)-21-carboxyhenicosa-3,7,9-trien-6-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
HMDB0185146	3,4,5-trihydroxy-6-{[(13Z,15E,19Z)-17-hydroxydocosa-13,15,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
HMDB0185149	3,4,5-trihydroxy-6-{[(16Z,19Z)-13-hydroxydocosa-14,16,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
HMDB0185151	6-{[(6Z,9Z)-21-carboxyhenicosa-4,6,9-trien-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
HMDB0185148	6-{[(3Z,6Z)-21-carboxyhenicosa-3,6,8-trien-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
HMDB0185152	3,4,5-trihydroxy-6-{[(13Z,16Z,18E)-hydroxydocosa-13,16,18-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
HMDB0185155	3,4,5-trihydroxy-6-{[(13Z,19Z)-16-hydroxydocosa-13,17,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
HMDB0185171	3,4,5-trihydroxy-6-{[(13Z,16Z,19Z)-2-hydroxydocosa-13,16,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7

	HMDB0185160	3,4,5-trihydroxy-6-{{[(13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadec-13-enoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
	HMDB0185154	6-{{[(3Z,9Z)-21-carboxyhenicosa-3,5,9-trien-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
	HMDB0185170	6-{{[(12Z,15Z,18Z)-1-carboxyhenicosa-12,15,18-trien-1-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
	HMDB0185163	6-{{[(13Z,16Z)-18-(3-ethyloxiran-2-yl)octadeca-13,16-dienoyl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
	HMDB0185157	3,4,5-trihydroxy-6-[(12-{3-[(2Z,5Z)-octa-2,5-dien-1-yl]oxiran-2-yl}dodecanoyl)oxy]oxane-2-carboxylic	C28H46O9	M+Na-2H	547.2888	2.7
	HMDB0185167	3,4,5-trihydroxy-6-{{[(13Z,16Z,19Z)-22-hydroxydocosa-13,16,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
	HMDB0185140	3,4,5-trihydroxy-6-{{[(13Z,16Z,19Z)-15-hydroxydocosa-13,16,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
	HMDB0185142	6-{{[(3Z)-21-carboxyhenicosa-3,6,9-trien-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
	HMDB0185133	6-{{[(3Z,6Z,9Z)-21-carboxyhenicosa-3,6,9-trien-11-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
	HMDB0185134	3,4,5-trihydroxy-6-{{[(13Z,16Z,19Z)-12-hydroxydocosa-13,16,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
	HMDB0185136	6-{{[(6Z,9Z)-21-carboxyhenicosa-3,6,9-trien-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
	HMDB0185137	3,4,5-trihydroxy-6-{{[(13Z,16Z,19Z)-21-hydroxydocosa-13,16,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
	HMDB0185139	6-{{[(6Z,9Z)-21-carboxyhenicosa-3,6,9-trien-8-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
	HMDB0185143	3,4,5-trihydroxy-6-{{[(13Z,16Z,19Z)-18-hydroxydocosa-13,16,19-trienoyl]oxy}oxane-2-carboxylic acid	C28H46O9	M+Na-2H	547.2888	2.7
554.1628	HMDB0135499	6-[4-(2-{{2-(3,4-dimethoxyphenyl)ethyl}-C-hydroxycarbonimidoyl}eth-1-en-1-yl)-2-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H31NO11	M+Na-2H	554.1644	-2.8
	HMDB0135495	6-[4-(2-{{3-(3,4-dimethoxyphenyl)-1-hydroxyprop-2-en-1-ylidene]amino}ethyl)-2-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H31NO11	M+Na-2H	554.1644	-2.8
	HMDB0135497	6-[5-(2-{{3-(3,4-dimethoxyphenyl)-1-hydroxyprop-2-en-1-ylidene]amino}ethyl)-2-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H31NO11	M+Na-2H	554.1644	-2.8
	HMDB0135493	6-[5-(2-{{2-(3,4-dimethoxyphenyl)ethyl}-C-hydroxycarbonimidoyl}eth-1-en-1-yl)-2-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H31NO11	M+Na-2H	554.1644	-2.8
556.1441	HMDB0035209	Cartormin	C27H29NO13	M-H20-H	556.1455	-2.5
	HMDB0177128	6-({1-[(3,4-dimethoxyphenyl)methyl]-8-hydroxy-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO11	M+Na-2H	556.1800	2.1
	HMDB0177129	6-({1-[(3,4-dimethoxyphenyl)methyl]-6-methoxy-2-methyl-2-oxo-1,2,3,4-tetrahydro-2H-isoquinolin-7-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO11	M+Na-2H	556.1800	2.1
	HMDB0177125	6-({1-[(3,4-dimethoxyphenyl)methyl]-4-hydroxy-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO11	M+Na-2H	556.1800	2.1
	HMDB0177127	6-({1-[(3,4-dimethoxyphenyl)methyl]-7-hydroxy-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-8-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO11	M+Na-2H	556.1800	2.1
	HMDB0177123	6-({1-[(3,4-dimethoxyphenyl)(hydroxy)methyl]-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO11	M+Na-2H	556.1800	2.1

556.1812	HMDB0177121	6-({1-[(3,4-dimethoxyphenyl)methyl]-1-hydroxy-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO11	M+Na-2H	556.1800	2.1
	HMDB0177120	6-({1-[(3,4-dimethoxyphenyl)methyl]-3-hydroxy-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO11	M+Na-2H	556.1800	2.1
	HMDB0135515	6-[4-(2-{{2-(3,4-dimethoxyphenyl)ethyl}-C-hydroxycarbonimidoyl}ethyl)-2-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO11	M+Na-2H	556.1800	2.1
	HMDB0135513	6-[5-(2-{{3-(3,4-dimethoxyphenyl)-1-hydroxypropylidene}amino}ethyl)-2-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO11	M+Na-2H	556.1800	2.1
	HMDB0135511	6-[4-(2-{{3-(3,4-dimethoxyphenyl)-1-hydroxypropylidene}amino}ethyl)-2-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO11	M+Na-2H	556.1800	2.1
	HMDB0135509	6-[5-(2-{{2-(3,4-dimethoxyphenyl)ethyl}-C-hydroxycarbonimidoyl}ethyl)-2-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H33NO11	M+Na-2H	556.1800	2.1
557.0399	HMDB0145878	3-[3,5-dihydroxy-4-(sulfooxy)phenyl]-6,11-dihydroxy-7-(4-hydroxy-3,5-dimethoxyphenyl)-2-ylidene-8-dioxatricyclo[7.3.1?]trideca-1(13),2,4,6,9,11-hexaen-2-ylum	C25H19O13S	M-H	557.0395	0.7
	HMDB0145879	7-[3,5-dimethoxy-4-(sulfooxy)phenyl]-6,11-dihydroxy-3-(3,4,5-trihydroxyphenyl)-2-ylidene-8-dioxatricyclo[7.3.1?]trideca-1(13),2,4,6,9,11-hexaen-2-ylum	C25H19O13S	M-H	557.0395	0.7
	HMDB0145886	7-[3,5-dimethoxy-4-(sulfooxy)phenyl]-6,11-dihydroxy-3-(2,4,5-trihydroxyphenyl)-2-ylidene-8-dioxatricyclo[7.3.1?]trideca-1(13),2,4,6,9,11-hexaen-2-ylum	C25H19O13S	M-H	557.0395	0.7
	HMDB0145893	3,8-dihydroxy-7-(4-hydroxy-3,5-dimethoxyphenyl)-12-[4-hydroxy-3-(sulfooxy)phenyl]-6-ylidene-11,13-trioxatetracyclo[7.4.1??]tetradeca-1,3,5(14),6,8-pentaen-6-ylum	C25H19O13S	M-H	557.0395	0.7
	HMDB0134851	4-[7-(3,4-dihydroxy-5-methoxyphenyl)-6,11-dihydroxy-2,8-dioxatricyclo[7.3.1?]trideca-1(13),4,6,9,11-pentaen-3-ylidene]cyclohexa-2,5-dien-1-ylidene hydrogen sulfuric acidium	C24H17O11S	M+FA-H	557.0395	0.7
	HMDB0152172	{5-[(1E)-3-[4-(5,7-dihydroxy-4-oxo-4H-chromen-2-yl)phenoxy]-3-oxoprop-1-en-1-yl]-2-hydroxyphenyl}oxidanesulfonic acid	C24H16O11S	M+FA-H	557.0395	0.7
558.1592	HMDB0034773	4-Demethylsimmondsin 2'-(E)-ferulate	C25H31NO12	M+Na-2H	558.1593	-0.2
	HMDB0034774	3-Demethylsimmondsin 2'-(Z)-ferulate	C25H31NO12	M+Na-2H	558.1593	-0.2
565.0474	HMDB0000286	Uridine diphosphate glucose	C15H24N2O17P2	M-H	565.0477	-0.6
	HMDB0000302	Uridine diphosphategalactose	C15H24N2O17P2	M-H	565.0477	-0.6
	HMDB0062573	Uridine diphosphategalactose	C15H24N2O17P2	M-H	565.0477	-0.6
	HMDB0060079	Uridine diphosphate glucose	C15H24N2O17P2	M-H	565.0477	-0.6
	HMDB0175875	[3,4,-trihydroxy-4a,9-bis(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-5-yl]oxidanesulfonic acid	C30H50O9S	M-H2O-H	567.2992	-0.1
	HMDB0175876	[8,9,-trihydroxy-4,8a-bis(hydroxymethyl)-4,6a,6b,11,11,14b-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-3-yl]oxidanesulfonic acid	C30H50O9S	M-H2O-H	567.2992	-0.1
	HMDB0175873	[4,5,-trihydroxy-4a,9-bis(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-3-yl]oxidanesulfonic acid	C30H50O9S	M-H2O-H	567.2992	-0.1

HMDB0175871	{[3,4,5,-tetrahydroxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-4a-yl]methoxy}sulfonic acid	C30H50O9S	M-H2O-H	567.2992	-0.1
HMDB0175872	{[3,8,9,-tetrahydroxy-8a-(hydroxymethyl)-4,6a,6b,11,11,14b-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-4-yl]methoxy}sulfonic acid	C30H50O9S	M-H2O-H	567.2992	-0.1
HMDB0175874	[3,5,-trihydroxy-4a,9-bis(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-4-yl]oxidanesulfonic acid	C30H50O9S	M-H2O-H	567.2992	-0.1
HMDB0182492	6-methyl-2-[(2S,15S)-2,6,6,15-tetramethyl-5-(sulfooxy)tetracyclo[8.7,,heptadec-1-en-14-yl]hept-5-enoic acid	C29H46O6S	M+FA-H	567.2997	-1.1
HMDB0175848	(2S,4aS,6aR,6bS,12aS)-12b-hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175853	(2S,4aS,6aR,6bR,12aS)-14-hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175844	(2S,4aS,6aR,6bR,12aS)-2-(hydroxymethyl)-4a,6a,6b,9,9,12a-hexamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175843	(2S,4aS,6aR,6bR,12aS)--hydroxy-4a,6a,6b,9,9,12a-hexamethyl-13-oxo-2-[(sulfooxy)methyl]-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175838	(2S,4aR,6aR,6bR,12aS)--hydroxy-2,6a,6b,9,9,12a-hexamethyl-13-oxo-4a-[(sulfooxy)methyl]-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175839	(2S,4aR,6aR,6bR,12aS)-4a-(hydroxymethyl)-2,6a,6b,9,9,12a-hexamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175852	(2S,4aS,6aR,6bR,12aS)--hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-13-oxo-14-(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0176019	[9-formyl-4,-dihydroxy-4a-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-5-yl]oxidanesulfonic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0178348	3-hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0178347	-hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-13-oxo-3-(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0176627	(2Z)-4,7-dihydroxy-2-methyl-6-[7,7,12,16-tetramethyl-6-(sulfooxy)pentacyclo[9.7,,,octadecan-15-yl]hept-2-enoic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0176629	(2Z)-4-hydroxy-6-[18-hydroxy-7,7,12,16-tetramethyl-6-(sulfooxy)pentacyclo[9.7octadecan-15-yl]-2-methylhept-2-enoic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0176020	[9-formyl-5,-dihydroxy-4a-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-4-yl]oxidanesulfonic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0176018	[4-formyl-8,9-dihydroxy-8a-(hydroxymethyl)-4,6a,6b,11,11,14b-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-3-yl]oxidanesulfonic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0176017	[(9-formyl-4,5,-trihydroxy-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-4a-yl)methoxy]sulfonic acid	C30H48O8S	M-H	567.2997	-1.1

567.2991

HMDB0176010	4,-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl-5-(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0176011	5,-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl-4-(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0176009	4,5-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl--(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175834	(2S,4aS,6aS,6bR,12aS)-6a-(hydroxymethyl)-2,4a,6b,9,9,12a-hexamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175833	(2S,4aS,6aS,6bR,12aS)--hydroxy-2,4a,6b,9,9,12a-hexamethyl-13-oxo-6a-[(sulfooxy)methyl]-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175828	(2S,4aS,6aR,6bR,12aR)--hydroxy-2,4a,6a,6b,9,9-hexamethyl-13-oxo-12a-[(sulfooxy)methyl]-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0169221	5,-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl-3-(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0169222	3,-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl-5-(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0169223	3,5-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl--(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175636	-hydroxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-11-(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175634	,11-dihydroxy-2,2,6a,6b,9,12a-hexamethyl-9-[(sulfooxy)methyl]-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175635	11-hydroxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl--(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175819	(2S,4aS,6aR,6bS,12aS)-6b-(hydroxymethyl)-2,4a,6a,9,9,12a-hexamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175818	(2S,4aS,6aR,6bS,12aS)--hydroxy-2,4a,6a,9,9,12a-hexamethyl-13-oxo-6b-[(sulfooxy)methyl]-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175823	(2S,4aS,6aR,6bR,12aS)--hydroxy-2,4a,6a,6b,9,12a-hexamethyl-13-oxo-9-[(sulfooxy)methyl]-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175824	(2S,4aS,6aR,6bR,12aS)-9-(hydroxymethyl)-2,4a,6a,6b,9,12a-hexamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0175829	(2S,4aS,6aR,6bR,12aR)-12a-(hydroxymethyl)-2,4a,6a,6b,9,9-hexamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M-H	567.2997	-1.1
HMDB0001278	Presqualene diphosphate	C30H52O7P2	M-H2O-H	567.3004	-2.4
HMDB0012188	All-trans-hexaprenyl diphosphate	C30H52O7P2	M-H2O-H	567.3004	-2.4

	HMDB0034101	Adouetine Y	C34H40N4O4	M-H	567.2977	2.5
	HMDB0029342	Ceanothine E	C34H40N4O4	M-H	567.2977	2.5
	HMDB0001097	Protoporphyrinogen IX	C34H40N4O4	M-H	567.2977	2.5
568.1813	HMDB0160574	5-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-4-hydroxydecanedioic acid	C20H33N3O11S	M+FA-H	568.1818	-0.8
	HMDB0160573	4-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-5-hydroxydecanedioic acid	C20H33N3O11S	M+FA-H	568.1818	-0.8
	HMDB0170548	4-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-5-hydroxy-2,7-dimethyloctanedioic acid	C20H33N3O11S	M+FA-H	568.1818	-0.8
	HMDB0060822	Doxorubicin-semiquinone	C27H33NO11	M+Na-2H	568.1800	2.2
570.3658	HMDB0178525	2-[2-oxo-2-({7,16,18-trihydroxy-19-[(1-hydroxyethylidene)amino]-5,9-dimethylicosan-6-yl}oxy)ethyl]butanedioic acid	C30H55NO10	M-H2O-H	570.3642	2.8
	HMDB0178526	2-[2-oxo-2-({6,16,18-trihydroxy-19-[(1-hydroxyethylidene)amino]-5,9-dimethylicosan-7-yl}oxy)ethyl]butanedioic acid	C30H55NO10	M-H2O-H	570.3642	2.8
578.0468	HMDB0180817	{[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)[(4,6-dimethoxypyrimidin-2-yl)-C-hydroxycarbonimidoyl]amino}(4-carboxy-3-chloro-1-methyl-1H-pyrazol-5-yl)hydroxy- $\dot{\nu}$?sulfanyl}oxidanyl	C18H22CIN6O13S	M-H2O-H	578.0470	-0.4
	HMDB0180819	{[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)[(4-hydroxy-6-methoxypyrimidin-2-yl)-C-hydroxycarbonimidoyl]amino}[3-chloro-4-(methoxycarbonyl)-1-methyl-1H-pyrazol-5-yl]hydroxy- $\dot{\nu}$?sulfanyl}oxidanyl	C18H22CIN6O13S	M-H2O-H	578.0470	-0.4
579.0266	HMDB0000935	Uridine diphosphate glucuronic acid	C15H22N2O18P2	M-H	579.0270	-0.7
	HMDB0012302	UDP-D-galacturonate	C15H22N2O18P2	M-H	579.0270	-0.7
	HMDB0012304	UDP-L-iduronate	C15H22N2O18P2	M-H	579.0270	-0.7
	HMDB0156314	3,4,5-trihydroxy-6-{{[4-hydroxy-5-({[hydroxy(phosphonooxy)phosphoryl]oxy}methyl)-2-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)oxolan-3-yl]oxy}oxane-2-carboxylic acid	C15H22N2O18P2	M-H	579.0270	-0.7
	HMDB0156315	3,4,5-trihydroxy-6-{{[4-hydroxy-2-({[hydroxy(phosphonooxy)phosphoryl]oxy}methyl)-5-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)oxolan-3-yl]oxy}oxane-2-carboxylic acid	C15H22N2O18P2	M-H	579.0270	-0.7
579.3050	HMDB0030459	Hordatine B	C29H40N8O5	M-H	579.3049	0.2
582.1825	HMDB0034773	4-Demethylsimmondsin 2'-(E)-ferulate	C25H31NO12	M+FA-H	582.1828	-0.6
	HMDB0034774	3-Demethylsimmondsin 2'-(Z)-ferulate	C25H31NO12	M+FA-H	582.1828	-0.6
582.1810	HMDB0151407	6-{{[6-butanoyl-8-(2-hydroxypropan-2-yl)-2-oxo-4-phenyl-2H,8H,9H-furo[2,3-h]chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H32O12	M-H	583.1821	-0.3
	HMDB0151406	3,4,5-trihydroxy-6-{{[8-(2-hydroxypropan-2-yl)-6-(2-methylpropanoyl)-2-oxo-4-phenyl-2H,8H,9H-furo[2,3-h]chromen-5-yl]oxy}oxane-2-carboxylic acid	C30H32O12	M-H	583.1821	-0.3

583.1817	HMDB0014609	(1R,3R,5S,8S,13R,14S)-1-hydroxy-14-(2-hydroxypropan-2-yl)-13-methyl-4,7,-trioxapentacyclo[6.4.1.1?,?]tetradecane-6,11-dione; (1R,5S,8S,13R,14R)-1-hydroxy-13-methyl-14-(prop-1-en-2-yl)-4,7,-trioxapentacyclo[6.4.1.1?,?]tetradecane-6,11-dione	C30H34O13	M-H2O-H	583.1816	0.6
583.2036	HMDB0175331	3,4,5-trihydroxy-6-[(9-hydroxy--methyl-4-[[[(2Z)-2-methylbut-2-enoyl]oxy]-3,6-dimethylidene-2-oxo-2H,3H,3aH,4H,5H,6H,7H,8H,9H,11aH-cyclodeca[b]furan-7-yl)oxy]oxane-2-carboxylic acid	C26H34O12	M+FA-H	583.2032	0.6
	HMDB0175330	3,4,5-trihydroxy-6-[(7-hydroxy--methyl-4-[[[(2Z)-2-methylbut-2-enoyl]oxy]-3,6-dimethylidene-2-oxo-2H,3H,3aH,4H,5H,6H,7H,8H,9H,11aH-cyclodeca[b]furan-9-yl)oxy]oxane-2-carboxylic acid	C26H34O12	M+FA-H	583.2032	0.6
	HMDB0039230	Citrusin A	C26H34O12	M+FA-H	583.2032	0.6
	HMDB0036783	Diosbulbinside F	C26H34O12	M+FA-H	583.2032	0.6
583.2200	HMDB0140664	6-[4-(3,7-dimethylocta-2,6-dien-1-yl)-2-hydroxy-5-(6-hydroxy-1-benzofuran-2-yl)-3-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140652	6-({2-[2-(3,7-dimethylocta-2,6-dien-1-yl)-5-hydroxy-3-methoxyphenyl]-6-hydroxy-1-benzofuran-7-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140657	6-[3-(4,6-dihydroxy-1-benzofuran-2-yl)-4-(3,7-dimethylocta-2,6-dien-1-yl)-5-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140656	6-({2-[2-(3,7-dimethylocta-2,6-dien-1-yl)-5-hydroxy-3-methoxyphenyl]-4-hydroxy-1-benzofuran-6-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140655	6-({2-[2-(3,7-dimethylocta-2,6-dien-1-yl)-5-hydroxy-3-methoxyphenyl]-6-hydroxy-1-benzofuran-4-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140658	6-[3-(3,7-dimethylocta-2,6-dien-1-yl)-6-hydroxy-2-(6-hydroxy-1-benzofuran-2-yl)-4-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140660	6-[4-(3,7-dimethylocta-2,6-dien-1-yl)-2-hydroxy-3-(6-hydroxy-1-benzofuran-2-yl)-5-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140662	6-[3-(3,7-dimethylocta-2,6-dien-1-yl)-6-hydroxy-4-(6-hydroxy-1-benzofuran-2-yl)-2-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140659	6-({2-[2-(3,7-dimethylocta-2,6-dien-1-yl)-5,6-dihydroxy-3-methoxyphenyl]-1-benzofuran-6-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140663	6-({2-[2-(3,7-dimethylocta-2,6-dien-1-yl)-4,5-dihydroxy-3-methoxyphenyl]-1-benzofuran-6-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140653	6-({2-[2-(3,7-dimethylocta-2,6-dien-1-yl)-5-hydroxy-3-methoxyphenyl]-7-hydroxy-1-benzofuran-6-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140636	3,4,5-trihydroxy-6-({2-[5-hydroxy-2-(8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-3-methoxyphenyl]-1-benzofuran-6-yl}oxy)oxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140637	3,4,5-trihydroxy-6-[3-(6-hydroxy-1-benzofuran-2-yl)-4-(8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-5-methoxyphenoxy]oxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140633	6-({2-[2-(3,7-dimethylocta-2,6-dien-1-yl)-5-hydroxy-3-methoxyphenyl]-6-hydroxy-1-benzofuran-5-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140634	6-({2-[2-(3,7-dimethylocta-2,6-dien-1-yl)-5-hydroxy-3-methoxyphenyl]-5-hydroxy-1-benzofuran-6-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140635	6-[3-(5,6-dihydroxy-1-benzofuran-2-yl)-4-(3,7-dimethylocta-2,6-dien-1-yl)-5-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6

	HMDB0140639	3,4,5-trihydroxy-6-[(2-{5-hydroxy-2-[4-hydroxy-3-(4-methylpent-3-en-1-yl)but-2-en-1-yl]-3-methoxyphenyl}-1-benzofuran-6-yl)oxy]oxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140651	3,4,5-trihydroxy-6-[3-(6-hydroxy-1-benzofuran-2-yl)-5-methoxy-4-{[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]methyl}phenoxy]oxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140654	6-[3-(6,7-dihydroxy-1-benzofuran-2-yl)-4-(3,7-dimethylocta-2,6-dien-1-yl)-5-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140648	6-[(2-{2-[5-(3,3-dimethyloxiran-2-yl)-3-methylpent-2-en-1-yl]-5-hydroxy-3-methoxyphenyl}-1-benzofuran-6-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140649	6-{4-[5-(3,3-dimethyloxiran-2-yl)-3-methylpent-2-en-1-yl]-3-(6-hydroxy-1-benzofuran-2-yl)-5-methoxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140650	3,4,5-trihydroxy-6-{[2-(5-hydroxy-3-methoxy-2-{[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]methyl}phenyl)-1-benzofuran-6-yl]oxy}oxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140643	3,4,5-trihydroxy-6-[3-(6-hydroxy-1-benzofuran-2-yl)-4-(4-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-5-methoxyphenoxy]oxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140646	3,4,5-trihydroxy-6-[3-(6-hydroxy-1-benzofuran-2-yl)-4-(5-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-5-methoxyphenoxy]oxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140645	3,4,5-trihydroxy-6-({2-[5-hydroxy-2-(5-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-3-methoxyphenyl]-1-benzofuran-6-yl}oxy)oxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140640	3,4,5-trihydroxy-6-[3-(6-hydroxy-1-benzofuran-2-yl)-4-[4-hydroxy-3-(4-methylpent-3-en-1-yl)but-2-en-1-yl]-5-methoxyphenoxy]oxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140642	3,4,5-trihydroxy-6-({2-[5-hydroxy-2-(4-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-3-methoxyphenyl]-1-benzofuran-6-yl}oxy)oxane-2-carboxylic acid	C31H36O11	M-H	583.2185	2.6
	HMDB0140670	6-[2-(3,7-dimethylocta-2,6-dien-1-yl)-3-(6-hydroxy-1-benzofuran-2-yl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H34O9	M+FA-H	583.2185	2.6
	HMDB0140669	6-({2-[2-(3,7-dimethylocta-2,6-dien-1-yl)-3-hydroxyphenyl]-1-benzofuran-6-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H34O9	M+FA-H	583.2185	2.6
583.3410	HMDB0029485	(+)-Isoxanthochymol	C38H50O6	M-H2O-H	583.3423	-2.3
	HMDB0039154	(-)-Guttiferone E	C38H50O6	M-H2O-H	583.3423	-2.3
	HMDB0030608	Xanthochymol	C38H50O6	M-H2O-H	583.3423	-2.3
	HMDB0039709	Guttiferone A	C38H50O6	M-H2O-H	583.3423	-2.3
584.1737	HMDB0135487	6-[1-(3,4-dimethoxyphenyl)-2-{[3-(3,4-dimethoxyphenyl)-1-hydroxyprop-2-en-1-ylidene]amino}ethoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H33NO12	M+Na-2H	584.1749	-2.1
	HMDB0135491	6-[6-(2-{[2-(3,4-dimethoxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl)-2,3-dimethoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H33NO12	M+Na-2H	584.1749	-2.1
	HMDB0135492	6-[2-(2-{[2-(3,4-dimethoxyphenyl)ethyl]-C-hydroxycarbonimidoyl}eth-1-en-1-yl)-4,5-dimethoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H33NO12	M+Na-2H	584.1749	-2.1
	HMDB0093004	DG(<i>i</i> -)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093002	DG(<i>l</i>)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093090	DG(<i>i</i> -12/18)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0092952	DG(8/22)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093003	DG(<i>i</i> -)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0092951	DG(8/22)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0094409	DG(22/8)	C33H64O5	M+FA-H	585.4736	-1.0

585.4730

HMDB0094121	DG(/)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093001	DG(/)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093894	DG(18/12)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093087	DG(12/18)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0092954	DG(8/i-22)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093092	DG(i-12/i-18)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093236	DG(13/i-17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093230	DG(i-13/a-17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093228	DG(a-13/i-17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093238	DG(13/a-17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093226	DG(i-13/17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093234	DG(i-13/i-17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093240	DG(a-13/a-17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093232	DG(a-13/17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093094	DG(12/i-18)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0092953	DG(8/i-22)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0094123	DG(i-/-)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0094411	DG(i-22/8)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093734	DG(a-17/i-13)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093089	DG(i-12/18)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093091	DG(i-12/i-18)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093225	DG(i-13/17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093229	DG(i-13/a-17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093233	DG(i-13/i-17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093363	DG(i-14/16)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093365	DG(i-14/i-16)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093480	DG(i-15/15)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093484	DG(i-15/a-15)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093488	DG(i-15/i-15)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093625	DG(i-16/14)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093627	DG(i-16/i-14)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093732	DG(i-17/13)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093736	DG(i-17/a-13)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093740	DG(i-17/i-13)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093896	DG(i-18/12)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093746	DG(a-17/a-13)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093738	DG(a-17/13)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093482	DG(a-15/i-15)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093093	DG(12/i-18)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093223	DG(13/17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093237	DG(13/a-17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093235	DG(13/i-17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093367	DG(14/i-16)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093492	DG(15/a-15)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093490	DG(15/i-15)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093629	DG(16/i-14)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093730	DG(17/13)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093744	DG(17/a-13)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093742	DG(17/i-13)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093900	DG(18/i-12)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093231	DG(a-13/17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093239	DG(a-13/a-17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093227	DG(a-13/i-17)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093486	DG(a-15/15)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093494	DG(a-15/a-15)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093898	DG(i-18/i-12)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0007011	DG(14/16)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0094124	DG(i-/-)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0094122	DG(/)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093899	DG(i-18/i-12)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093901	DG(18/i-12)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093897	DG(i-18/12)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093743	DG(17/i-13)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0093731	DG(17/13)	C33H64O5	M+FA-H	585.4736	-1.0
HMDB0094412	DG(i-22/8)	C33H64O5	M+FA-H	585.4736	-1.0

	HMDB0094410	DG(22/8)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0007068	DG(15/15)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0007095	DG(16/14)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0055981	DG(15/15)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093895	DG(12/18)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093624	DG(14/16)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0055954	DG(14/16)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093088	DG(18/12)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093735	DG(a-17/i-13)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093224	DG(13/17)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093483	DG(a-15/i-15)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093493	DG(15/a-15)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093481	DG(i-15/i-15)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093489	DG(i-15/i-15)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093495	DG(a-15/a-15)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093487	DG(a-15/i-15)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093368	DG(14/i-16)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093366	DG(i-14/i-16)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093364	DG(i-14/16)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093485	DG(i-15/a-15)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093733	DG(i-17/13)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093739	DG(a-17/13)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093741	DG(i-17/i-13)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093745	DG(17/a-13)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093737	DG(i-17/a-13)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093747	DG(a-17/a-13)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093491	DG(15/i-15)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093626	DG(i-16/14)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093628	DG(i-16/i-14)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0093630	DG(16/i-14)	C33H64O5	M+FA-H	585.4736	-1.0
	HMDB0173859	3,4,5-trihydroxy-6-(octacosyloxy)oxane-2-carboxylic acid	C34H66O7	M-H	585.4736	-1.0
586.1913	HMDB0135503	6-[1-(3,4-dimethoxyphenyl)-2-{{2-(3,4-dimethoxyphenyl)ethyl}-C-hydroxycarbonimidoyl}ethoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H35NO12	M+Na-2H	586.1906	1.2
	HMDB0135505	6-[1-(3,4-dimethoxyphenyl)-2-{{3-(3,4-dimethoxyphenyl)-1-hydroxypropylidene}amino}ethoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H35NO12	M+Na-2H	586.1906	1.2
	HMDB0135507	6-[2-(3,4-dimethoxyphenyl)-1-{{2-(3,4-dimethoxyphenyl)ethyl}-C-hydroxycarbonimidoyl}ethoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H35NO12	M+Na-2H	586.1906	1.2
586.5166	HMDB0000829	N-Stearoylsphingosine	C36H71NO3	M+Na-2H	586.5181	-2.5
	HMDB0011763	Cer(d18/18:1(9Z))	C36H71NO3	M+Na-2H	586.5181	-2.5
	HMDB0011762	Cer(d18/18:1(11Z))	C36H71NO3	M+Na-2H	586.5181	-2.5
	HMDB0004950	Ceramide (d18:1/18)	C36H71NO3	M+Na-2H	586.5181	-2.5
	HMDB0145440	(6S,12aR)-4-(dimethylamino)-6,,11a,12a-tetrahydroxy-6-methyl-1,3,11,12-tetraoxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximide acid	C27H33N3O9	M+FA-H	588.2199	-1.8
	HMDB0145346	N-[(4aS,11S)-2,4a,7,11-tetrahydroxy-11-methyl-4,5,6-trioxo-3-{{[(pyrrolidin-1-yl)methyl]-C-hydroxycarbonimidoyl}-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-1-yl]-N-methylmethanamine oxide	C27H33N3O9	M+FA-H	588.2199	-1.8
	HMDB0145347	(6S,12aS)-4-(dimethylamino)-3,6,,12a-tetrahydroxy-6-methyl-1,11,12-trioxo-N-[(1-oxo-1-yl?pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximide acid	C27H33N3O9	M+FA-H	588.2199	-1.8
	HMDB0145344	(6S,12aS)-4-(dimethylamino)-3,5,6,,12a-pentahydroxy-6-methyl-1,11,12-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximide acid	C27H33N3O9	M+FA-H	588.2199	-1.8

HMDB0145345	(6S,12aS)-4-(dimethylamino)-3,4a,6,,12a-pentahydroxy-6-methyl-1,11,12-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145343	(6R,12aS)-4-(dimethylamino)-3,5a,6,,12a-pentahydroxy-6-methyl-1,11,12-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145342	(6S,12aR)-4-(dimethylamino)-3,6,,11a,12a-pentahydroxy-6-methyl-1,11,12-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145341	(6S,12aS)-4-(dimethylamino)-3,6,,12a-tetrahydroxy-6-methyl-1,11,12-trioxo-N-[[4-oxobutyl]amino]methyl]-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145338	(6S,12aS)-4-(dimethylamino)-3,6,9,,12a-pentahydroxy-6-methyl-1,11,12-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145334	(6S,12aS)-4-(dimethylamino)-3,4,6,,12a-pentahydroxy-6-methyl-1,11,12-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145337	(6S,12aS)-4-(dimethylamino)-3,6,8,,12a-pentahydroxy-6-methyl-1,11,12-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145348	(6S,12aS)-4-(dimethylamino)-3,6,,12a-tetrahydroxy-N-[(2-hydroxypyrrolidin-1-yl)methyl]-6-methyl-1,11,12-trioxo-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145354	(6S,12aS)-4-(dimethylamino)-4,6,,12a-tetrahydroxy-6-methyl-1,3,11,12-tetraoxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145358	(6S,12aS)-4-(dimethylamino)-6,,12a-trihydroxy-6-(hydroxymethyl)-1,3,11,12-tetraoxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145438	(6S,12aS)-4-(dimethylamino)-2,6,,12a-tetrahydroxy-6-methyl-1,3,11,12-tetraoxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145424	(6S,12aS)-4-(dimethylamino)-6,,12a-trihydroxy-N-[(2-hydroxypyrrolidin-1-yl)methyl]-6-methyl-1,3,11,12-tetraoxo-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145419	(6S,12aS)-4-(dimethylamino)-6,,12a-trihydroxy-6-methyl-1,3,11,12-tetraoxo-N-[(1-oxo-1H-pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145415	N-[(4aS,11S)-4a,7,11-trihydroxy-11-methyl-2,4,5,6-tetraoxo-3-[[pyrrolidin-1-yl)methyl]-C-hydroxycarbonimidoyl]-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-1-yl]-N-methylmethanamine oxide	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145411	(6S,12aS)-4-(dimethylamino)-4a,6,,12a-tetrahydroxy-6-methyl-1,3,11,12-tetraoxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145407	(6R,12aS)-4-(dimethylamino)-5a,6,,12a-tetrahydroxy-6-methyl-1,3,11,12-tetraoxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8

HMDB0145403	(6S,12aS)-4-(dimethylamino)-5,6,,12a-tetrahydroxy-6-methyl-1,3,11,12-tetraoxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145384	(6S,12aS)-4-(dimethylamino)-6,,12a-trihydroxy-6-methyl-1,3,11,12-tetraoxo-N-[[4-(oxobutyl)amino]methyl]-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145371	(6S,12aS)-4-(dimethylamino)-6,9,,12a-tetrahydroxy-6-methyl-1,3,11,12-tetraoxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145367	(6S,12aS)-4-(dimethylamino)-6,8,,12a-tetrahydroxy-6-methyl-1,3,11,12-tetraoxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,11a,12,12a-dodecahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145335	(6S,12aS)-4-(dimethylamino)-3,6,,12a-tetrahydroxy-6-(hydroxymethyl)-1,11,12-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,11a,12,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145332	(6S,12aS)-4-(dimethylamino)-6,,12,12a-tetrahydroxy-6-methyl-1,3,11-trioxo-N-[(1-oxo-1-yl?pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145288	(4aS,5aS,6S,12aS)-4-(dimethylamino)-3,6,,12,12a-pentahydroxy-N-[(2-hydroxypyrrolidin-1-yl)methyl]-6-methyl-1,11-dioxo-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145282	(4aS,5aS,6S,12aS)-4-(dimethylamino)-3,6,,12,12a-pentahydroxy-6-methyl-1,11-dioxo-N-[[4-(oxobutyl)amino]methyl]-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145285	(5aS,6S,12aR)-4-(dimethylamino)-3,4a,6,,12,12a-hexahydroxy-6-methyl-1,11-dioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145284	(4aS,6R,12aS)-4-(dimethylamino)-3,5a,6,,12,12a-hexahydroxy-6-methyl-1,11-dioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145283	(4aR,5aR,6S,12aS)-4-(dimethylamino)-3,5,6,,12,12a-hexahydroxy-6-methyl-1,11-dioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145278	(4aS,5aS,6S,12aS)-4-(dimethylamino)-3,6,8,,12,12a-hexahydroxy-6-methyl-1,11-dioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145279	(4aS,5aS,6S,12aS)-4-(dimethylamino)-3,6,9,,12,12a-hexahydroxy-6-methyl-1,11-dioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145276	(4aS,5aS,6S,12aS)-4-(dimethylamino)-3,6,,12,12a-pentahydroxy-6-(hydroxymethyl)-1,11-dioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145275	(4aR,5aS,6S,12aS)-4-(dimethylamino)-3,4,6,,12,12a-hexahydroxy-6-methyl-1,11-dioxo-N-[(pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
HMDB0145286	N-[(4aS,11S,11aS,12aS)-2,4a,5,7,11-pentahydroxy-11-methyl-4,6-dioxo-3-[[pyrrolidin-1-yl)methyl]-C-hydroxycarbonimidoyl]-1,4,4a,6,11,11a,12,12a-octahydrotetracene-1-yl]-N-methylmethanamine oxide	C27H33N3O9	M+FA-H	588.2199	-1.8

	HMDB0145287	(4aS,5aS,6S,12aS)-4-(dimethylamino)-3,6,,12,12a-pentahydroxy-6-methyl-1,11-dioxo-N-[(1-oxo-1- β -pyrrolidin-1-yl)methyl]-1,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
	HMDB0145319	(6S,12aS)-4-(dimethylamino)-4,6,,12,12a-pentahydroxy-6-methyl-1,3,11-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
	HMDB0145333	(6S,12aS)-4-(dimethylamino)-6,,12,12a-tetrahydroxy-N-[(2-hydroxypyrrolidin-1-yl)methyl]-6-methyl-1,3,11-trioxo-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
	HMDB0145331	N-[(4aS,11S)-4a,5,7,11-tetrahydroxy-11-methyl-2,4,6-trioxo-3-{{(pyrrolidin-1-yl)methyl}-C-hydroxycarbonimidoyl}-1,2,3,4,4a,6,11,11a,12,12a-decahydrotetracene-1-yl]-N-methylmethanamine oxide	C27H33N3O9	M+FA-H	588.2199	-1.8
	HMDB0145330	(6S,12aR)-4-(dimethylamino)-4a,6,,12,12a-pentahydroxy-6-methyl-1,3,11-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
	HMDB0145327	(6S,12aS)-4-(dimethylamino)-2,6,,12,12a-pentahydroxy-6-methyl-1,3,11-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
	HMDB0145328	(6R,12aS)-4-(dimethylamino)-5a,6,,12,12a-pentahydroxy-6-methyl-1,3,11-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
	HMDB0145329	(6S,12aS)-4-(dimethylamino)-5,6,,12,12a-pentahydroxy-6-methyl-1,3,11-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
	HMDB0145326	(6S,12aS)-4-(dimethylamino)-6,,12,12a-tetrahydroxy-6-methyl-1,3,11-trioxo-N-[(4-oxobutyl)amino]methyl]-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
	HMDB0145322	(6S,12aS)-4-(dimethylamino)-6,8,,12,12a-pentahydroxy-6-methyl-1,3,11-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
	HMDB0145323	(6S,12aS)-4-(dimethylamino)-6,9,,12,12a-pentahydroxy-6-methyl-1,3,11-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
	HMDB0145320	(6S,12aS)-4-(dimethylamino)-6,,12,12a-tetrahydroxy-6-(hydroxymethyl)-1,3,11-trioxo-N-[(pyrrolidin-1-yl)methyl]-1,2,3,4,4a,5,5a,6,11,12a-decahydrotetracene-2-carboximidic acid	C27H33N3O9	M+FA-H	588.2199	-1.8
593.1253	HMDB0029405	Neobetainin	C24H24N2O13	M+FA-H	593.1260	-1.2
595.1891	HMDB0006825	Tetrahydrofolyl-[Glu](2)	C24H30N8O9	M+Na-2H	595.1882	1.4
595.2223	HMDB0061015	<i>ortho</i>-hydroxyatorvastatin	C33H35FN2O6	M+Na-2H	595.2226	-0.5
	HMDB0061014	<i>para</i>-hydroxyatorvastatin	C33H35FN2O6	M+Na-2H	595.2226	-0.5
596.0854	HMDB0145160	(6-{{(3S)-3-acetyl-3,5,12-trihydroxy-6,11-dioxo-1,2,3,4,6,11-hexahydrotetracene-1-yl}oxy}-4-amino-2-methylideneoxan-3-yl)oxidanefulfonic acid	C26H25NO12S	M+Na-2H	596.0844	1.7
	HMDB0180161	{{(3,8-dihydroxy-6-methoxy-9-oxo-9,9-dihydroacridin-4-yl)oxy}-8,8-dimethyl-2-oxo-2H,8H,9H,H-pyrano[2,3-h]chromen-9-yl}oxidanefulfonic acid	C28H23NO12S	M-H	596.0868	-2.4
597.4009	HMDB0015680	Nonoxynol-9	C33H60O10	M-H2O-H	597.4003	1.1

599.1970	HMDB0170833	6-([3,5-dihydroxy-2-methyl-6-({3,4,5-trihydroxy-6-[4-(prop-2-en-1-yl)phenoxy]oxan-2-yl}methoxy)oxan-4-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H38O16	M-H2O-H	599.1976	-1.0
	HMDB0170834	6-([4,5-dihydroxy-6-methyl-2-({3,4,5-trihydroxy-6-[4-(prop-2-en-1-yl)phenoxy]oxan-2-yl}methoxy)oxan-3-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H38O16	M-H2O-H	599.1976	-1.0
	HMDB0170836	6-({3,5-dihydroxy-2-[4-(prop-2-en-1-yl)phenoxy]-6-[[3,4,5-trihydroxy-6-methyloxan-2-yl]oxy]methyl}oxan-4-yl)oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H38O16	M-H2O-H	599.1976	-1.0
	HMDB0170832	6-([4,5-dihydroxy-2-methyl-6-({3,4,5-trihydroxy-6-[4-(prop-2-en-1-yl)phenoxy]oxan-2-yl}methoxy)oxan-3-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H38O16	M-H2O-H	599.1976	-1.0
	HMDB0170837	6-({4,5-dihydroxy-2-[4-(prop-2-en-1-yl)phenoxy]-6-[[3,4,5-trihydroxy-6-methyloxan-2-yl]oxy]methyl}oxan-3-yl)oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H38O16	M-H2O-H	599.1976	-1.0
	HMDB0170835	6-({4,5-dihydroxy-6-[4-(prop-2-en-1-yl)phenoxy]-2-[[3,4,5-trihydroxy-6-methyloxan-2-yl]oxy]methyl}oxan-3-yl)oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C27H38O16	M-H2O-H	599.1976	-1.0
	HMDB0041413	Marmesin rutinoside	C26H34O13	M+FA-H	599.1981	-1.9
599.3187	HMDB0061696	1-Stearoylglycerophosphoinositol	C27H53O12P	M-H	599.3202	-2.5
	HMDB0240261	1-Stearoylglycerophosphoinositol	C27H53O12P	M-H	599.3202	-2.5
	HMDB0061704	2-Stearoylglycerophosphoinositol	C27H53O12P	M-H	599.3202	-2.5
	HMDB0062777	[(2R)-2-hydroxy-3-(octadecanoyloxy)propoxy]({[(2R,3R,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid	C27H53O12P	M-H	599.3202	-2.5
599.4511	HMDB0072714	TG(8//i-12)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0072669	TG(8/8/i-14)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0072663	TG(i-12/8)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0072557	TG(8/12)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0094822	TG(12/8/)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0094821	TG(i-12/8/)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0094879	TG(i-12//8)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0094880	TG(12//8)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0099171	TG(i-14/8/8)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0099172	TG(14/8/8)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0072383	TG(8//12)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0072172	TG(8/8/14)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0072155	TG(8/i-12/)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0000548	TG(//)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0071897	TG(/8/i-12)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0071392	TG(/12/8)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0071111	TG(8/12/)	C33H62O6	M+FA-H	599.4528	-2.9
	HMDB0173871	3,4,5-trihydroxy-6-[(1-oxooctacosan-2-yl)oxy]oxane-2-carboxylic acid	C34H64O8	M-H	599.4528	-2.9
	HMDB0173867	3,4,5-trihydroxy-6-[(28-oxooctacosan-2-yl)oxy]oxane-2-carboxylic acid	C34H64O8	M-H	599.4528	-2.9
	HMDB0173869	3,4,5-trihydroxy-6-[(28-oxooctacosyl)oxy]oxane-2-carboxylic acid	C34H64O8	M-H	599.4528	-2.9
	HMDB0166341	3,4,5-trihydroxy-6-[(22-oxooctacosyl)oxy]oxane-2-carboxylic acid	C34H64O8	M-H	599.4528	-2.9
	HMDB0173873	3,4,5-trihydroxy-6-(octacosanoyloxy)oxane-2-carboxylic acid	C34H64O8	M-H	599.4528	-2.9
601.3663	HMDB0039143	beta-Doradecin	C40H52O3	M+Na-2H	601.3663	0.0
601.4907	HMDB0112215	2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,,]heptadec-7-en-5-yl 5-(3-methyl-5-pentylfuran-2-yl)pentanoate	C42H68O3	M-H2O-H	601.4985	2.1

601.4277	HMDB0112223	2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,]heptadec-7-en-5-yl 7-(3-methyl-5-propylfuran-2-yl)heptanoate	C42H68O3	M-H2O-H	601.4985	2.1
601.8272	HMDB0160460	2-amino-3-[4-(4-hydroxyphenoxy)-3,5-diiodophenyl]-3-(sulfooxy)propanoic acid	C15H13I2NO8S	M-H2O-H	601.8267	0.8
605.1899	HMDB0158297	6-[(2S,15R)-2,15-dimethyl-3,5-dioxo-13-(sulfooxy)tetracyclo[8.7.,heptadecan-4-yl]-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H36O12S	M+FA-H	605.1909	-1.7
605.4801	HMDB0029959	Asiminenin A	C37H66O6	M-H	605.4787	2.4
	HMDB0030940	Squamocin N	C37H66O6	M-H	605.4787	2.4
	HMDB0031886	Rollidecin D	C37H66O6	M-H	605.4787	2.4
	HMDB0037117	Neoannonin B	C37H66O6	M-H	605.4787	2.4
	HMDB0034967	cis-Reticulatacin--one	C37H66O6	M-H	605.4787	2.4
606.0747	HMDB0060522	UDP-N-acetyl-alpha-D-galactosamine	C17H27N3O17P2	M-H	606.0743	0.7
	HMDB0000290	Uridine diphosphate-N-acetylglucosamine	C17H27N3O17P2	M-H	606.0743	0.7
	HMDB0062760	Uridine diphosphate-N-acetylgalactosamine	C17H27N3O17P2	M-H	606.0743	0.7
	HMDB0000304	Uridine diphosphate-N-acetylgalactosamine	C17H27N3O17P2	M-H	606.0743	0.7
	HMDB0013112	UDP-N-acetyl-D-mannosamine	C17H27N3O17P2	M-H	606.0743	0.7
608.5261	HMDB0004948	Ceramide (d18:1/9Z-18:1)	C36H69NO3	M+FA-H	608.5259	0.3
	HMDB0011774	Cer(d18:1/18:1(11Z))	C36H69NO3	M+FA-H	608.5259	0.3
	HMDB0240362	CHEBI:136461	C36H69NO3	M+FA-H	608.5259	0.3
609.4723	HMDB0056137	DG(14:1n5/18:1n9)	C35H64O5	M+FA-H	609.4736	-2.1
	HMDB0056136	DG(14:1n5/18:1n7)	C35H64O5	M+FA-H	609.4736	-2.1
	HMDB0056156	DG(16:1n7/16:1n7)	C35H64O5	M+FA-H	609.4736	-2.1
	HMDB0032094	Panatellicin	C35H64O5	M+FA-H	609.4736	-2.1
	HMDB0032732	cis-Solamin	C35H64O5	M+FA-H	609.4736	-2.1
	HMDB0031390	Annotemoyin 1	C35H64O5	M+FA-H	609.4736	-2.1
	HMDB0007240	DG(18:2(9Z,12Z)/14)	C35H64O5	M+FA-H	609.4736	-2.1
	HMDB0007212	DG(18:1(9Z)/14:1(9Z))	C35H64O5	M+FA-H	609.4736	-2.1
	HMDB0007183	DG(18:1(11Z)/14:1(9Z))	C35H64O5	M+FA-H	609.4736	-2.1
	HMDB0007128	DG(16:1(9Z)/16:1(9Z))	C35H64O5	M+FA-H	609.4736	-2.1
	HMDB0007043	DG(14:1(9Z)/18:1(11Z))	C35H64O5	M+FA-H	609.4736	-2.1
	HMDB0007044	DG(14:1(9Z)/18:1(9Z))	C35H64O5	M+FA-H	609.4736	-2.1
	HMDB0007016	DG(14/18:2(9Z,12Z))	C35H64O5	M+FA-H	609.4736	-2.1
611.1451	HMDB0003337	Glutathione disulfide	C20H32N6O12S2	M-H	611.1447	0.7
611.4879	HMDB0056040	DG(18/14:1n5)	C35H66O5	M+FA-H	611.4892	-2.2
	HMDB0056015	DG(16/16:1n7)	C35H66O5	M+FA-H	611.4892	-2.2
	HMDB0055961	DG(14/18:1n7)	C35H66O5	M+FA-H	611.4892	-2.2
	HMDB0055962	DG(14/18:1n9)	C35H66O5	M+FA-H	611.4892	-2.2
	HMDB0007211	DG(18:1(9Z)/14)	C35H66O5	M+FA-H	611.4892	-2.2
	HMDB0007182	DG(18:1(11Z)/14)	C35H66O5	M+FA-H	611.4892	-2.2
	HMDB0007154	DG(18/14:1(9Z))	C35H66O5	M+FA-H	611.4892	-2.2
	HMDB0007127	DG(16:1(9Z)/16)	C35H66O5	M+FA-H	611.4892	-2.2
	HMDB0007099	DG(16/16:1(9Z))	C35H66O5	M+FA-H	611.4892	-2.2
	HMDB0007042	DG(14:1(9Z)/18)	C35H66O5	M+FA-H	611.4892	-2.2
	HMDB0007014	DG(14/18:1(11Z))	C35H66O5	M+FA-H	611.4892	-2.2
	HMDB0007015	DG(14/18:1(9Z))	C35H66O5	M+FA-H	611.4892	-2.2
	HMDB0142035	6-(4-{3-[3,4-bis(2-hydroxyethoxy)phenyl]-2-oxopropanoyl}-3,5-dihydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H28O15	M+FA-H	613.1410	-0.7
	HMDB0137976	6-(2-benzoyl-3-hydroxy-5-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}phenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H28O15	M+FA-H	613.1410	-0.7
	HMDB0138008	3,4,5-trihydroxy-6-{[2-(1-hydroxy-4-oxocyclohex-2-en-1-yl)-3,6,7,8-tetramethoxy-4-oxo-4H-chromen-5-yl]oxy}oxane-2-carboxylic acid	C25H28O15	M+FA-H	613.1410	-0.7
	HMDB0142029	6-({2-[3,4-bis(2-hydroxyethoxy)phenyl]-3,7-dihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-5-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H28O15	M+FA-H	613.1410	-0.7

613.1406	HMDB0142030	6-({2-[3,4-bis(2-hydroxyethoxy)phenyl]-3,5-dihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-7-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H28O15	M+FA-H	613.1410	-0.7
	HMDB0142034	6-(2-{3-[3,4-bis(2-hydroxyethoxy)phenyl]-2-oxopropanoyl}-3,5-dihydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H28O15	M+FA-H	613.1410	-0.7
	HMDB0154272	6-{4-[3-(3,4-dihydroxyphenyl)propanoyl]-3,5-dihydroxy-2-[(3,4,5-trihydroxyoxan-2-yl)oxy]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H30O17	M-H	613.1410	-0.7
	HMDB0154274	3,4,5-trihydroxy-6-[2-hydroxy-5-(3-oxo-3-{2,4,6-trihydroxy-3-[(3,4,5-trihydroxyoxan-2-yl)oxy]phenyl}propyl)phenoxy]oxane-2-carboxylic acid	C26H30O17	M-H	613.1410	-0.7
	HMDB0154273	3,4,5-trihydroxy-6-[2-hydroxy-4-(3-oxo-3-{2,4,6-trihydroxy-3-[(3,4,5-trihydroxyoxan-2-yl)oxy]phenyl}propyl)phenoxy]oxane-2-carboxylic acid	C26H30O17	M-H	613.1410	-0.7
	HMDB0154275	6-{2-[3-(3,4-dihydroxyphenyl)propanoyl]-3,5-dihydroxy-4-[(3,4,5-trihydroxyoxan-2-yl)oxy]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H30O17	M-H	613.1410	-0.7
	HMDB0154276	6-{2-[3-(3,4-dihydroxyphenyl)propanoyl]-3,5-dihydroxy-6-[(3,4,5-trihydroxyoxan-2-yl)oxy]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H30O17	M-H	613.1410	-0.7
	HMDB0062695	2-[(3,4-dihydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-2-yl)methoxy](hydroxy)phosphoryl]oxy]-4-hydroxy-5-[(1-hydroxyethylidene)amino]-6-(1,2,3-trihydroxypropyl)oxane-2-carboxylic acid	C20H31N4O16P	M-H	613.1400	1.0
	HMDB0001176	Cytidine 5'-monophosphate-N-acetylneuraminic acid	C20H31N4O16P	M-H	613.1400	1.0
	HMDB0178348	3-hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
	HMDB0175848	(2S,4aS,6aR,6bS,12aS)-12b-hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
	HMDB0175844	(2S,4aS,6aR,6bR,12aS)-2-(hydroxymethyl)-4a,6a,6b,9,9,12a-hexamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
	HMDB0175843	(2S,4aS,6aR,6bR,12aS)--hydroxy-4a,6a,6b,9,9,12a-hexamethyl-13-oxo-2-[(sulfooxy)methyl]-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
	HMDB0175838	(2S,4aR,6aR,6bR,12aS)--hydroxy-2,6a,6b,9,9,12a-hexamethyl-13-oxo-4a-[(sulfooxy)methyl]-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
	HMDB0175839	(2S,4aR,6aR,6bR,12aS)-4a-(hydroxymethyl)-2,6a,6b,9,9,12a-hexamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
	HMDB0175834	(2S,4aS,6aS,6bR,12aS)-6a-(hydroxymethyl)-2,4a,6b,9,9,12a-hexamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
	HMDB0175833	(2S,4aS,6aS,6bR,12aS)--hydroxy-2,4a,6b,9,9,12a-hexamethyl-13-oxo-6a-[(sulfooxy)methyl]-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
	HMDB0175829	(2S,4aS,6aR,6bR,12aR)-12a-(hydroxymethyl)-2,4a,6a,6b,9,9-hexamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
	HMDB0175828	(2S,4aS,6aR,6bR,12aR)--hydroxy-2,4a,6a,6b,9,9-hexamethyl-13-oxo-12a-[(sulfooxy)methyl]-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
	HMDB0175852	(2S,4aS,6aR,6bR,12aS)--hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-13-oxo-14-(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3

HMDB0175853	(2S,4aS,6aR,6bR,12aS)-14-hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0178347	-hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-13-oxo-3-(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0176019	[9-formyl-4,-dihydroxy-4a-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-5-yl]oxidanesulfonic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0176018	[4-formyl-8,9-dihydroxy-8a-(hydroxymethyl)-4,6a,6b,11,11,14b-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricene-3-yl]oxidanesulfonic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0176017	[(9-formyl-4,5,-trihydroxy-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-yl)methoxy]sulfonic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0176010	4,-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl-5-(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0176011	5,-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl-4-(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0176009	4,5-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl--(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0175824	(2S,4aS,6aR,6bR,12aS)-9-(hydroxymethyl)-2,4a,6a,6b,9,12a-hexamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0175823	(2S,4aS,6aR,6bR,12aS)--hydroxy-2,4a,6a,6b,9,12a-hexamethyl-13-oxo-9-[(sulfooxy)methyl]-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0169221	5,-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl-3-(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0169222	3,-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl-5-(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0169223	3,5-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl--(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0175636	-hydroxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-11-(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0175634	,11-dihydroxy-2,2,6a,6b,9,12a-hexamethyl-9-[(sulfooxy)methyl]-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0175635	11-hydroxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl--(sulfooxy)-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0175819	(2S,4aS,6aR,6bS,12aS)-6b-(hydroxymethyl)-2,4a,6a,9,9,12a-hexamethyl-13-oxo--(sulfooxy)-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3
HMDB0175818	(2S,4aS,6aR,6bS,12aS)--hydroxy-2,4a,6a,9,9,12a-hexamethyl-13-oxo-6b-[(sulfooxy)methyl]-docosahydricene-2-carboxylic acid	C30H48O8S	M+FA-H	613.3052	1.3

	HMDB0176020	[9-formyl-5,-dihydroxy-4a-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricen-4-yl]oxidanesulfonic acid	C30H48O8S	M+FA-H	613.3052	1.3
	HMDB0015129	Neomycin	C23H46N6O13	M-H	613.3050	1.6
613.3856	HMDB0115842	PA(i-/8)	C31H61O8P	M+Na-2H	613.3851	0.9
	HMDB0115816	PA(i-14/i-14)	C31H61O8P	M+Na-2H	613.3851	0.9
	HMDB0115802	PA(i-13/i-15)	C31H61O8P	M+Na-2H	613.3851	0.9
	HMDB0115795	PA(i-13/a-15)	C31H61O8P	M+Na-2H	613.3851	0.9
	HMDB0115785	PA(i-12/i-16)	C31H61O8P	M+Na-2H	613.3851	0.9
	HMDB0115706	PA(a-13/i-15)	C31H61O8P	M+Na-2H	613.3851	0.9
	HMDB0115699	PA(a-13/a-15)	C31H61O8P	M+Na-2H	613.3851	0.9
	HMDB0115693	PA(8/i-)	C31H61O8P	M+Na-2H	613.3851	0.9
	HMDB0115617	PA(i-/18)	C31H61O8P	M+Na-2H	613.3851	0.9
	HMDB0115491	PA(8/)	C31H61O8P	M+Na-2H	613.3851	0.9
	HMDB0115090	PA(8/)	C31H61O8P	M+Na-2H	613.3851	0.9
	HMDB0094415	DG(i-22/)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093012	DG(/22)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093014	DG(/i-22)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093108	DG(i-12/i-)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093106	DG(i-12/)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0092956	DG(8/i-24)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093011	DG(/22)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0094129	DG(i-/i-12)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0094127	DG(i-/12)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0092955	DG(8/i-24)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0094131	DG(/i-12)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093013	DG(/i-22)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0094413	DG(22/)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0094125	DG(/12)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093103	DG(12/)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093110	DG(12/i-)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093254	DG(13/19)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093382	DG(i-14/18)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093386	DG(14/i-18)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093384	DG(i-14/i-18)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093264	DG(13/i-19)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093104	DG(12/)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093260	DG(a-13/19)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093256	DG(i-13/19)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093258	DG(a-13/i-19)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093262	DG(i-13/i-19)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0094522	DG(i-24/8)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0094019	DG(i-19/i-13)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093508	DG(i-15/17)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093383	DG(i-14/i-18)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093381	DG(i-14/18)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093261	DG(i-13/i-19)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093255	DG(i-13/19)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093107	DG(i-12/i-)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093105	DG(i-12/)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093764	DG(a-17/i-15)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093512	DG(i-15/a-17)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093516	DG(i-15/i-17)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093642	DG(i-16/16)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0094017	DG(i-19/a-13)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0094015	DG(i-19/13)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093917	DG(i-18/i-14)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093915	DG(i-18/14)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093770	DG(i-17/i-15)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093766	DG(i-17/a-15)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093762	DG(i-17/15)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093644	DG(i-16/i-16)	C35H68O5	M+FA-H	613.5049	1.5
	HMDB0093776	DG(a-17/a-15)	C35H68O5	M+FA-H	613.5049	1.5

613.5058

HMDB0093768	DG(a-17/15)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093760	DG(17/15)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093646	DG(16/i-16)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093518	DG(15/i-17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093520	DG(15/a-17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093506	DG(15/17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093385	DG(14/i-18)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093263	DG(13/i-19)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093253	DG(13/19)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093774	DG(17/a-15)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093772	DG(17/i-15)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093919	DG(18/i-14)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093510	DG(a-15/i-17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093522	DG(a-15/a-17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093514	DG(a-15/17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093257	DG(a-13/i-19)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093259	DG(a-13/19)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094021	DG(19/i-13)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094023	DG(19/a-13)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094013	DG(19/13)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093109	DG(12/i-)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093523	DG(a-15/a-17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093918	DG(i-18/i-14)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094022	DG(19/i-13)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094014	DG(19/13)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094128	DG(i-/12)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094130	DG(i-/i-12)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094018	DG(i-19/a-13)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093920	DG(18/i-14)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094016	DG(i-19/13)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094020	DG(i-19/i-13)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094024	DG(19/a-13)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094132	DG(/i-12)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0031011	DG(16/16)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0056009	DG(16/16)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0007153	DG(18/14)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0007098	DG(16/16)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093914	DG(14/18)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0055955	DG(14/18)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094126	DG(/12)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094414	DG(22/)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094416	DG(i-22/)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0094523	DG(i-24/8)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0007013	DG(14/18)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093509	DG(i-15/17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093507	DG(15/17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093519	DG(15/i-17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093645	DG(i-16/i-16)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093643	DG(i-16/16)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093513	DG(i-15/a-17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093765	DG(i-15/a-17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093511	DG(a-15/i-17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093515	DG(a-15/17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093521	DG(15/a-17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093517	DG(i-15/i-17)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093647	DG(16/i-16)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093773	DG(17/i-15)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093767	DG(i-17/a-15)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093761	DG(17/15)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093775	DG(17/a-15)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093777	DG(a-17/a-15)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093769	DG(a-17/15)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093763	DG(i-17/15)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093771	DG(i-17/i-15)	C35H68O5	M+FA-H	613.5049	1.5
HMDB0093916	DG(i-18/14)	C35H68O5	M+FA-H	613.5049	1.5

614.2181	HMDB0145595	2-[[[(6R,12Z,17E,19E)-14,21-dihydroxy-11,19-dimethyl-2,8,23-trioxo--(propan-2-yl)-9,26-dioxo-3,15,28-triazatricyclo[23.2.1,octacos-1(27),12,14,17,19,25(28)-hexaen-6-yl]sulfonyl}acetaldehyde	C30H39N3O10S	M-H2O-H	614.2172	1.4
	HMDB0164180	7-benzyl-5,8-dihydroxy-4- {[1-hydroxy-4-methyl-2-(sulfooxy)pentylidene]amino}-3-(propan-2-yl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C30H39N3O10S	M-H2O-H	614.2172	1.4
	HMDB0183601	2-amino-3- {[[(7E,9E,11Z)-1-[3-(hydrogen phosphonatoxy)-2-oxopropoxy]-5-hydroxy-1-oxoicos-7,9,11-trien-6-yl]sulfanyl} propanoate	C26H42NO10PS	M+Na-2H	614.2170	1.8
617.1865	HMDB0128923	3,4,5-trihydroxy-6- {2-[(3-methylbut-2-enoyl)oxy]-2-[9-[(3-methylbut-2-enoyl)oxy]-2-oxo-2H,8H,9H-furo[2,3-h]chromen-8-yl]propoxy} oxane-2-carboxylic acid	C30H34O14	M-H	617.1876	-1.7
	HMDB0132485	3,4,5-trihydroxy-6- {2-[(2-methylbut-2-enoyl)oxy]-2-[9- {[[(2E)-2-methylbut-2-enoyl]oxy}-2-oxo-2H,8H,9H-furo[2,3-h]chromen-8-yl]propoxy} oxane-2-carboxylic acid	C30H34O14	M-H	617.1876	-1.7
618.0912	HMDB0174254	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-({1-hydroxy-3-[(2Z)-3-(prop-2-en-1-yl)disulfanyl]prop-2-ene-1-sulfonyl}propan-2-yl} sulfanyl)ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C19H31N3O9S4	M+FA-H	618.0925	-2.1
	HMDB0174255	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1-hydroxy-3- {[[(1Z)-3-(prop-2-ene-1-sulfonyl]prop-1-en-1-yl]disulfanyl} propan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C19H31N3O9S4	M+FA-H	618.0925	-2.1
619.3501	HMDB0030011	Scutigeral	C34H52O10	M-H	619.3488	2.1
	HMDB0171679	6-[1-hydroxy-1-(3-hydroxy-2,15-dimethyl-5- {[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy} tetracyclo[8.7.,,heptadec-7-en-14-yl]ethyl]-3,4-dimethyl-5,6-dihydro-2H-pyran-2-one	C34H52O10	M-H	619.3488	2.1
	HMDB0041049	Physagulin D	C34H52O10	M-H	619.3488	2.1
619.4326	HMDB0114833	PA(16/14)	C33H65O8P	M-H	619.4344	-3.0
	HMDB0115708	PA(a-13/i-17)	C33H65O8P	M-H	619.4344	-3.0
	HMDB0115787	PA(i-12/i-18)	C33H65O8P	M-H	619.4344	-3.0
	HMDB0115796	PA(i-13/a-17)	C33H65O8P	M-H	619.4344	-3.0
	HMDB0115804	PA(i-13/i-17)	C33H65O8P	M-H	619.4344	-3.0
	HMDB0115818	PA(i-14/i-16)	C33H65O8P	M-H	619.4344	-3.0
	HMDB0115830	PA(i-/-)	C33H65O8P	M-H	619.4344	-3.0
	HMDB0115902	PA(i-22/8)	C33H65O8P	M-H	619.4344	-3.0
	HMDB0115700	PA(a-13/a-17)	C33H65O8P	M-H	619.4344	-3.0
	HMDB0115695	PA(8/i-22)	C33H65O8P	M-H	619.4344	-3.0
	HMDB0114772	PA(8/22)	C33H65O8P	M-H	619.4344	-3.0
	HMDB0115058	PA(/)	C33H65O8P	M-H	619.4344	-3.0
	HMDB0115269	PA(22/8)	C33H65O8P	M-H	619.4344	-3.0
	HMDB0115619	PA(i-/-)	C33H65O8P	M-H	619.4344	-3.0
	HMDB0097345	TG(i-13/a-15/8)[rac]	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0096594	TG(13/8/a-15)[rac]	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0096592	TG(13/8/15)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0096593	TG(13/8/i-15)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0096590	TG(i-13/8/a-15)[rac]	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0096588	TG(a-13/8/i-15)[rac]	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0096589	TG(i-13/8/i-15)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0096591	TG(i-13/8/15)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0096587	TG(a-13/8/15)[rac]	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0096586	TG(a-13/8/a-15)[rac]	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0095519	TG(12/16/8)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0095518	TG(i-12/16/8)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0095516	TG(12/i-16/8)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0095517	TG(i-12/i-16/8)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0096662	TG(a-13/13)[rac]	C39H74O6	M-H2O-H	619.5302	-1.2

HMDB0096661	TG(a-13/a-13/)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0096930	TG(i-13/13/)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0096929	TG(a-13/i-13/)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0096928	TG(a-13/13/)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0096926	TG(i-13/a-13/)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0096925	TG(13/a-13/)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0096927	TG(13/i-13/)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0096668	TG(13//i-13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0096669	TG(13//a-13)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0096664	TG(i-13/i-13/)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0096667	TG(13/13/)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0096665	TG(i-13//a-13)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0096666	TG(i-13//13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0096663	TG(a-13//i-13)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0095233	TG(12/14/)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0095232	TG(i-12/14/)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0072835	TG(8/i-12/i-16)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0072814	TG(a-13/13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0072778	TG(8/8/)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0072774	TG(/12/i-14)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0072770	TG(8/18)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0072737	TG(8/i-14/14)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0072556	TG(8/14/14)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0072542	TG(i-13/a-13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0072502	TG(8/i-13/15)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0072491	TG(8/15/13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0072479	TG(8/15/i-13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0072405	TG(8/i-13/a-15)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0072396	TG(8/14/i-14)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0094843	TG(i-12/8/i-16)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0094844	TG(i-12/8/16)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0095231	TG(i-12/i-14/)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0095230	TG(12/i-14/)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0094947	TG(i-12/12/12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0094944	TG(i-12/i-12/12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0094943	TG(12/12/i-12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0094946	TG(i-12/i-12/i-12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0094945	TG(12/i-12/i-12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0094895	TG(12//14)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0094896	TG(12//i-14)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0094893	TG(i-12//i-14)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0094894	TG(i-12//14)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0094846	TG(12/8/i-16)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0094845	TG(12/8/16)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0072357	TG(i-12/i-14)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0097346	TG(a-13/a-15/8)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0103535	TG(16//)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0103534	TG(i-16//)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0103479	TG(16/8/i-12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0103478	TG(16/8/12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0103476	TG(i-16/8/i-12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0103477	TG(i-16/8/12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0101252	TG(15/13/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0101250	TG(i-15/i-13/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0101251	TG(i-15/13/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0101249	TG(a-15/i-13/8)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0101248	TG(a-15/13/8)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0101244	TG(15/a-13/8)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0101247	TG(15/i-13/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0103592	TG(16/i-12/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0103594	TG(i-16/12/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0107867	TG(18//8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0107866	TG(i-18//8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0107808	TG(i-18/8/)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0107809	TG(18/8/)	C39H74O6	M-H20-H	619.5302	-1.2

HMDB0103595	TG(16/12/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0103593	TG(i-16/i-12/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0101245	TG(i-15/a-13/8)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0100904	TG(15/8/a-13)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0099236	TG(i-14/12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0099238	TG(14/i-12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0099235	TG(i-14/i-12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0099188	TG(14/8/i-14)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0099187	TG(14/14/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0099186	TG(i-14/8/14)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0099185	TG(i-14/i-14/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0097352	TG(13/15/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0097350	TG(i-13/i-15/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0097349	TG(a-13/i-15/8)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0097348	TG(a-13/15/8)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0097351	TG(i-13/15/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0097347	TG(13/i-15/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0099237	TG(14//12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0099295	TG(14/i-12/)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0100901	TG(i-15/8/13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0100902	TG(15/8/13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0100903	TG(15/8/i-13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0100898	TG(a-15/8/i-13)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0100897	TG(a-15/8/13)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0100900	TG(i-15/8/a-13)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0100899	TG(i-15/8/i-13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0100896	TG(a-15/8/a-13)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0099592	TG(i-14/14/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0099591	TG(14/i-14/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0099296	TG(i-14/i-12/)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0099298	TG(14/12/)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0099297	TG(i-14/12/)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0097344	TG(13/a-15/8)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0101246	TG(a-15/a-13/8)[rac]	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071342	TG(8/15/a-13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071389	TG(/13/i-13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071390	TG(/18/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071397	TG(8/i-14/i-14)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071444	TG(8/i-15/a-13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071467	TG(8/a-15/a-13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071477	TG(8/i-15/13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071482	TG(8/a-13/i-15)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071551	TG(8/a-15/i-13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071563	TG(8//i-18)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071607	TG(/i-14/i-12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071617	TG(/8/i-18)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071622	TG(/i-12/14)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071640	TG(8/16/i-12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071320	TG(/13/13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071315	TG(8/i-13/i-15)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071305	TG(/a-13/a-13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071608	TG(/16)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071114	TG(/12/14)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0011188	TG(12/12/12)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0063783	TG(i-8/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0064269	TG(/8/8)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071110	TG(8/13/15)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071131	TG(/i-13/13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071162	TG(8/12/16)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071254	TG(8/i-15/i-13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071778	TG(/a-13/i-13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071784	TG(8/12/i-16)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0072303	TG(8/a-15/13)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071976	TG(8/a-13/a-15)	C39H74O6	M-H20-H	619.5302	-1.2
HMDB0071986	TG(8/i-12/16)	C39H74O6	M-H20-H	619.5302	-1.2

	HMDB0071998	TG(8/13/a-15)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0072051	TG(8//18)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0072056	TG(8/18/)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0072131	TG(/i-14/12)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0072173	TG(8/i-18/)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0072208	TG(/14/12)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0072215	TG(8/a-13/15)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0072236	TG(8/i-16/12)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0072296	TG(8/i-16/i-12)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0072344	TG(/14/i-12)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0071718	TG(8/16/12)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0071935	TG(8/8/i-)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0071908	TG(/13/a-13)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0071958	TG(/i-16)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0071916	TG(/i-13/i-13)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0071902	TG(8/13/i-15)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0072346	TG(/i-18/8)	C39H74O6	M-H2O-H	619.5302	-1.2
	HMDB0056178	DG(18:1n7/18:1n9)	C39H72O5	M-H	619.5307	-2.1
	HMDB0056177	DG(18:1n7/18:1n7)	C39H72O5	M-H	619.5307	-2.1
	HMDB0056197	DG(18:1n9/18:1n9)	C39H72O5	M-H	619.5307	-2.1
	HMDB0007161	DG(18/18:2(9Z,12Z))	C39H72O5	M-H	619.5307	-2.1
	HMDB0007188	DG(18:1(11Z)/18:1(11Z))	C39H72O5	M-H	619.5307	-2.1
	HMDB0007189	DG(18:1(11Z)/18:1(9Z))	C39H72O5	M-H	619.5307	-2.1
	HMDB0007217	DG(18:1(9Z)/18:1(11Z))	C39H72O5	M-H	619.5307	-2.1
	HMDB0007218	DG(18:1(9Z)/18:1(9Z))	C39H72O5	M-H	619.5307	-2.1
	HMDB0007245	DG(18:2(9Z,12Z)/18)	C39H72O5	M-H	619.5307	-2.1
	HMDB0007137	DG(16:1(9Z)/:1(11Z))	C39H72O5	M-H	619.5307	-2.1
	HMDB0007109	DG(16:/2(11Z,14Z))	C39H72O5	M-H	619.5307	-2.1
	HMDB0007058	DG(14:1(9Z)/22:1(13Z))	C39H72O5	M-H	619.5307	-2.1
	HMDB0007646	DG(22:2(13Z,16Z)/14)	C39H72O5	M-H	619.5307	-2.1
	HMDB0007618	DG(22:1(13Z)/14:1(9Z))	C39H72O5	M-H	619.5307	-2.1
	HMDB0007417	DG(:2(11Z,14Z)/16)	C39H72O5	M-H	619.5307	-2.1
	HMDB0007030	DG(14/22:2(13Z,16Z))	C39H72O5	M-H	619.5307	-2.1
	HMDB0007389	DG(:1(11Z)/16:1(9Z))	C39H72O5	M-H	619.5307	-2.1
	HMDB0055972	DG(14/22:2n6)	C39H72O5	M-H	619.5307	-2.1
	HMDB0056024	DG(16:/2n6)	C39H72O5	M-H	619.5307	-2.1
	HMDB0056140	DG(14:1n5/22:1n9)	C39H72O5	M-H	619.5307	-2.1
	HMDB0056159	DG(16:1n7/:1n9)	C39H72O5	M-H	619.5307	-2.1
620.0878	HMDB0160045	2-[(9-{3-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-4-hydroxy-5-[(phosphonooxy)methyl]oxolan-2-yl}-9H-purin-6-yl)amino]butanedioic acid	C20H26N5O17P	M-H2O-H	620.0877	0.1
	HMDB0160046	2-[(9-{4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-3-hydroxy-5-[(phosphonooxy)methyl]oxolan-2-yl}-9H-purin-6-yl)amino]butanedioic acid	C20H26N5O17P	M-H2O-H	620.0877	0.1
	HMDB0160048	6-({3-carboxy-3-[(9-{3,4-dihydroxy-5-[(phosphonooxy)methyl]oxolan-2-yl}-9H-purin-6-yl)amino]propanoyl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H26N5O17P	M-H2O-H	620.0877	0.1
	HMDB0160047	6-({3-carboxy-2-[(9-{3,4-dihydroxy-5-[(phosphonooxy)methyl]oxolan-2-yl}-9H-purin-6-yl)amino]propanoyl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C20H26N5O17P	M-H2O-H	620.0877	0.1
621.1690	HMDB0182994	6-{[2-({6-[carboxy(phenyl)methoxy]-3,4,5-trihydroxyoxan-2-yl}methoxy)-4,5-dihydroxyoxan-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H34O18	M-H	621.1672	2.8
	HMDB0182993	6-{[2-({6-[carboxy(phenyl)methoxy]-3,4,5-trihydroxyoxan-2-yl}methoxy)-3,5-dihydroxyoxan-4-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H34O18	M-H	621.1672	2.8
	HMDB0182995	6-({6-[carboxy(phenyl)methoxy]-4,5-dihydroxy-2-[(3,4,5-trihydroxyoxan-2-yl)oxy]methyl}oxan-3-yl)oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H34O18	M-H	621.1672	2.8
	HMDB0182997	6-({2-[carboxy(phenyl)methoxy]-4,5-dihydroxy-6-[(3,4,5-trihydroxyoxan-2-yl)oxy]methyl}oxan-3-yl)oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H34O18	M-H	621.1672	2.8

	HMDB0182996	6-({2-[carboxy(phenyl)methoxy]-3,5-dihydroxy-6- {[(3,4,5-trihydroxyoxan-2-yl)oxy]methyl}oxan-4- yl)oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H34O18	M-H	621.1672	2.8
	HMDB0182999	3,4,5-trihydroxy-6-({2-phenyl-2-[(3,4,5-trihydroxy-6- {[(3,4,5-trihydroxyoxan-2-yl)oxy]methyl}oxan-2- yl)oxy]acetyl}oxy)oxane-2-carboxylic acid	C25H34O18	M-H	621.1672	2.8
	HMDB0182998	6-({6-({6-[carboxy(phenyl)methoxy]-3,4,5- trihydroxyoxan-2-yl}methoxy)-4,5-dihydroxyoxan-3- yl)oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C25H34O18	M-H	621.1672	2.8
625.0202	HMDB0155749	6-({9-[3,4-dihydroxy-5- ([hydroxy(phosphonooxy)phosphoryl]oxy)methyl]ox olan-2-yl]-9H-purin-6-yl}oxy)-3,4,5-trihydroxyoxane- 2-carboxylic acid	C16H22N4O1 7P2	M+Na-2H	625.0202	0.0
	HMDB0187547	3,4,5-trihydroxy-6-({4-hydroxy-5- ([hydroxy(phosphonooxy)phosphoryl]oxy)methyl)-2- (6-hydroxy-9H-purin-9-yl)oxolan-3-yl]oxy}oxane-2- carboxylic acid	C16H22N4O1 7P2	M+Na-2H	625.0202	0.0
	HMDB0187548	3,4,5-trihydroxy-6-({4-hydroxy-2- ([hydroxy(phosphonooxy)phosphoryl]oxy)methyl)-5- (6-hydroxy-9H-purin-9-yl)oxolan-3-yl]oxy}oxane-2- carboxylic acid	C16H22N4O1 7P2	M+Na-2H	625.0202	0.0
626.5860	HMDB0240679	(5Z,9Z)-N-[(2S,3R)-1,3-dihydroxyoctadec-4-en-2- yl]tetracos-5,9-dienimidic acid	C42H79NO3	M-H20-H	626.5876	-2.6
	HMDB0240680	(15Z)-N-[(2S,3R,14Z)-1,3-dihydroxyoctadeca-4,14- dien-2-yl]tetracos-15-enimidic acid	C42H79NO3	M-H20-H	626.5876	-2.6
627.1360	HMDB0138879	6-{5-[5-(5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1- benzopyran-2-yl)-7-hydroxy-3-(hydroxymethyl)-2,3- dihydro-1-benzofuran-2-yl]-2-hydroxyphenoxy}-3,4,5- trihydroxyoxane-2-carboxylic acid	C30H28O15	M-H	627.1355	0.7
	HMDB0138876	6-({2-[2-(3,4-dihydroxyphenyl)-7-hydroxy-3- (hydroxymethyl)-2,3-dihydro-1-benzofuran-5-yl]-7- hydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-5- yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H28O15	M-H	627.1355	0.7
	HMDB0138877	6-({5-(5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1- benzopyran-2-yl)-2-(3,4-dihydroxyphenyl)-3- (hydroxymethyl)-2,3-dihydro-1-benzofuran-7-yl]oxy}- 3,4,5-trihydroxyoxane-2-carboxylic acid	C30H28O15	M-H	627.1355	0.7
	HMDB0138878	6-{4-[5-(5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1- benzopyran-2-yl)-7-hydroxy-3-(hydroxymethyl)-2,3- dihydro-1-benzofuran-2-yl]-2-hydroxyphenoxy}-3,4,5- trihydroxyoxane-2-carboxylic acid	C30H28O15	M-H	627.1355	0.7
	HMDB0138875	6-({2-[2-(3,4-dihydroxyphenyl)-7-hydroxy-3- (hydroxymethyl)-2,3-dihydro-1-benzofuran-5-yl]-5- hydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-7- yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C30H28O15	M-H	627.1355	0.7
628.0469	HMDB0180824	{[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)[(4-hydroxy-6- methoxypyrimidin-2-yl)-C- hydroxycarbonimidoyl]amino](4-carboxy-3-chloro-1- methyl-1H-pyrazol-5-yl)hydroxy- ~~4~~ ?sulfanyl}oxidanyl	C17H20ClN6 O13S	M+FA-H	628.0480	-1.7
628.6029	HMDB0004953	Cer(d18:1/24:1(15Z))	C42H81NO3	M-H20-H	628.6033	-0.6
630.0072	HMDB0180619	6-[(2,4-dichloro-3-{5,7-dimethoxy-[1,2,4]triazolo[1,5- a]pyrimidine-2-sulfonamido}phenyl)methoxy]-3,4,5- trihydroxyoxane-2-carboxylic acid	C20H21Cl2N5 O11S	M+Na-2H	630.0082	-1.6
	HMDB0180624	6-(2,4-dichloro-3-{5,7-dimethoxy-[1,2,4]triazolo[1,5- a]pyrimidine-2-sulfonamido}-5-methylphenoxy)-3,4,5- trihydroxyoxane-2-carboxylic acid	C20H21Cl2N5 O11S	M+Na-2H	630.0082	-1.6
	HMDB0180622	6-(3,5-dichloro-4-{5,7-dimethoxy-[1,2,4]triazolo[1,5- a]pyrimidine-2-sulfonamido}-2-methylphenoxy)-3,4,5- trihydroxyoxane-2-carboxylic acid	C20H21Cl2N5 O11S	M+Na-2H	630.0082	-1.6
	HMDB0126235	2-{2,6-dihydroxy-4-[6-hydroxy-7-(3-methylbut-2-en-1- yl)-1-benzofuran-2-yl]phenyl}-6-(2,4-dihydroxy-5- methoxyphenyl)-4-methylcyclohex-3-ene-1-carboxylic acid	C34H34O9	M+FA-H	631.2185	0.0

631.2185	HMDB0126228	2-{2,6-dihydroxy-4-[6-hydroxy-7-(3-methylbut-2-en-1-yl)-1-benzofuran-2-yl]-3-methoxyphenyl}-6-(2,4-dihydroxyphenyl)-4-methylcyclohex-3-ene-1-carboxylic acid	C34H34O9	M+FA-H	631.2185	0.0
	HMDB0059949	Rhodin G7	C34H34N4O7	M+Na-2H	631.2174	1.7
	HMDB0041621	6'-Sialyllactosamine	C23H40N2O18	M-H	631.2203	-2.9
	HMDB0006607	3'-Sialyllactosamine	C23H40N2O18	M-H	631.2203	-2.9
631.3650	HMDB0040650	3-trans-Caffeoyltormentic acid	C39H54O8	M-H2O-H	631.3635	2.4
	HMDB0040682	23-trans-p-Coumaroyloxytormentic acid	C39H54O8	M-H2O-H	631.3635	2.4
631.4616	HMDB0164344	{[11-hydroxy--(5-methyl-2-oxooxolan-3-yl)triacontan-12-yl]oxy}sulfonic acid	C35H68O7S	M-H	631.4613	0.5
	HMDB0164345	{[12-hydroxy--(5-methyl-2-oxooxolan-3-yl)triacontan-11-yl]oxy}sulfonic acid	C35H68O7S	M-H	631.4613	0.5
	HMDB0164353	{[13-hydroxy--(5-methyl-2-oxooxolan-3-yl)triacontan-14-yl]oxy}sulfonic acid	C35H68O7S	M-H	631.4613	0.5
	HMDB0164354	{[14-hydroxy--(5-methyl-2-oxooxolan-3-yl)triacontan-13-yl]oxy}sulfonic acid	C35H68O7S	M-H	631.4613	0.5
	HMDB0164362	{[16-hydroxy-1-(5-methyl-2-oxooxolan-3-yl)triacontan-15-yl]oxy}sulfonic acid	C35H68O7S	M-H	631.4613	0.5
	HMDB0164363	{[16-hydroxy--(5-methyl-2-oxooxolan-3-yl)triacontan-15-yl]oxy}sulfonic acid	C35H68O7S	M-H	631.4613	0.5
	HMDB0164372	{[13-hydroxy-1-(5-methyl-2-oxooxolan-3-yl)triacontan-14-yl]oxy}sulfonic acid	C35H68O7S	M-H	631.4613	0.5
	HMDB0164371	{[14-hydroxy-1-(5-methyl-2-oxooxolan-3-yl)triacontan-13-yl]oxy}sulfonic acid	C35H68O7S	M-H	631.4613	0.5
632.2275	HMDB0164184	2-amino-3-[4-(1-[(1-carboxy-2-phenylethyl)-C-hydroxycarbonimidoyl]-1-{[1-hydroxy-4-methyl-2-(sulfooxy)pentylidene]amino}-3-methylbutan-2-yl]oxy]phenyl]propanoic acid	C30H41N3O11S	M-H2O-H	632.2278	-0.5
	HMDB0164182	3-(4-{2-[(2-amino-1-hydroxy-3-phenylpropylidene)amino]-2-carboxyethyl}phenoxy)-2-{[1-hydroxy-4-methyl-2-(sulfooxy)pentylidene]amino}-4-methylpentanoic acid	C30H41N3O11S	M-H2O-H	632.2278	-0.5
	HMDB0145634	(2E)-5-[(E)-1-[2-(9-amino-4-hydroxy-6-methyl-2-oxonona-5,7-dien-1-yl)-1,3-oxazole-4-carbonyl]-3-(2-oxoethanesulfonyl)pyrrolidine-2-carbonyloxy]-4,6-dimethylhept-2-enoic acid	C30H41N3O11S	M-H2O-H	632.2278	-0.5
	HMDB0134650	2-amino-4-(1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(3-hydroxy-5-oxo-1,7-diphenylheptan-4-yl)sulfanyl]ethyl)-C-hydroxycarbonimidoyl]butanoic acid	C29H37N3O8S	M+FA-H	632.2283	-1.3
	HMDB0134649	2-amino-4-(1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(4-hydroxy-5-oxo-1,7-diphenylheptan-3-yl)sulfanyl]ethyl)-C-hydroxycarbonimidoyl]butanoic acid	C29H37N3O8S	M+FA-H	632.2283	-1.3
	HMDB0133948	2-amino-4-(1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(2-hydroxy-5-oxo-1,7-diphenylheptyl)sulfanyl]ethyl)-C-hydroxycarbonimidoyl]butanoic acid	C29H37N3O8S	M+FA-H	632.2283	-1.3
	HMDB0133949	2-amino-4-(1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1-hydroxy-5-oxo-1,7-diphenylheptan-2-yl)sulfanyl]ethyl)-C-hydroxycarbonimidoyl]butanoic acid	C29H37N3O8S	M+FA-H	632.2283	-1.3
	HMDB0164180	7-benzyl-5,8-dihydroxy-4-{[1-hydroxy-4-methyl-2-(sulfooxy)pentylidene]amino}-3-(propan-2-yl)-2-oxa-6,9-diazabicyclo[2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C30H39N3O10S	M-H	632.2283	-1.3
	HMDB0183618	6-[(25-carboxypentacosan-2-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H60O9	M+FA-H	633.4219	1.4
	HMDB0183619	3,4,5-trihydroxy-6-[(25-hydroxyhexacosanoyl)oxy]oxane-2-carboxylic acid	C32H60O9	M+FA-H	633.4219	1.4

633.4228	HMDB0183621	6-[(25-carboxypentacosyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H60O9	M+FA-H	633.4219	1.4
	HMDB0183622	3,4,5-trihydroxy-6-[(26-hydroxyhexacosanoyl)oxy]oxane-2-carboxylic acid	C32H60O9	M+FA-H	633.4219	1.4
	HMDB0183625	3,4,5-trihydroxy-6-[(2-hydroxyhexacosanoyl)oxy]oxane-2-carboxylic acid	C32H60O9	M+FA-H	633.4219	1.4
	HMDB0183624	6-[(1-carboxypentacosyl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H60O9	M+FA-H	633.4219	1.4
633.5604	HMDB0034841	Faradiol myristate	C44H76O3	M-H2O-H	633.5611	-1.0
635.4879	HMDB0056144	DG(14:1n5/:2n6)	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0056030	DG(16/18:3n3)	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0056023	DG(16/18:3n6)	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0055970	DG(14/:3n6)	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0055964	DG(14/:3n9)	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0007472	DG(:3(8Z,11Z,14Z)/14)	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0007443	DG(:3(5Z,8Z,11Z)/14)	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0007415	DG(:2(11Z,14Z)/14:1(9Z))	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0007301	DG(18:3(9Z,12Z,15Z)/16)	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0007272	DG(18:3(6Z,9Z,12Z)/16)	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0007244	DG(18:2(9Z,12Z)/16:1(9Z))	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0007132	DG(16:1(9Z)/18:2(9Z,12Z))	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0007104	DG(16/18:3(6Z,9Z,12Z))	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0007105	DG(16/18:3(9Z,12Z,15Z))	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0007051	DG(14:1(9Z)/:2(11Z,14Z))	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0007024	DG(14/:3(8Z,11Z,14Z))	C37H66O5	M+FA-H	635.4892	-2.1
	HMDB0007023	DG(14/:3(5Z,8Z,11Z))	C37H66O5	M+FA-H	635.4892	-2.1
635.5246	HMDB0032475	Polyoxyethylene dioleate	C38H70O4	M+FA-H	635.5256	-1.6
637.3832	HMDB0115775	PA(i-12/18:2(9Z,11Z))	C33H61O8P	M+Na-2H	637.3851	-2.9
	HMDB0114853	PA(16:1(9Z)/14:1(9Z))	C33H61O8P	M+Na-2H	637.3851	-2.9
637.5034	HMDB0055969	DG(14/:2n6)	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0056157	DG(16:1n7/18:1n7)	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0056158	DG(16:1n7/18:1n9)	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0056138	DG(14:1n5/:1n9)	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0055995	DG(15/18:2n6)	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0034560	cis-Uvariamicin IV	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0032714	cis-Uvariamicin IB	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0034302	Reticulatain 2	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0034924	Neoreticulatain A	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0007414	DG(:2(11Z,14Z)/14)	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0007386	DG(:1(11Z)/14:1(9Z))	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0007243	DG(18:2(9Z,12Z)/16)	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0007215	DG(18:1(9Z)/16:1(9Z))	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0007186	DG(18:1(11Z)/16:1(9Z))	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0007130	DG(16:1(9Z)/18:1(11Z))	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0007131	DG(16:1(9Z)/18:1(9Z))	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0007103	DG(16/18:2(9Z,12Z))	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0007050	DG(14:1(9Z)/:1(11Z))	C37H68O5	M+FA-H	637.5049	-2.3
	HMDB0007022	DG(14/:2(11Z,14Z))	C37H68O5	M+FA-H	637.5049	-2.3
639.1851	HMDB0184456	[(2S,15R)-2,15-dimethyl-5-sulfo-14-{4-[(2-sulfoethyl)-C-hydroxycarbonimidoyl]butan-2-yl}-16-(sulfooxy)tetracyclo-heptadecan-9-yl]oxidanyl	C26H44NO12S3	M-H2O-H	639.1842	1.4
639.2421	HMDB0059795	Gluten exorphin B5	C30H38N6O11	M-H2O-H	639.2415	1.0
	HMDB0060661	Pyruvaldehyde	C33H38N4O8	M+Na-2H	639.2436	-2.4
	HMDB0181787	3-{15-hydroxy-15-[5-(1-hydroxytridecyl)oxolan-2-yl]pentadecyl}-5-methyloxolan-2-one	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0176309	3-{11-hydroxy-11-[5-(1-hydroxyheptadecyl)oxolan-2-yl]undecyl}-5-methyloxolan-2-one	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0172633	3-(16-{[5-(1-hydroxyundecyl)oxolan-2-yl]methoxy}hexadecyl)-5-methyloxolan-2-one	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0056041	DG(18/16:1n7)	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0056016	DG(16/18:1n7)	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0055963	DG(14/:1n9)	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0056065	DG(/14:1n5)	C37H70O5	M+FA-H	639.5205	-1.6

639.5195	HMDB0007385	DG:(1(11Z)/14)	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0007357	DG(/14:1(9Z))	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0007214	DG(18:1(9Z)/16)	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0007185	DG(18:1(11Z)/16)	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0007157	DG(18/16:1(9Z))	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0007129	DG(16:1(9Z)/18)	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0007102	DG(16/18:1(9Z))	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0007101	DG(16/18:1(11Z))	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0007049	DG(14:1(9Z)/)	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0056017	DG(16/18:1n9)	C37H70O5	M+FA-H	639.5205	-1.6
	HMDB0007021	DG(14/1:1(11Z))	C37H70O5	M+FA-H	639.5205	-1.6
640.0847	HMDB0038405	6-Sinapoylglucoraphenin	C23H31NO14S3	M-H	640.0834	2.0
641.2868	HMDB0036361	Pipercyclobutanamide B	C36H40N2O6	M+FA-H	641.2868	-0.1
	HMDB0165881	1-{[4-hydroxy-3-({6-methoxy-1-[(4-methoxyphenyl)methyl]-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-yl}oxy)phenyl]methyl}-2-methyl-1,2,3,4-tetrahydroisoquinoline-6,7-diol	C36H40N2O6	M+FA-H	641.2868	-0.1
	HMDB0165882	7-{2-hydroxy-5-[(7-hydroxy-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl]phenoxy}-1-[(4-methoxyphenyl)methyl]-2-methyl-1,2,3,4-tetrahydroisoquinolin-6-ol	C36H40N2O6	M+FA-H	641.2868	-0.1
	HMDB0165883	Nelumboferine	C36H40N2O6	M+FA-H	641.2868	-0.1
	HMDB0165886	1-{[4-hydroxy-3-({6-methoxy-1-[(4-methoxyphenyl)methyl]-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-yl}oxy)phenyl]methyl}-6-methoxy-1,2,3,4-tetrahydroisoquinolin-7-ol	C36H40N2O6	M+FA-H	641.2868	-0.1
	HMDB0165887	1-{[4-hydroxy-3-({6-methoxy-1-[(4-methoxyphenyl)methyl]-1,2,3,4-tetrahydroisoquinolin-7-yl}oxy)phenyl]methyl}-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-ol	C36H40N2O6	M+FA-H	641.2868	-0.1
	HMDB0165963	4-hydroxy-4-[(7-{3-[(7-hydroxy-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl]phenoxy}-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl]cyclohexa-2,5-dien-1-one	C36H40N2O6	M+FA-H	641.2868	-0.1
	HMDB0167991	1-{[4-hydroxy-3-({1-[(4-hydroxyphenyl)methyl]-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-yl}oxy)phenyl]methyl}-7-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-6-ol	C36H40N2O6	M+FA-H	641.2868	-0.1
	HMDB0167990	7-{5-[(6,7-dimethoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl]-2-hydroxyphenoxy}-1-[(4-hydroxyphenyl)methyl]-2-methyl-1,2,3,4-tetrahydroisoquinolin-6-ol	C36H40N2O6	M+FA-H	641.2868	-0.1
	HMDB0167995	4-[(6,7-dimethoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl]-2-({1-[(4-hydroxyphenyl)methyl]-6-methoxy-1,2,3,4-tetrahydroisoquinolin-7-yl}oxy)phenol	C36H40N2O6	M+FA-H	641.2868	-0.1
	HMDB0040521	Dipiperamide D	C36H40N2O6	M+FA-H	641.2868	-0.1
	HMDB0167994	4-[(6,7-dimethoxy-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl]-2-({1-[(4-hydroxyphenyl)methyl]-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-7-yl}oxy)phenol	C36H40N2O6	M+FA-H	641.2868	-0.1
642.4499	HMDB0008825	PE(14/16:1(9Z))	C35H68NO8P	M-H2O-H	642.4499	0.1
	HMDB0113839	PE-NMe2(14/14:1(9Z))	C35H68NO8P	M-H2O-H	642.4499	0.1
	HMDB0113018	PE-NMe(15/14:1(9Z))	C35H68NO8P	M-H2O-H	642.4499	0.1
	HMDB0112938	PE-NMe(14:1(9Z)/15)	C35H68NO8P	M-H2O-H	642.4499	0.1
	HMDB0008857	PE(14:1(9Z)/16)	C35H68NO8P	M-H2O-H	642.4499	0.1

	HMDB0008921	PE(16/14:1(9Z))	C35H68NO8P	M-H2O-H	642.4499	0.1
	HMDB0008953	PE(16:1(9Z)/14)	C35H68NO8P	M-H2O-H	642.4499	0.1
	HMDB0113899	PE-NMe2(14:1(9Z)/14)	C35H68NO8P	M-H2O-H	642.4499	0.1
643.0523	HMDB0129226	(3-{8-[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro-2H-1-benzopyran-3-yl]-5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl}phenyl)oxidanesulfonic acid	C30H22O13S	M+Na-2H	643.0528	-0.7
	HMDB0129233	{5-[8-(5,7-dihydroxy-4-oxo-2-phenyl-3,4-dihydro-2H-1-benzopyran-3-yl)-5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl]-2-hydroxyphenyl}oxidanesulfonic acid	C30H22O13S	M+Na-2H	643.0528	-0.7
	HMDB0151092	(4-{4'-[(E)-2-(3,5-dihydroxy-4-methoxyphenyl)ethenyl]-4,6,6'-trihydroxy-2'-oxo-2H,2'H-3,3'-spirobi[[1]benzofuran]-2-yl}phenyl)oxidanesulfonic acid	C30H22O13S	M+Na-2H	643.0528	-0.7
643.1462	HMDB0040537	Kaempferol 3-(2'',3''-diacetyl-4''-p-coumaroyl)rhannoside	C34H30O14	M-H2O-H	643.1452	1.6
644.3655	HMDB0039897	Hydroxyhomodestruxin B	C31H53N5O8	M+Na-2H	644.3641	2.2
644.5960	HMDB0011765	Cer(d18/22)	C40H81NO3	M+Na-2H	644.5963	-0.5
645.3924	HMDB0114803	PA(14:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C37H61O8P	M-H2O-H	645.3920	0.6
	HMDB0115199	PA(:5(5Z,8Z,11Z,14Z,17Z)/14:1(9Z))	C37H61O8P	M-H2O-H	645.3920	0.6
645.4490	HMDB0184751	(8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraen-1-yl 7-[3-hydroxy-2-(3-hydroxyoctyl)-5-oxocyclopentyl]heptanoate	C40H64O5	M+Na-2H	645.4500	-1.6
	HMDB0184729	(8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraen-1-yl 7-{3,5-dihydroxy-2-[(1E)-3-hydroxyoct-1-en-1-yl]cyclopentyl}heptanoate	C40H64O5	M+Na-2H	645.4500	-1.6
	HMDB0114921	PA(18:1(9Z)/14)	C35H67O8P	M-H	645.4501	-1.7
	HMDB0114896	PA(18:1(11Z)/14)	C35H67O8P	M-H	645.4501	-1.7
	HMDB0114874	PA(18/14:1(9Z))	C35H67O8P	M-H	645.4501	-1.7
	HMDB0114855	PA(16:1(9Z)/16)	C35H67O8P	M-H	645.4501	-1.7
	HMDB0031131	Glycerol 1-(9Z-octadecenoate) 2-tetradecanoate 3-phosphate	C35H67O8P	M-H	645.4501	-1.7
646.3395	HMDB0037300	Jubanine C	C39H47N5O5	M-H2O-H	646.3393	0.3
	HMDB0170627	3-(4-{2-[(2-amino-1-hydroxy-3-methylpentylidene)amino]ethenyl}-3-hydroxyphenoxy)-2-{[2-(dimethylamino)-1-hydroxy-3-phenylpropylidene]amino}-3-phenylpropanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
	HMDB0170609	2-({3-[4-(2-aminoethenyl)-3-hydroxyphenoxy]-2-[(2-(dimethylamino)-1-hydroxy-3-phenylpropylidene]amino}-1-hydroxy-3-phenylpropylidene}amino)-3-methylpentanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
	HMDB0170606	2-({3-[4-(2-aminoethenyl)phenoxy]-2-[(2-(dimethylamino)-1-hydroxy-3-phenylpropylidene]amino}-1-hydroxy-3-phenylpropylidene}amino)-5-hydroxy-3-methylpentanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
	HMDB0170608	2-({3-[4-(2-aminoethenyl)phenoxy]-2-[(2-(dimethylamino)-1-hydroxy-3-(2-hydroxyphenyl)propylidene]amino}-1-hydroxy-3-phenylpropylidene}amino)-3-methylpentanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
	HMDB0170607	2-({3-[4-(2-aminoethenyl)phenoxy]-2-[(2-(dimethylamino)-1-hydroxy-3-phenylpropylidene]amino}-1-hydroxy-3-(2-hydroxyphenyl)propylidene}amino)-3-methylpentanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3

HMDB0170602	2-({3-[4-(2-aminoethenyl)phenoxy]-2-{{2-(dimethylamino)-1-hydroxy-3-phenylpropylidene}amino}-1-hydroxy-3-(4-hydroxyphenyl)propylidene}amino)-3-methylpentanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
HMDB0170603	2-({3-[4-(2-aminoethenyl)phenoxy]-2-{{2-(dimethylamino)-1-hydroxy-3-(4-hydroxyphenyl)propylidene}amino}-1-hydroxy-3-phenylpropylidene}amino)-3-methylpentanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
HMDB0170601	2-({3-[4-(2-aminoethenyl)phenoxy]-2-{{2-(dimethylamino)-1-hydroxy-3-(3-hydroxyphenyl)propylidene}amino}-1-hydroxy-3-phenylpropylidene}amino)-3-methylpentanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
HMDB0170604	2-({3-[4-(2-aminoethenyl)phenoxy]-2-{{2-(dimethylamino)-1-hydroxy-3-phenylpropylidene}amino}-1-hydroxy-3-phenylpropylidene}amino)-4-hydroxy-3-methylpentanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
HMDB0170600	2-({3-[4-(2-aminoethenyl)phenoxy]-2-{{2-(dimethylamino)-1-hydroxy-3-phenylpropylidene}amino}-1-hydroxy-3-(3-hydroxyphenyl)propylidene}amino)-3-methylpentanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
HMDB0170599	2-({3-[4-(2-aminoethenyl)phenoxy]-2-{{2-(dimethylamino)-1,3-dihydroxy-3-phenylpropylidene}amino}-1-hydroxy-3-phenylpropylidene}amino)-3-methylpentanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
HMDB0170595	2-({3-[4-(2-aminoethenyl)phenoxy]-2-{{2-(dimethylamino)-1,2-dihydroxy-3-phenylpropylidene}amino}-1-hydroxy-3-phenylpropylidene}amino)-3-methylpentanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
HMDB0170610	2-({3-[4-(2-aminoethenyl)phenoxy]-2-{{2-(dimethyl-oxo-5-azanyl)-1-hydroxy-3-phenylpropylidene}amino}-1-hydroxy-3-phenylpropylidene}amino)-3-methylpentanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
HMDB0170613	3-(4-{2-[(2-amino-1-hydroxy-3-methylpentylidene)amino]ethenyl}phenoxy)-2-{{2-(dimethylamino)-1,2-dihydroxy-3-phenylpropylidene}amino}-3-phenylpropanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
HMDB0170626	3-(4-{2-[(2-amino-1-hydroxy-3-methylpentylidene)amino]ethenyl}phenoxy)-2-{{2-(dimethylamino)-1-hydroxy-3-(2-hydroxyphenyl)propylidene}amino}-3-phenylpropanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
HMDB0170628	3-(4-{2-[(2-amino-1-hydroxy-3-methylpentylidene)amino]ethenyl}phenoxy)-2-{{2-(dimethyl-oxo-5-azanyl)-1-hydroxy-3-phenylpropylidene}amino}-3-phenylpropanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
HMDB0170622	3-(4-{2-[(2-amino-1,4-dihydroxy-3-methylpentylidene)amino]ethenyl}phenoxy)-2-{{2-(dimethylamino)-1-hydroxy-3-phenylpropylidene}amino}-3-phenylpropanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
HMDB0170621	3-(4-{2-[(2-amino-1-hydroxy-3-methylpentylidene)amino]ethenyl}phenoxy)-2-{{2-(dimethylamino)-1-hydroxy-3-(4-hydroxyphenyl)propylidene}amino}-3-phenylpropanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
HMDB0170624	3-(4-{2-[(2-amino-1,5-dihydroxy-3-methylpentylidene)amino]ethenyl}phenoxy)-2-{{2-(dimethylamino)-1-hydroxy-3-phenylpropylidene}amino}-3-phenylpropanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
HMDB0170623	3-(4-{2-[(2-amino-3-ethyl-1,4-dihydroxybutylidene)amino]ethenyl}phenoxy)-2-{{2-(dimethylamino)-1-hydroxy-3-phenylpropylidene}amino}-3-phenylpropanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3

	HMDB0170620	3-(4-{2-[(2-amino-1-hydroxy-3-methylpentylidene)amino]ethenyl}phenoxy)-2-{[2-(dimethylamino)-1-hydroxy-3-phenylpropylidene]amino}-3-(4-hydroxyphenyl)propanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
	HMDB0170618	3-(4-{2-[(2-amino-1-hydroxy-3-methylpentylidene)amino]ethenyl}phenoxy)-2-{[2-(dimethylamino)-1-hydroxy-3-phenylpropylidene]amino}-3-(3-hydroxyphenyl)propanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
	HMDB0170617	3-(4-{2-[(2-amino-1-hydroxy-3-methylpentylidene)amino]ethenyl}phenoxy)-2-{[2-(dimethylamino)-1,3-dihydroxy-3-phenylpropylidene]amino}-3-phenylpropanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
	HMDB0170619	3-(4-{2-[(2-amino-1-hydroxy-3-methylpentylidene)amino]ethenyl}phenoxy)-2-{[2-(dimethylamino)-1-hydroxy-3-(3-hydroxyphenyl)propylidene]amino}-3-phenylpropanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
	HMDB0170614	3-(4-{2-[(2-amino-1,3-dihydroxy-3-methylpentylidene)amino]ethenyl}phenoxy)-2-{[2-(dimethylamino)-1-hydroxy-3-phenylpropylidene]amino}-3-phenylpropanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
	HMDB0170596	2-{[3-[4-(2-aminoethenyl)phenoxy]-2-{[2-(dimethylamino)-1-hydroxy-3-phenylpropylidene]amino}-1-hydroxy-3-phenylpropylidene}amino]-3-hydroxy-3-methylpentanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
	HMDB0170625	3-(4-{2-[(2-amino-1-hydroxy-3-methylpentylidene)amino]ethenyl}phenoxy)-2-{[2-(dimethylamino)-1-hydroxy-3-phenylpropylidene]amino}-3-(2-hydroxyphenyl)propanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
	HMDB0170605	2-{[3-[4-(2-aminoethenyl)phenoxy]-2-{[2-(dimethylamino)-1-hydroxy-3-phenylpropylidene]amino}-1-hydroxy-3-phenylpropylidene}amino]-3-(hydroxymethyl)pentanoic acid	C34H42N4O6	M+FA-H	647.3086	0.3
647.3606	HMDB0029485	(+)-Isoxanthochymol	C38H50O6	M+FA-H	647.3589	2.6
	HMDB0039154	(-)-Guttiiferone E	C38H50O6	M+FA-H	647.3589	2.6
	HMDB0030608	Xanthochymol	C38H50O6	M+FA-H	647.3589	2.6
	HMDB0039709	Guttiiferone A	C38H50O6	M+FA-H	647.3589	2.6
	HMDB0039580	Sucrose monostearate	C30H58O13	M+Na-2H	647.3624	-2.8
647.4647	HMDB0056291	DG(18:2n6/18:4n3)	C40H66O5	M+Na-2H	647.4657	-1.5
	HMDB0056008	DG(15/22:6n3)	C40H66O5	M+Na-2H	647.4657	-1.5
	HMDB0007092	DG(15/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C40H66O5	M+Na-2H	647.4657	-1.5
	HMDB0007764	DG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/15)	C40H66O5	M+Na-2H	647.4657	-1.5
	HMDB0115789	PA(i-12/i-)	C35H69O8P	M-H	647.4657	-1.6
	HMDB0115806	PA(i-13/i-19)	C35H69O8P	M-H	647.4657	-1.6
	HMDB0115831	PA(i-/12)	C35H69O8P	M-H	647.4657	-1.6
	HMDB0115848	PA(i-/i-12)	C35H69O8P	M-H	647.4657	-1.6
	HMDB0115890	PA(i-22/)	C35H69O8P	M-H	647.4657	-1.6
	HMDB0115932	PA(i-24/8)	C35H69O8P	M-H	647.4657	-1.6
	HMDB0115710	PA(a-13/i-19)	C35H69O8P	M-H	647.4657	-1.6
	HMDB0115696	PA(8/i-24)	C35H69O8P	M-H	647.4657	-1.6
	HMDB0115634	PA(/i-12)	C35H69O8P	M-H	647.4657	-1.6
	HMDB0000674	PA(16/16)	C35H69O8P	M-H	647.4657	-1.6
	HMDB0114777	PA(22)	C35H69O8P	M-H	647.4657	-1.6
	HMDB0114873	PA(18/14)	C35H69O8P	M-H	647.4657	-1.6
	HMDB0115059	PA(/12)	C35H69O8P	M-H	647.4657	-1.6
	HMDB0115237	PA(22/)	C35H69O8P	M-H	647.4657	-1.6
	HMDB0115621	PA(/i-22)	C35H69O8P	M-H	647.4657	-1.6

648.2213	HMDB0136727	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-({1,3-dihydroxy-8-[(7-methoxy-2-oxo-2H-chromen-5-yl)oxy]-2,6-dimethyloct-6-en-2-yl)sulfanyl}ethyl)-C-hydroxycarbonimidoyl}butanoic acid	C30H41N3O12S	M-H2O-H	648.2227	-2.2
	HMDB0164249	2-amino-3-(4-{[1-({1-carboxy-2-[4-(sulfooxy)phenyl]ethyl)-C-hydroxycarbonimidoyl]-1-[(1,2-dihydroxy-4-methylpentylidene)amino]-3-methylbutan-2-yl}oxy}phenyl)propanoic acid	C30H41N3O12S	M-H2O-H	648.2227	-2.2
	HMDB0164250	2-amino-3-{4-[(1-{[1-carboxy-2-(4-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}-1-{[1-hydroxy-4-methyl-2-(sulfooxy)pentylidene]amino}-3-methylbutan-2-	C30H41N3O12S	M-H2O-H	648.2227	-2.2
	HMDB0164246	2-amino-3-(4-{[1-({1-carboxy-2-[3-(sulfooxy)phenyl]ethyl)-C-hydroxycarbonimidoyl]-1-[(1,2-dihydroxy-4-methylpentylidene)amino]-3-methylbutan-2-yl}oxy}phenyl)propanoic acid	C30H41N3O12S	M-H2O-H	648.2227	-2.2
	HMDB0164244	2-amino-3-{4-[(1-{[1-carboxy-2-(2-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}-1-{[1-hydroxy-4-methyl-2-(sulfooxy)pentylidene]amino}-3-methylbutan-2-	C30H41N3O12S	M-H2O-H	648.2227	-2.2
	HMDB0164241	2-amino-3-[4-({1-[(1-carboxy-2-phenylethyl)-C-hydroxycarbonimidoyl]-1-{[1,2-dihydroxy-4-methyl-5-(sulfooxy)pentylidene]amino}-3-methylbutan-2-yl}oxy)phenyl]propanoic acid	C30H41N3O12S	M-H2O-H	648.2227	-2.2
	HMDB0164242	2-amino-3-[4-({1-[(1-carboxy-2-phenylethyl)-C-hydroxycarbonimidoyl]-1-{[1,5-dihydroxy-4-methyl-2-(sulfooxy)pentylidene]amino}-3-methylbutan-2-yl}oxy)phenyl]propanoic acid	C30H41N3O12S	M-H2O-H	648.2227	-2.2
	HMDB0164238	2-amino-3-[4-({1-[(1-carboxy-2-phenylethyl)-C-hydroxycarbonimidoyl]-4-hydroxy-1-{[1-hydroxy-4-methyl-2-(sulfooxy)pentylidene]amino}-3-methylbutan-2-yl}oxy)phenyl]propanoic acid	C30H41N3O12S	M-H2O-H	648.2227	-2.2
	HMDB0164237	2-amino-3-[4-({1-[(1-carboxy-2-phenylethyl)-C-hydroxycarbonimidoyl]-1-[(1,2-dihydroxy-4-methylpentylidene)amino]-3-methyl-4-(sulfooxy)butan-2-yl}oxy)phenyl]propanoic acid	C30H41N3O12S	M-H2O-H	648.2227	-2.2
	HMDB0164232	2-amino-3-[4-({1-[(1-carboxy-2-phenylethyl)-C-hydroxycarbonimidoyl]-1-{[1,4-dihydroxy-4-methyl-2-(sulfooxy)pentylidene]amino}-3-methylbutan-2-yl}oxy)phenyl]propanoic acid	C30H41N3O12S	M-H2O-H	648.2227	-2.2
	HMDB0164229	2-amino-3-[4-({1-[(1-carboxy-2-phenylethyl)-C-hydroxycarbonimidoyl]-3-hydroxy-1-{[1-hydroxy-4-methyl-2-(sulfooxy)pentylidene]amino}-3-methylbutan-2-yl}oxy)phenyl]propanoic acid	C30H41N3O12S	M-H2O-H	648.2227	-2.2
	HMDB0164225	2-({3-[4-(2-amino-2-carboxyethyl)phenoxy]-2-[(1,2-dihydroxy-4-methylpentylidene)amino]-1-hydroxy-4-methylpentylidene}amino)-3-phenyl-3-(sulfooxy)propanoic acid	C30H41N3O12S	M-H2O-H	648.2227	-2.2
	HMDB0164226	2-({3-[4-(2-amino-2-carboxyethyl)phenoxy]-1-hydroxy-2-{[1-hydroxy-4-methyl-2-(sulfooxy)pentylidene]amino}-4-methylpentylidene}amino)-3-hydroxy-3-phenylpropanoic acid	C30H41N3O12S	M-H2O-H	648.2227	-2.2
	HMDB0164222	2-amino-3-[4-({1-[(1-carboxy-2-phenylethyl)-C-hydroxycarbonimidoyl]-1-{[1-hydroxy-4-methyl-2-(sulfooxy)pentylidene]amino}-3-methylbutan-2-yl}oxy)phenyl]-3-hydroxypropanoic acid	C30H41N3O12S	M-H2O-H	648.2227	-2.2
	HMDB0164221	2-amino-3-[4-({1-[(1-carboxy-2-phenylethyl)-C-hydroxycarbonimidoyl]-1-[(1,2-dihydroxy-4-methylpentylidene)amino]-3-methylbutan-2-yl}oxy)phenyl]-3-(sulfooxy)propanoic acid	C30H41N3O12S	M-H2O-H	648.2227	-2.2

	HMDB0136730	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-({2,6-dihydroxy-1-[(7-methoxy-2-oxo-2H-chromen-5-yl)oxy]-3,7-dimethyloct-7-en-3-yl} sulfanyl)ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C30H41N3O12S	M-H2O-H	648.2227	-2.2
	HMDB0164247	2-amino-3-{4-[(1-{[1-carboxy-2-(3-hydroxyphenyl)ethyl]-C-hydroxycarbonimidoyl}-1-{[1-hydroxy-4-methyl-2-(sulfooxy)pentylidene]amino}-3-methylbutan-2-	C30H41N3O12S	M-H2O-H	648.2227	-2.2
648.2933	HMDB0015641	Dabigatran etexilate	C34H41N7O5	M+Na-2H	648.2916	2.6
648.9250	HMDB0032285	trisodium 3-sulfo-6-sulfonato-1-[2-(4-sulfonatophthalen-1-yl)diazen-1-yl]naphthalen-2-olate	C20H11N2Na3O10S3	M+FA-H	648.9251	-0.1
649.1966	HMDB0175056	6-{{6-(4-ethenylphenoxy)-4-hydroxy-2-(hydroxymethyl)-5-[(3,4,5-trihydroxy-6-methyloxan-2-yl)oxy]oxan-3-yl}oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H36O16	M+FA-H	649.1985	-3.0
	HMDB0175053	6-[(2-{[2-(4-ethenylphenoxy)-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy}-3,5-dihydroxy-6-methyloxan-4-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H36O16	M+FA-H	649.1985	-3.0
	HMDB0175054	6-[(2-{[2-(4-ethenylphenoxy)-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy}-4,5-dihydroxy-6-methyloxan-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H36O16	M+FA-H	649.1985	-3.0
	HMDB0175055	6-{{2-(4-ethenylphenoxy)-5-hydroxy-6-(hydroxymethyl)-3-[(3,4,5-trihydroxy-6-methyloxan-2-yl)oxy]oxan-4-yl}oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H36O16	M+FA-H	649.1985	-3.0
	HMDB0175052	6-[(6-{[2-(4-ethenylphenoxy)-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy}-4,5-dihydroxy-2-methyloxan-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H36O16	M+FA-H	649.1985	-3.0
	HMDB0175057	6-{{6-(4-ethenylphenoxy)-3,4-dihydroxy-5-[(3,4,5-trihydroxy-6-methyloxan-2-yl)oxy]oxan-2-yl}methoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H36O16	M+FA-H	649.1985	-3.0
	HMDB0034682	cis-Ferulic acid [arabinosyl-(1->3)-[glucosyl-(1->6)]-glucosyl] ester	C27H38O18	M-H	649.1985	-3.0
649.3304	HMDB0015429	Metocurine	C40H48N2O6	M-H	649.3294	1.5
651.4037	HMDB0033408	4-Methoxycinnamoyloleanolic acid methyl ester	C41H58O5	M+Na-2H	651.4031	0.9
654.2934	HMDB0165918	4-[(7-{5-[(2-acetyl-7-hydroxy-6-methoxy-2-methyl-1,2,3,4-tetrahydro-2H-isoquinolin-1-yl)methyl]-2-hydroxyphenoxy}-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl]-4-hydroxycyclohexa-2,5-dien-1-one	C38H43N2O8	M-H	654.2947	-1.9
	HMDB0165936	4-[(2-acetyl-7-{2-hydroxy-5-[(7-hydroxy-6-methoxy-2-methyl-1,2,3,4-tetrahydroisoquinolin-1-yl)methyl]phenoxy}-6-methoxy-2-methyl-1,2,3,4-tetrahydro-2H-isoquinolin-1-yl)methyl]-4-hydroxycyclohexa-2,5-dien-1-one	C38H43N2O8	M-H	654.2947	-1.9
656.0790	HMDB0180815	{{[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)][(4,6-dimethoxypyrimidin-2-yl)-C-hydroxycarbonimidoyl]amino}[3-chloro-4-(methoxycarbonyl)-1-methyl-1H-pyrazol-5-yl]hydroxy-yl sulfanyl} oxidanyl	C19H24ClN6O13S	M+FA-H	656.0793	-0.4
	HMDB0112941	PE-NMe(14:1(9Z)/16)	C36H70NO8P	M-H2O-H	656.4655	1.2
	HMDB0112940	PE-NMe(14/16:1(9Z))	C36H70NO8P	M-H2O-H	656.4655	1.2
	HMDB0113840	PE-NMe2(14:1(9Z)/15)	C36H70NO8P	M-H2O-H	656.4655	1.2
	HMDB0113918	PE-NMe2(15/14:1(9Z))	C36H70NO8P	M-H2O-H	656.4655	1.2

656.4663	HMDB0113061	PE-NMe(16:1(9Z)/14)	C36H70NO8P	M-H2O-H	656.4655	1.2
	HMDB0113040	PE-NMe(16/14:1(9Z))	C36H70NO8P	M-H2O-H	656.4655	1.2
	HMDB0008955	PE(16:1(9Z)/15)	C36H70NO8P	M-H2O-H	656.4655	1.2
	HMDB0008891	PE(15/16:1(9Z))	C36H70NO8P	M-H2O-H	656.4655	1.2
	HMDB0007899	PC(14:1(9Z)/14)	C36H70NO8P	M-H2O-H	656.4655	1.2
	HMDB0007867	PC(14/14:1(9Z))	C36H70NO8P	M-H2O-H	656.4655	1.2
	HMDB0038620	Acidissiminin epoxide	C43H65NO5	M-H2O-H	656.4679	-2.4
657.4484	HMDB0056306	DG(18:3n6/:5n3)	C41H64O5	M+Na-2H	657.4500	-2.5
	HMDB0056337	DG(:4n6/18:4n3)	C41H64O5	M+Na-2H	657.4500	-2.5
	HMDB0056369	DG(18:3n3/:5n3)	C41H64O5	M+Na-2H	657.4500	-2.5
	HMDB0056373	DG(18:4n3/:4n3)	C41H64O5	M+Na-2H	657.4500	-2.5
	HMDB0007288	DG(18:3(6Z,9Z,12Z)/:5(5Z,8Z,11Z,14Z,17Z))	C41H64O5	M+Na-2H	657.4500	-2.5
	HMDB0007317	DG(18:3(9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C41H64O5	M+Na-2H	657.4500	-2.5
	HMDB0007344	DG(18:4(6Z,9Z,12Z,15Z)/:4(5Z,8Z,11Z,14Z))	C41H64O5	M+Na-2H	657.4500	-2.5
	HMDB0007345	DG(18:4(6Z,9Z,12Z,15Z)/:4(8Z,11Z,14Z,17Z))	C41H64O5	M+Na-2H	657.4500	-2.5
	HMDB0007512	DG(:4(5Z,8Z,11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C41H64O5	M+Na-2H	657.4500	-2.5
	HMDB0007541	DG(:4(8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C41H64O5	M+Na-2H	657.4500	-2.5
	HMDB0007568	DG(:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z))	C41H64O5	M+Na-2H	657.4500	-2.5
	HMDB0007569	DG(:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	C41H64O5	M+Na-2H	657.4500	-2.5
	HMDB0114948	PA(18:2(9Z,12Z)/15)	C36H67O8P	M-H	657.4501	-2.6
	HMDB0114815	PA(15/18:2(9Z,12Z))	C36H67O8P	M-H	657.4501	-2.6
659.1287	HMDB0124773	({6-[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro-2H-1-benzopyran-8-yl]-3,4-dihydroxy-5-[(3,4,5-trihydroxy-6-methyloxan-2-yl)oxy]oxan-2-yl)methoxy)sulfonic acid	C27H32O17S	M-H	659.1287	-0.1
	HMDB0126880	(6-{5,7-dihydroxy-4-oxo-2-phenyl-8-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-3,4-dihydro-2H-1-benzopyran-6-yl}-4,5-dihydroxy-2-(hydroxymethyl)oxan-3-yl)oxidanesulfonic acid	C27H32O17S	M-H	659.1287	-0.1
	HMDB0126879	(6-{5,7-dihydroxy-4-oxo-2-phenyl-6-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-3,4-dihydro-2H-1-benzopyran-8-yl}-4,5-dihydroxy-2-(hydroxymethyl)oxan-3-yl)oxidanesulfonic acid	C27H32O17S	M-H	659.1287	-0.1
	HMDB0126878	(2-{5,7-dihydroxy-4-oxo-2-phenyl-6-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-3,4-dihydro-2H-1-benzopyran-8-yl}-3,5-dihydroxy-6-(hydroxymethyl)oxan-4-yl)oxidanesulfonic acid	C27H32O17S	M-H	659.1287	-0.1
	HMDB0126881	(2-{5,7-dihydroxy-4-oxo-2-phenyl-8-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-3,4-dihydro-2H-1-benzopyran-6-yl}-3,5-dihydroxy-6-(hydroxymethyl)oxan-4-yl)oxidanesulfonic acid	C27H32O17S	M-H	659.1287	-0.1
	HMDB0126877	(2-{5,7-dihydroxy-4-oxo-2-phenyl-6-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-3,4-dihydro-2H-1-benzopyran-8-yl}-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl)oxidanesulfonic acid	C27H32O17S	M-H	659.1287	-0.1
	HMDB0126875	[(6-{5,7-dihydroxy-4-oxo-2-phenyl-6-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-3,4-dihydro-2H-1-benzopyran-8-yl}-3,4,5-trihydroxyoxan-2-yl)methoxy]sulfonic acid	C27H32O17S	M-H	659.1287	-0.1
	HMDB0126876	[(6-{5,7-dihydroxy-4-oxo-2-phenyl-8-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-3,4-dihydro-2H-1-benzopyran-6-yl}-3,4,5-trihydroxyoxan-2-yl)methoxy]sulfonic acid	C27H32O17S	M-H	659.1287	-0.1
	HMDB0124774	{6-[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro-2H-1-benzopyran-8-yl]-4-hydroxy-2-(hydroxymethyl)-5-[(3,4,5-trihydroxy-6-methyloxan-2-yl)oxy]oxan-3-yl}oxidanesulfonic acid	C27H32O17S	M-H	659.1287	-0.1

	HMDB0124775	{2-[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro-2H-1-benzopyran-8-yl]-5-hydroxy-6-(hydroxymethyl)-3-[(3,4,5-trihydroxy-6-methyloxan-2-yl)oxy]oxan-4-yl} oxidanesulfonic acid	C27H32O17S	M-H	659.1287	-0.1
	HMDB0124772	(4-{8-[4,5-dihydroxy-6-(hydroxymethyl)-3-[(3,4,5-trihydroxy-6-methyloxan-2-yl)oxy]oxan-2-yl]-5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl}phenyl)oxidanesulfonic acid	C27H32O17S	M-H	659.1287	-0.1
	HMDB0126882	(2-{5,7-dihydroxy-4-oxo-2-phenyl-8-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-3,4-dihydro-2H-1-benzopyran-6-yl}-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl)oxidanesulfonic acid	C27H32O17S	M-H	659.1287	-0.1
659.2277	HMDB0030112	Kuwanon J	C40H38O10	M-H2O-H	659.2281	-0.6
	HMDB0035964	Artonin C	C40H38O10	M-H2O-H	659.2281	-0.6
	HMDB0126375	3-(2,4-dihydroxyphenyl)-1-{3-[5-(2,4-dihydroxyphenyl)-6-(5-hydroxy-2,2-dimethyl-2H-chromene-6-carbonyl)-3-methylcyclohex-2-en-1-yl]-2,4-dihydroxyphenyl}propan-1-one	C40H38O10	M-H2O-H	659.2281	-0.6
659.5031	HMDB0056295	DG(18:2n6/22:6n3)	C44H70O5	M-H2O-H	659.5039	-1.3
659.5978	HMDB0056021	DG(16/24:1n9)	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0056046	DG(18/22:1n9)	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0056069	DG(/:1n9)	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0056091	DG(22/18:1n7)	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0056092	DG(22/18:1n9)	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0056113	DG(24/16:1n7)	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0007123	DG(16/24:1(15Z))	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0007823	DG(24:1(15Z)/16)	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0007795	DG(24/16:1(9Z))	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0007622	DG(22:1(13Z)/18)	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0007151	DG(16:1(9Z)/24)	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0007174	DG(18/22:1(13Z))	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0007202	DG(18:1(11Z)/22)	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0007231	DG(18:1(9Z)/22)	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0007369	DG(/:1(11Z))	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0007397	DG(:1(11Z)/)	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0007594	DG(22/18:1(11Z))	C43H82O5	M-H2O-H	659.5978	-0.1
	HMDB0007595	DG(22/18:1(9Z))	C43H82O5	M-H2O-H	659.5978	-0.1
660.3886	HMDB0015616	Telaprevir	C36H53N7O6	M-H2O-H	660.3873	1.9
	HMDB0185449	11-(2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl)sulfanyl)-12-hydroxydocosanoic acid	C32H59N3O9S	M-H	660.3899	-2.0
	HMDB0185450	12-(2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl)sulfanyl)-11-hydroxydocosanoic acid	C32H59N3O9S	M-H	660.3899	-2.0
660.4988	HMDB0008916	PE(15/P-16)	C36H72NO7P	M-H	660.4974	2.2
	HMDB0011337	PE(P-16/15)	C36H72NO7P	M-H	660.4974	2.2
	HMDB0029221	LysoPC(28:1(5Z))	C36H72NO7P	M-H	660.4974	2.2
661.4245	HMDB0034770	6-Geranylgeranyl 8'-methyl 6,8'-diapocarotene-6,8'-dioate	C43H60O4	M+Na-2H	661.4238	1.0
	HMDB0114823	PA(15/:5(5Z,8Z,11Z,14Z,17Z))	C38H65O8P	M-H2O-H	661.4233	1.8
	HMDB0115200	PA(:5(5Z,8Z,11Z,14Z,17Z)/15)	C38H65O8P	M-H2O-H	661.4233	1.8
	HMDB0056203	DG(18:1n9/18:3n6)	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0056210	DG(18:1n9/18:3n3)	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007113	DG(16/:4(8Z,11Z,14Z,17Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0056191	DG(18:1n7/18:3n3)	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0056184	DG(18:1n7/18:3n6)	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0056166	DG(16:1n7/:3n6)	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0055973	DG(14/22:4n6)	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0056026	DG(16/:4n6)	C39H68O5	M+FA-H	661.5049	-0.7

661.5044	HMDB0056032	DG(16/:4n3)	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0056057	DG(18/18:4n3)	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0056160	DG(16:1n7/:3n9)	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007031	DG(14/22:4(7Z,Z,13Z,16Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007305	DG(18:3(9Z,12Z,15Z)/18:1(9Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007304	DG(18:3(9Z,12Z,15Z)/18:1(11Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007332	DG(18:4(6Z,9Z,12Z,15Z)/18)	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007447	DG(:3(5Z,8Z,11Z)/16:1(9Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007476	DG(:3(8Z,11Z,14Z)/16:1(9Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007504	DG(:4(5Z,8Z,11Z,14Z)/16)	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007533	DG(:4(8Z,11Z,14Z,17Z)/16)	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007675	DG(22:4(7Z,Z,13Z,16Z)/14)	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007275	DG(18:3(6Z,9Z,12Z)/18:1(11Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007276	DG(18:3(6Z,9Z,12Z)/18:1(9Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007248	DG(18:2(9Z,12Z)/18:2(9Z,12Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007112	DG(16/:4(5Z,8Z,11Z,14Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007139	DG(16:1(9Z)/:3(5Z,8Z,11Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007140	DG(16:1(9Z)/:3(8Z,11Z,14Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007164	DG(18/18:4(6Z,9Z,12Z,15Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007191	DG(18:1(11Z)/18:3(6Z,9Z,12Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007192	DG(18:1(11Z)/18:3(9Z,12Z,15Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007220	DG(18:1(9Z)/18:3(6Z,9Z,12Z))	C39H68O5	M+FA-H	661.5049	-0.7
	HMDB0007221	DG(18:1(9Z)/18:3(9Z,12Z,15Z))	C39H68O5	M+FA-H	661.5049	-0.7
662.1014	HMDB0039421	Fenugreekine	C21H27N7O14P2	M-H	662.1018	-0.7
	HMDB0000902	NAD+	C21H27N7O14P2	M-H	662.1018	-0.7
	HMDB0155854	1-{5-[(1-[(5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy}(hydroxy)phosphoryl)oxy](hydroxy)phosphoryl]oxy)methyl}-3,4-dihydroxyoxolan-2-yl}-3-(C-hydroxycarbonimidoyl)-1-pyridin-1-ylum	C21H28N7O14P2	M-H	662.1018	-0.7
662.2405	HMDB0150235	2-amino-4-(1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-(4-[2-(2,4-dihydroxyphenyl)-7-methoxy-3,4-dihydro-2H-1-benzopyran-8-yl]-3-hydroxy-2-methylbutan-2-yl)sulfanyl)ethyl)-C-hydroxycarbonimidoyl)butanoic acid	C31H41N3O11S	M-H	662.2389	2.4
663.4390	HMDB0114821	PA(15/:4(5Z,8Z,11Z,14Z))	C38H67O8P	M-H2O-H	663.4390	0.1
	HMDB0114822	PA(15/:4(8Z,11Z,14Z,17Z))	C38H67O8P	M-H2O-H	663.4390	0.1
	HMDB0115146	PA(:4(5Z,8Z,11Z,14Z)/15)	C38H67O8P	M-H2O-H	663.4390	0.1
	HMDB0115173	PA(:4(8Z,11Z,14Z,17Z)/15)	C38H67O8P	M-H2O-H	663.4390	0.1
663.5190	HMDB0168955	6-(dotriacontyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C38H74O7	M+Na-2H	663.5181	1.3
	HMDB0168953	6-(dotriacontan-2-yloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C38H74O7	M+Na-2H	663.5181	1.3
	HMDB0240593	(2S)-1-(hexadecanoyloxy)-3-hydroxypropan-2-yl (11Z,14Z,17Z)-icosa-11,14,17-trienoate	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0056165	DG(16:1n7/:2n6)	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0056147	DG(14:1n5/22:2n6)	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0056056	DG(18/18:3n3)	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0056049	DG(18/18:3n6)	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0056025	DG(16/:3n6)	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0056019	DG(16/:3n9)	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0007647	DG(22:2(13Z,16Z)/14:1(9Z))	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0007475	DG(:3(8Z,11Z,14Z)/16)	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0007446	DG(:3(5Z,8Z,11Z)/16)	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0007418	DG(:2(11Z,14Z)/16:1(9Z))	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0007303	DG(18:3(9Z,12Z,15Z)/18)	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0007274	DG(18:3(6Z,9Z,12Z)/18)	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0007247	DG(18:2(9Z,12Z)/18:1(9Z))	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0007246	DG(18:2(9Z,12Z)/18:1(11Z))	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0007219	DG(18:1(9Z)/18:2(9Z,12Z))	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0007190	DG(18:1(11Z)/18:2(9Z,12Z))	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0007163	DG(18/18:3(9Z,12Z,15Z))	C39H70O5	M+FA-H	663.5205	-2.3

	HMDB0007162	DG(18/18:3(6Z,9Z,12Z))	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0007138	DG(16:1(9Z):2(11Z,14Z))	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0007111	DG(16/:3(8Z,11Z,14Z))	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0007110	DG(16/:3(5Z,8Z,11Z))	C39H70O5	M+FA-H	663.5205	-2.3
	HMDB0007059	DG(14:1(9Z)/22:2(13Z,16Z))	C39H70O5	M+FA-H	663.5205	-2.3
664.1593	HMDB0126127	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-({5,9-dihydroxy-8,8-dimethyl-2-oxo-4-phenyl-2H,8H,9H,H-pyrano[2,3-h]chromen--yl}sulfanyl)ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C30H33N3O11S	M+Na-2H	664.1582	1.6
	HMDB0126128	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-({5,-dihydroxy-8,8-dimethyl-2-oxo-4-phenyl-2H,8H,9H,H-pyrano[2,3-h]chromen-9-yl}sulfanyl)ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C30H33N3O11S	M+Na-2H	664.1582	1.6
665.2152	HMDB0144794	N-(3-{3-hydroxy-1-[(6R)-2-hydroxy-4-oxo-6-(2-phenylethyl)-6-propyloxan-3-yl]propyl}phenyl)-5-(trifluoromethyl)pyridine-2-sulfonamide	C31H35F3N2O6S	M+FA-H	665.2150	0.3
	HMDB0144793	N-(3-{1-[(6S)-2-hydroxy-6-(2-hydroxypropyl)-4-oxo-6-(2-phenylethyl)oxan-3-yl]propyl}phenyl)-5-(trifluoromethyl)pyridine-2-sulfonamide	C31H35F3N2O6S	M+FA-H	665.2150	0.3
	HMDB0144792	N-(3-{2-hydroxy-1-[(6R)-2-hydroxy-4-oxo-6-(2-phenylethyl)-6-propyloxan-3-yl]propyl}phenyl)-5-(trifluoromethyl)pyridine-2-sulfonamide	C31H35F3N2O6S	M+FA-H	665.2150	0.3
	HMDB0144795	N-(3-{1-[(6S)-2-hydroxy-6-(3-hydroxypropyl)-4-oxo-6-(2-phenylethyl)oxan-3-yl]propyl}phenyl)-5-(trifluoromethyl)pyridine-2-sulfonamide	C31H35F3N2O6S	M+FA-H	665.2150	0.3
	HMDB0144800	N-(3-{1-hydroxy-1-[(6R)-2-hydroxy-4-oxo-6-(2-phenylethyl)-6-propyloxan-3-yl]propyl}phenyl)-5-(trifluoromethyl)pyridine-2-sulfonamide	C31H35F3N2O6S	M+FA-H	665.2150	0.3
	HMDB0144799	N-(3-{1-[(6R)-2,5-dihydroxy-4-oxo-6-(2-phenylethyl)-6-propyloxan-3-yl]propyl}phenyl)-5-(trifluoromethyl)pyridine-2-sulfonamide	C31H35F3N2O6S	M+FA-H	665.2150	0.3
	HMDB0144801	N-(3-{1-[(6R)-2-hydroxy-6-(2-hydroxy-2-phenylethyl)-4-oxo-6-propyloxan-3-yl]propyl}phenyl)-5-(trifluoromethyl)pyridine-2-sulfonamide	C31H35F3N2O6S	M+FA-H	665.2150	0.3
	HMDB0144798	N-(3-{1-[(6R)-2,3-dihydroxy-4-oxo-6-(2-phenylethyl)-6-propyloxan-3-yl]propyl}phenyl)-5-(trifluoromethyl)pyridine-2-sulfonamide	C31H35F3N2O6S	M+FA-H	665.2150	0.3
	HMDB0144804	N-(3-{1-[(6R)-2-hydroxy-4-oxo-6-(2-phenylethyl)-6-propyloxan-3-yl]propyl}phenyl)-1-oxo-5-(trifluoromethyl)-1H-pyridine-2-sulfonamide	C31H35F3N2O6S	M+FA-H	665.2150	0.3
	HMDB0144803	N-(3-{1-[(6R)-2-hydroxy-6-[2-(4-hydroxyphenyl)ethyl]-4-oxo-6-propyloxan-3-yl]propyl}phenyl)-5-(trifluoromethyl)pyridine-2-sulfonamide	C31H35F3N2O6S	M+FA-H	665.2150	0.3
	HMDB0144805	N-(3-{1-[(6R)-2-hydroxy-6-[2-(2-hydroxyphenyl)ethyl]-4-oxo-6-propyloxan-3-yl]propyl}phenyl)-5-(trifluoromethyl)pyridine-2-sulfonamide	C31H35F3N2O6S	M+FA-H	665.2150	0.3
	HMDB0144802	N-(3-{1-[(6R)-2-hydroxy-6-[2-(3-hydroxyphenyl)ethyl]-4-oxo-6-propyloxan-3-yl]propyl}phenyl)-5-(trifluoromethyl)pyridine-2-sulfonamide	C31H35F3N2O6S	M+FA-H	665.2150	0.3
	HMDB0176707	6-({[3,5-dihydroxy-6-(hydroxymethyl)-4-{[3,4,5-trihydroxy-6-({[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}methyl)oxan-2-yl]oxy}oxan-2-yl]oxy}methyl)oxane-2,3,4,5-tetrol	C24H42O21	M-H	665.2146	0.9
	HMDB0187421	2-{[4,5-dihydroxy-2-(hydroxymethyl)-6-[(3,4,5-trihydroxy-6-([4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy}oxan-2-yl)methoxy]oxan-3-yl]oxy}-6-(hydroxymethyl)oxane-3,4,5-triol	C24H42O21	M-H	665.2146	0.9
	HMDB0187422	AC1NBP2P	C24H42O21	M-H	665.2146	0.9
	HMDB0040182	Fagopyritol A3	C24H42O21	M-H	665.2146	0.9

	HMDB0039176	Nystose	C24H42O21	M-H	665.2146	0.9
	HMDB0038871	Sesamose	C24H42O21	M-H	665.2146	0.9
	HMDB0039173	3-beta-Glucosylcellotriose	C24H42O21	M-H	665.2146	0.9
	HMDB0038490	Bifurcose	C24H42O21	M-H	665.2146	0.9
	HMDB0035323	Fagopyritol B3	C24H42O21	M-H	665.2146	0.9
	HMDB0038870	Neobifurcose	C24H42O21	M-H	665.2146	0.9
	HMDB0039174	3-beta-Cellobiosylcellobiose	C24H42O21	M-H	665.2146	0.9
	HMDB0003553	Stachyose	C24H42O21	M-H	665.2146	0.9
	HMDB0001296	Maltotetraose	C24H42O21	M-H	665.2146	0.9
	HMDB0000757	Glycogen	C24H42O21	M-H	665.2146	0.9
	HMDB0029931	Mannan	C24H42O21	M-H	665.2146	0.9
	HMDB0041435	Citbismine C	C37H36N2O11	M-H2O-H	665.2135	2.5
	HMDB0139498	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(2-hydroxy-1-{[2-hydroxy-2-(4-methoxyphenyl)ethyl]-C-hydroxycarbonimidoyl}-2-phenylethyl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C28H36N4O10S	M+FA-H	665.2134	2.7
	HMDB0139497	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(2-hydroxy-2-{[2-hydroxy-2-(4-methoxyphenyl)ethyl]-C-hydroxycarbonimidoyl}-1-phenylethyl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C28H36N4O10S	M+FA-H	665.2134	2.7
665.5345	HMDB0056024	DG(16/:2n6)	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0055972	DG(14/22:2n6)	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0056140	DG(14:1n5/22:1n9)	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0056159	DG(16:1n7/:1n9)	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0007030	DG(14/22:2(13Z,16Z))	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0007417	DG(:2(11Z,14Z)/16)	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0007618	DG(22:1(13Z)/14:1(9Z))	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0007646	DG(22:2(13Z,16Z)/14)	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0007389	DG(:1(11Z)/16:1(9Z))	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0007245	DG(18:2(9Z,12Z)/18)	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0007058	DG(14:1(9Z)/22:1(13Z))	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0007109	DG(16/:2(11Z,14Z))	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0007137	DG(16:1(9Z):1(11Z))	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0007161	DG(18/18:2(9Z,12Z))	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0007188	DG(18:1(11Z)/18:1(11Z))	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0007189	DG(18:1(11Z)/18:1(9Z))	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0007217	DG(18:1(9Z)/18:1(11Z))	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0007218	DG(18:1(9Z)/18:1(9Z))	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0056177	DG(18:1n7/18:1n7)	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0056197	DG(18:1n9/18:1n9)	C39H72O5	M+FA-H	665.5362	-2.5
	HMDB0056178	DG(18:1n7/18:1n9)	C39H72O5	M+FA-H	665.5362	-2.5
665.9213	HMDB0059647	Adenosine 5'-pentaphosphate	C10H18N5O19P5	M-H	665.9211	0.3
667.5508	HMDB0056089	DG(22/14:1n5)	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0055965	DG(14/22:1n9)	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0056018	DG(16/:1n9)	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0056066	DG(/16:1n7)	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0056043	DG(18/18:1n9)	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0007589	DG(22/14:1(9Z))	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0007617	DG(22:1(13Z)/14)	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0007388	DG(:1(11Z)/16)	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0007360	DG(/16:1(9Z))	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0007029	DG(14/22:1(13Z))	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0007057	DG(14:1(9Z)/22)	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0007108	DG(16/:1(11Z))	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0007136	DG(16:1(9Z)/)	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0007160	DG(18/18:1(9Z))	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0007159	DG(18/18:1(11Z))	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0007187	DG(18:1(11Z)/18)	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0007216	DG(18:1(9Z)/18)	C39H74O5	M+FA-H	667.5518	-1.5
	HMDB0056042	DG(18/18:1n7)	C39H74O5	M+FA-H	667.5518	-1.5
668.5948	HMDB0004953	Cer(d18:1/24:1(15Z))	C42H81NO3	M+Na-2H	668.5963	-2.3

669.1672	HMDB0125110	7-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-3,5-bis([3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)-1位?chromen-1-ylum	C28H33O16	M+FA-H	669.1672	-0.1
	HMDB0125115	3-{[4,5-dihydroxy-6-(hydroxymethyl)-3-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}oxan-2-yl]oxy}-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-1位?chromen-1-ylum	C28H33O16	M+FA-H	669.1672	-0.1
	HMDB0127030	5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-3,6-bis[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-4H-chromen-4-one	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0151388	5,7-dihydroxy-2-(3-methoxy-4-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}phenyl)-6-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-4H-chromen-4-one	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0038813	Scoparin 2"-glucoside	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0037746	Keioside	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0037422	Isoscoparin 2"-O-glucoside	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0146614	Isoscoparin 7-glucoside	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0037500	Subulin	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0037361	Azaleatin 3-rutinoside	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0037743	Pasternoside	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0037443	Sexangularetin 3-glucoside 7-rhamnoside	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0037410	6,8-Diglucosyldiosmetin	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0037745	Calendoflavoside	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0037744	Isorhamnetin 3-O-[b-L-rhamnofuranosyl-(1->6)-D-glucopyranoside]	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0037375	Isorhamnetin 3-glucoside 4'-rhamnoside	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0037409	3,8-Diglucosyldiosmetin	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0037085	Isorhamnetin 3-O-[b-D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside]	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0039124	Crosatoside A	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0126961	5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-6,8-bis[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-4H-chromen-4-one	C28H32O16	M+FA-H	669.1672	-0.1
	HMDB0127850	6-[(2-{3-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl]oxy]-4-(methoxymethyl)phenyl}-3,5-dihydroxy-3,4-dihydro-2H-1-benzopyran-7-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C29H34O18	M-H	669.1672	-0.1
	HMDB0037469	Spinacetin 3-gentiobioside	C29H34O18	M-H	669.1672	-0.1
	HMDB0041766	Quercetin 3'-sulfate	C28H33O16	M+FA-H	669.1678	-0.9
	HMDB0041677	5,7-Dihydroxy-8,4'-dimethoxyisoflavone	C28H33O16	M+FA-H	669.1678	-0.9
	HMDB0038098	4-Hydroxy-3-prenylbenzoic acid glucoside	C28H33O16	M+FA-H	669.1678	-0.9
	HMDB0038099	Petunidin 3-rhamnoside 5-glucoside	C28H33O16	M+FA-H	669.1678	-0.9
669.3461	HMDB0039553	Lyciumoside III	C32H56O13	M+Na-2H	669.3468	-1.0
669.3846	HMDB0173070	6-{[14-(3,4-dihydroxy-6-methyl-5-methylideneheptan-2-yl)-4-hydroxy-2,15-dimethyltetracyclo[8.7.,heptadecan-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H56O10	M+FA-H	669.3855	-1.4
	HMDB0168866	6-{[(2S,15S)-14-(3,4-dihydroxy-5,6-dimethylheptan-2-yl)-2,15-dimethyl-4-oxotetracyclo[8.7.,heptadecan-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H56O10	M+FA-H	669.3855	-1.4
	HMDB0174690	6-{[14-(3,4-dihydroxy-5,6-dimethylheptan-2-yl)-2,15-dimethyl-8-oxotetracyclo[8.7.,heptadecan-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C34H56O10	M+FA-H	669.3855	-1.4
	HMDB0056230	DG(:1n9/:4n3)	C43H74O5	M-H	669.5463	0.8
	HMDB0056084	DG(/:5n3)	C43H74O5	M-H	669.5463	0.8
	HMDB0056189	DG(18:1n7/22:4n6)	C43H74O5	M-H	669.5463	0.8
	HMDB0056208	DG(18:1n9/22:4n6)	C43H74O5	M-H	669.5463	0.8
	HMDB0056224	DG(:1n9/:4n6)	C43H74O5	M-H	669.5463	0.8
	HMDB0056262	DG(22:1n9/18:4n3)	C43H74O5	M-H	669.5463	0.8
	HMDB0056300	DG(18:3n6/22:2n6)	C43H74O5	M-H	669.5463	0.8
	HMDB0056345	DG(22:2n6/18:3n3)	C43H74O5	M-H	669.5463	0.8
	HMDB0056310	DG(:2n6/:3n6)	C43H74O5	M-H	669.5463	0.8
	HMDB0056239	DG(:3n9/:2n6)	C43H74O5	M-H	669.5463	0.8
	HMDB0056060	DG(18/22:5n3)	C43H74O5	M-H	669.5463	0.8

669.5469	HMDB0056055	DG(18/22:5n6)	C43H74O5	M-H	669.5463	0.8
	HMDB0007177	DG(18/22:5(4Z,7Z,Z,13Z,16Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007514	DG(4(5Z,8Z,11Z,14Z):1(11Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007543	DG(4(8Z,11Z,14Z,17Z):1(11Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007571	DG(5(5Z,8Z,11Z,14Z,17Z)/)	C43H74O5	M-H	669.5463	0.8
	HMDB0007628	DG(22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007655	DG(22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007656	DG(22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007681	DG(22:4(7Z,Z,13Z,16Z)/18:1(11Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007682	DG(22:4(7Z,Z,13Z,16Z)/18:1(9Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007709	DG(22:5(4Z,7Z,Z,13Z,16Z)/18)	C43H74O5	M-H	669.5463	0.8
	HMDB0007738	DG(22:5(7Z,Z,13Z,16Z,19Z)/18)	C43H74O5	M-H	669.5463	0.8
	HMDB0007486	DG(3(8Z,11Z,14Z):2(11Z,14Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007457	DG(3(5Z,8Z,11Z):2(11Z,14Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007178	DG(18/22:5(7Z,Z,13Z,16Z,19Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007205	DG(18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007234	DG(18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007291	DG(18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007320	DG(18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007348	DG(18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007375	DG(/:5(5Z,8Z,11Z,14Z,17Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007403	DG(1(11Z):4(8Z,11Z,14Z,17Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007402	DG(1(11Z):4(5Z,8Z,11Z,14Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007429	DG(2(11Z,14Z):3(5Z,8Z,11Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0007430	DG(2(11Z,14Z):3(8Z,11Z,14Z))	C43H74O5	M-H	669.5463	0.8
	HMDB0034840	Faradiol laurate	C42H72O3	M+FA-H	669.5463	0.8
670.2088	HMDB0178468	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{[3-(3,4-dimethoxyphenyl)-1-hydroxy-5-methoxy-4-oxo-2,4,5,6-tetrahydro-1H-phenalen-2-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C32H37N3O11S	M-H	670.2076	1.8
	HMDB0178469	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{[3-(3,4-dimethoxyphenyl)-2-hydroxy-5-methoxy-4-oxo-2,4,5,6-tetrahydro-1H-phenalen-1-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C32H37N3O11S	M-H	670.2076	1.8
	HMDB0178471	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{[7-(3,4-dimethoxyphenyl)-1-hydroxy-5-methoxy-6-oxo-2,4,5,6-tetrahydro-1H-phenalen-2-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C32H37N3O11S	M-H	670.2076	1.8
	HMDB0178470	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{[7-(3,4-dimethoxyphenyl)-2-hydroxy-5-methoxy-6-oxo-2,4,5,6-tetrahydro-1H-phenalen-1-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C32H37N3O11S	M-H	670.2076	1.8
670.6100	HMDB0000831	N-Lignoceroylsphingosine	C42H83NO3	M+Na-2H	670.6120	-2.9
	HMDB0011769	Cer(d18/24:1(15Z))	C42H83NO3	M+Na-2H	670.6120	-2.9
	HMDB0004956	Ceramide (d18:1/24)	C42H83NO3	M+Na-2H	670.6120	-2.9
671.1115	HMDB0034258	Amritoside	C26H26O18	M+FA-H	671.1101	2.1
	HMDB0169576	6-({2-[6-(carboxymethyl)-3,4,5-trihydroxyoxan-2-yl]-1,6,7-trihydroxy-9-oxo-9H-xanthen-3-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H26O18	M+FA-H	671.1101	2.1
	HMDB0169577	6-({7-[6-(carboxymethyl)-3,4,5-trihydroxyoxan-2-yl]-2,6,8-trihydroxy-9-oxo-9H-xanthen-3-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H26O18	M+FA-H	671.1101	2.1
	HMDB0169578	6-({7-[6-(carboxymethyl)-3,4,5-trihydroxyoxan-2-yl]-3,6,8-trihydroxy-9-oxo-9H-xanthen-2-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H26O18	M+FA-H	671.1101	2.1
	HMDB0169579	6-({2-[6-(carboxymethyl)-3,4,5-trihydroxyoxan-2-yl]-3,6,7-trihydroxy-9-oxo-9H-xanthen-1-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C26H26O18	M+FA-H	671.1101	2.1
	HMDB0169580	3,4,5-trihydroxy-6-({2-[3,4,5-trihydroxy-6-(1,3,6,7-tetrahydroxy-9-oxo-9H-xanthen-2-yl)oxan-2-yl]acetyl}oxy)oxane-2-carboxylic acid	C26H26O18	M+FA-H	671.1101	2.1

671.2339	HMDB0036526	Myricanol 5-(6-galloylglucoside)	C34H40O14	M-H	671.2345	-0.9
	HMDB0184539	3,4,5-trihydroxy-6-({5-hydroxy-4-[(2S)-16-hydroxy-2-methyl-5-(sulfooxy)tetraacyclo[8.7.,heptadecan-14-yl]pentanoyl}oxy)oxane-2-carboxylic acid	C29H46O14S	M+Na-2H	671.2355	-2.4
	HMDB0039340	Ichangin 4-glucoside	C32H42O14	M+Na-2H	671.2321	2.6
671.3094	HMDB0015032	Benzylpenicilloyl polylysine	C28H46N6O8S	M+FA-H	671.3080	2.1
	HMDB0015429	Metocurine	C40H48N2O6	M+Na-2H	671.3114	-2.9
671.4649	HMDB0114900	PA(18:1(11Z)/16:1(9Z))	C37H69O8P	M-H	671.4657	-1.2
	HMDB0114925	PA(18:1(9Z)/16:1(9Z))	C37H69O8P	M-H	671.4657	-1.2
	HMDB0114949	PA(18:2(9Z,12Z)/16)	C37H69O8P	M-H	671.4657	-1.2
	HMDB0115092	PA(:1(11Z)/14:1(9Z))	C37H69O8P	M-H	671.4657	-1.2
	HMDB0115504	PA(14:2(11Z,14Z))	C37H69O8P	M-H	671.4657	-1.2
	HMDB0115532	PA(:2(11Z,14Z)/14)	C37H69O8P	M-H	671.4657	-1.2
	HMDB0007860	PA(16/18:2(9Z,12Z))	C37H69O8P	M-H	671.4657	-1.2
671.5636	HMDB0056309	DG(:2n6/:2n6)	C43H76O5	M-H	671.5620	2.4
	HMDB0056261	DG(22:1n9/18:3n3)	C43H76O5	M-H	671.5620	2.4
	HMDB0056254	DG(22:1n9/18:3n6)	C43H76O5	M-H	671.5620	2.4
	HMDB0056223	DG(:1n9/:3n6)	C43H76O5	M-H	671.5620	2.4
	HMDB0056217	DG(:1n9/:3n9)	C43H76O5	M-H	671.5620	2.4
	HMDB0056106	DG(22/18:4n3)	C43H76O5	M-H	671.5620	2.4
	HMDB0056083	DG(/:4n3)	C43H76O5	M-H	671.5620	2.4
	HMDB0056077	DG(/:4n6)	C43H76O5	M-H	671.5620	2.4
	HMDB0056054	DG(18/22:4n6)	C43H76O5	M-H	671.5620	2.4
	HMDB0007456	DG(:3(5Z,8Z,11Z)/:1(11Z))	C43H76O5	M-H	671.5620	2.4
	HMDB0007485	DG(:3(8Z,11Z,14Z)/:1(11Z))	C43H76O5	M-H	671.5620	2.4
	HMDB0007513	DG(:4(5Z,8Z,11Z,14Z)/)	C43H76O5	M-H	671.5620	2.4
	HMDB0007542	DG(:4(8Z,11Z,14Z,17Z)/)	C43H76O5	M-H	671.5620	2.4
	HMDB0007599	DG(22/18:4(6Z,9Z,12Z,15Z))	C43H76O5	M-H	671.5620	2.4
	HMDB0007627	DG(22:1(13Z)/18:3(9Z,12Z,15Z))	C43H76O5	M-H	671.5620	2.4
	HMDB0007626	DG(22:1(13Z)/18:3(6Z,9Z,12Z))	C43H76O5	M-H	671.5620	2.4
	HMDB0007654	DG(22:2(13Z,16Z)/18:2(9Z,12Z))	C43H76O5	M-H	671.5620	2.4
	HMDB0007428	DG(:2(11Z,14Z)/:2(11Z,14Z))	C43H76O5	M-H	671.5620	2.4
	HMDB0007400	DG(:1(11Z)/:3(5Z,8Z,11Z))	C43H76O5	M-H	671.5620	2.4
	HMDB0007197	DG(18:1(11Z)/:3(5Z,8Z,11Z))	C43H76O5	M-H	671.5620	2.4
	HMDB0007262	DG(18:2(9Z,12Z)/22:2(13Z,16Z))	C43H76O5	M-H	671.5620	2.4
	HMDB0007290	DG(18:3(6Z,9Z,12Z)/22:1(13Z))	C43H76O5	M-H	671.5620	2.4
	HMDB0007319	DG(18:3(9Z,12Z,15Z)/22:1(13Z))	C43H76O5	M-H	671.5620	2.4
	HMDB0007347	DG(18:4(6Z,9Z,12Z,15Z)/22)	C43H76O5	M-H	671.5620	2.4
	HMDB0007373	DG(/:4(5Z,8Z,11Z,14Z))	C43H76O5	M-H	671.5620	2.4
	HMDB0007374	DG(/:4(8Z,11Z,14Z,17Z))	C43H76O5	M-H	671.5620	2.4
	HMDB0007401	DG(:1(11Z)/:3(8Z,11Z,14Z))	C43H76O5	M-H	671.5620	2.4
	HMDB0007680	DG(22:4(7Z,Z,13Z,16Z)/18)	C43H76O5	M-H	671.5620	2.4
	HMDB0007176	DG(18/22:4(7Z,Z,13Z,16Z))	C43H76O5	M-H	671.5620	2.4
672.2363	HMDB0000445	Alpha-Tetrascaccharide	C26H45NO20	M-H20-H	672.2351	1.8
672.2456	HMDB0176927	2-amino-4-[(2-{[3,5-bis(acetyloxy)-2-hydroxy-4-(3-hydroxy-6-methylhepta-1,5-dien-2-yl)-1-methyl-6-oxocyclohexyl]sulfanyl}-1-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl)-C-hydroxycarbonimidoyl]butanoic acid	C29H43N3O13S	M-H	672.2444	1.8
	HMDB0006698	Tri-N-acetylchitotriose	C24H41N3O16	M+FA-H	672.2469	-1.9
	HMDB0003362	Chitin	C24H41N3O16	M+FA-H	672.2469	-1.9
	HMDB0113841	PE-NMe2(15/15)	C37H74NO8P	M-H20-H	672.4968	-1.8
	HMDB0029174	3-Sn-phosphatidylethanolamine	C37H74NO8P	M-H20-H	672.4968	-1.8
	HMDB0113940	PE-NMe2(16/14)	C37H74NO8P	M-H20-H	672.4968	-1.8
	HMDB0113041	PE-NMe(16/15)	C37H74NO8P	M-H20-H	672.4968	-1.8

672.4956	HMDB0113845	PE-NMe2(14/16)	C37H74NO8P	M-H20-H	672.4968	-1.8
	HMDB0007868	PC(14/15)	C37H74NO8P	M-H20-H	672.4968	-1.8
	HMDB0007932	PC(15/14)	C37H74NO8P	M-H20-H	672.4968	-1.8
	HMDB0008826	PE(14/18)	C37H74NO8P	M-H20-H	672.4968	-1.8
	HMDB0008923	PE(16/16)	C37H74NO8P	M-H20-H	672.4968	-1.8
	HMDB0008986	PE(18/14)	C37H74NO8P	M-H20-H	672.4968	-1.8
	HMDB0112964	PE-NMe(15/16)	C37H74NO8P	M-H20-H	672.4968	-1.8
	HMDB0008884	PE(14:1(9Z)/P-18)	C37H72NO7P	M-H	672.4974	-2.6
	HMDB0008852	PE(14/P-18:1(11Z))	C37H72NO7P	M-H	672.4974	-2.6
	HMDB0011434	PE(P-18:1(9Z)/14)	C37H72NO7P	M-H	672.4974	-2.6
	HMDB0011401	PE(P-18:1(11Z)/14)	C37H72NO7P	M-H	672.4974	-2.6
	HMDB0011369	PE(P-18/14:1(9Z))	C37H72NO7P	M-H	672.4974	-2.6
	HMDB0011339	PE(P-16/16:1(9Z))	C37H72NO7P	M-H	672.4974	-2.6
	HMDB0008982	PE(16:1(9Z)/P-16)	C37H72NO7P	M-H	672.4974	-2.6
	HMDB0008853	PE(14/P-18:1(9Z))	C37H72NO7P	M-H	672.4974	-2.6
673.3077	HMDB0184186	6-[(6-{{(6E,E,14E)-15-carboxy-13-hydroxy-3,7,11,15-tetramethylpentadeca-1,6,,14-tetraen-3-yl]oxy}-3,4,5-trihydroxyoxan-2-yl)methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H50O15	M-H	673.3077	0.0
	HMDB0184185	6-[(2-{{(6E,E,14E)-15-carboxy-13-hydroxy-3,7,11,15-tetramethylpentadeca-1,6,,14-tetraen-3-yl]oxy}-3,5-dihydroxy-6-(hydroxymethyl)oxan-4-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H50O15	M-H	673.3077	0.0
	HMDB0183226	6-[(5E,9E)-1-carboxy-1,5,9,13-tetramethyl-13-{{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}pentadeca-1,5,9,14-tetraen-3-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H50O15	M-H	673.3077	0.0
	HMDB0183223	6-[(2-{{(6E,E,14E)-15-carboxy-13-hydroxy-3,7,11,15-tetramethylpentadeca-1,6,,14-tetraen-3-yl]oxy}-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H50O15	M-H	673.3077	0.0
	HMDB0183227	3,4,5-trihydroxy-6-{{(2E,6E,E)-4-hydroxy-2,6,,14-tetramethyl-14-{{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}hexadeca-2,6,,15-tetraenoyl]oxy}oxane-2-carboxylic acid	C32H50O15	M-H	673.3077	0.0
	HMDB0183224	6-[(6-{{(6E,E,14E)-15-carboxy-13-hydroxy-3,7,11,15-tetramethylpentadeca-1,6,,14-tetraen-3-yl]oxy}-4,5-dihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H50O15	M-H	673.3077	0.0
	HMDB0169445	3,4,5-trihydroxy-6-{{(2Z,6Z,Z)-4-hydroxy-2,6,,14-tetramethyl-14-{{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}hexadeca-2,6,,15-tetraenoyl]oxy}oxane-2-carboxylic acid	C32H50O15	M-H	673.3077	0.0
	HMDB0169444	6-[(1Z,5Z,9Z)-1-carboxy-1,5,9,13-tetramethyl-13-{{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}pentadeca-1,5,9,14-tetraen-3-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H50O15	M-H	673.3077	0.0

	HMDB0169442	6-[(6-{[(6Z,Z,14Z)-15-carboxy-13-hydroxy-3,7,11,15-tetramethylpentadeca-1,6,,14-tetraen-3-yl]oxy}-4,5-dihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H50O15	M-H	673.3077	0.0
	HMDB0169440	6-[(2-{[(6Z,14Z)-15-carboxy-13-hydroxy-3,7,11,15-tetramethylpentadeca-1,6,,14-tetraen-3-yl]oxy}-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H50O15	M-H	673.3077	0.0
	HMDB0169443	6-[(6-{[(6Z,Z,14Z)-15-carboxy-13-hydroxy-3,7,11,15-tetramethylpentadeca-1,6,,14-tetraen-3-yl]oxy}-3,4,5-trihydroxyoxan-2-yl)methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H50O15	M-H	673.3077	0.0
	HMDB0169441	6-[(2-{[(6Z,Z,14Z)-15-carboxy-13-hydroxy-3,7,11,15-tetramethylpentadeca-1,6,,14-tetraen-3-yl]oxy}-3,5-dihydroxy-6-(hydroxymethyl)oxan-4-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C32H50O15	M-H	673.3077	0.0
	HMDB0037125	Pisumoside B	C32H52O16	M-H2O-H	673.3071	0.8
673.4810	HMDB0056293	DG(18:2n6/:5n3)	C42H68O5	M+Na-2H	673.4813	-0.5
	HMDB0007858	PA(16/18:1(11Z))	C37H71O8P	M-H	673.4814	-0.6
	HMDB0114899	PA(18:1(11Z)/16)	C37H71O8P	M-H	673.4814	-0.6
	HMDB0114924	PA(18:1(9Z)/16)	C37H71O8P	M-H	673.4814	-0.6
	HMDB0115062	PA(/14:1(9Z))	C37H71O8P	M-H	673.4814	-0.6
	HMDB0115091	PA(:1(11Z)/14)	C37H71O8P	M-H	673.4814	-0.6
	HMDB0007859	PA(16/18:1(9Z))	C37H71O8P	M-H	673.4814	-0.6
	HMDB0031130	9-Octadecenoic acid 1-[[[(1-oxohexadecyl)oxy]methyl]-2-(phosphonoxy)ethyl ester	C37H71O8P	M-H	673.4814	-0.6
	HMDB0114877	PA(18/16:1(9Z))	C37H71O8P	M-H	673.4814	-0.6
674.5111	HMDB0008851	PE(14/P-18)	C37H74NO7P	M-H	674.5130	-2.8
	HMDB0011368	PE(P-18/14)	C37H74NO7P	M-H	674.5130	-2.8
	HMDB0011158	PE(P-16/16)	C37H74NO7P	M-H	674.5130	-2.8
	HMDB0008949	PE(16/P-16)	C37H74NO7P	M-H	674.5130	-2.8
675.1639	HMDB0129135	3-(3,4-dihydroxyphenyl)-11,19-bis(4-hydroxyphenyl)-4,12,-trioxaheptacyclo[16.6.1.1.1,?1?,??heptacos-1(25),5,7,9(27),13,15,17(26),21,23-nonaene-7,15,23-triol	C42H30O10	M-H2O-H	675.1655	-2.4
675.3750	HMDB0182483	3,4,5-trihydroxy-6-[(6-methyl-2-{2,6,6,11,15-pentamethyl-5-oxotetracyclo[8.7.,heptadec-1()-en-14-yl]hept-5-enoyl}oxy]oxane-2-carboxylic acid	C36H54O9	M+FA-H	675.3750	0.0
	HMDB0182490	3,4,5-trihydroxy-6-[(6-methyl-2-[(2S,11S,15S)-2,6,6,11,15-pentamethyl-5-oxotetracyclo[8.7.,heptadec-1()-en-14-yl]hept-5-enoyl}oxy]oxane-2-carboxylic acid	C36H54O9	M+FA-H	675.3750	0.0
	HMDB0034503	2,3,23-Triacetylsericic acid	C36H54O9	M+FA-H	675.3750	0.0
	HMDB0035725	Ganoderic acid Mc	C36H54O9	M+FA-H	675.3750	0.0
	HMDB0035336	Ganoderic acid Mb	C36H54O9	M+FA-H	675.3750	0.0
	HMDB0097790	TG(a-13/a-17/)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
	HMDB0099258	TG(14/i-16)	C43H82O6	M-H2O-H	675.5928	-1.3
	HMDB0099319	TG(14/14/i-12)	C43H82O6	M-H2O-H	675.5928	-1.3
	HMDB0099320	TG(i-14/i-14/12)	C43H82O6	M-H2O-H	675.5928	-1.3
	HMDB0099323	TG(i-14/i-14/i-12)	C43H82O6	M-H2O-H	675.5928	-1.3
	HMDB0099321	TG(14/i-12/i-14)	C43H82O6	M-H2O-H	675.5928	-1.3
	HMDB0099322	TG(i-14/i-12/14)	C43H82O6	M-H2O-H	675.5928	-1.3
	HMDB0099324	TG(i-14/12/14)	C43H82O6	M-H2O-H	675.5928	-1.3
	HMDB0099326	TG(14/12/i-14)	C43H82O6	M-H2O-H	675.5928	-1.3
	HMDB0099325	TG(14/14/12)	C43H82O6	M-H2O-H	675.5928	-1.3
	HMDB0099435	TG(14/a-13/a-13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
	HMDB0099436	TG(i-14/a-13/a-13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
	HMDB0099439	TG(i-14/a-13/13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
	HMDB0099437	TG(i-14/a-13/i-13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
	HMDB0099438	TG(14/a-13/13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
	HMDB0099440	TG(14/a-13/i-13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3

HMDB0099443	TG(i-14/i-13/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099257	TG(14/16)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099256	TG(i-14/16)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0097792	TG(a-13/17)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0097795	TG(i-13/17/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0097794	TG(i-13/i-17/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0097793	TG(a-13/i-17)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0097796	TG(13/17/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0098215	TG(a-13/19/8)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0098214	TG(13/i-19/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0098217	TG(i-13/i-19/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0098218	TG(i-13/19/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0098219	TG(13/19/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0098216	TG(a-13/i-19/8)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099205	TG(i-14/8/i-18)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099207	TG(14/8/18)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099206	TG(i-14/8/18)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099208	TG(14/8/i-18)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099255	TG(i-14/i-16)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099442	TG(i-14/13/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099441	TG(14/i-13/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071836	TG(8/i-22)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0100145	TG(14/i-18/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0100146	TG(i-14/i-18/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0100147	TG(i-14/18/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0100148	TG(14/18/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0100927	TG(a-15/8/17)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0100926	TG(a-15/8/a-17)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0100928	TG(a-15/8/i-17)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0100932	TG(15/8/17)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0100931	TG(i-15/8/17)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0100929	TG(i-15/8/i-17)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0100930	TG(i-15/8/a-17)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0100934	TG(15/8/a-17)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0100933	TG(15/8/i-17)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101001	TG(a-15/a-15/)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101002	TG(a-15/15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072693	TG(12/i-18)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099864	TG(i-14/16/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099445	TG(14/i-13/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099446	TG(i-14/i-13/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099444	TG(14/i-13/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099447	TG(i-14/13/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099451	TG(14/13/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099448	TG(i-14/i-13/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099450	TG(14/13/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099449	TG(i-14/13/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099452	TG(14/13/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099595	TG(14/i-14/12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099596	TG(i-14/14/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099597	TG(14/i-14/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099598	TG(i-14/14/12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099862	TG(14/i-16/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099863	TG(i-14/i-16/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0099865	TG(14/16/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101004	TG(i-15/i-15/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0097789	TG(i-13/a-17/)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096699	TG(13//a-17)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096810	TG(13/12/a-15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096809	TG(13/12/i-15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096808	TG(13/12/15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096963	TG(i-13/a-13/i-14)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096967	TG(13/a-13/i-14)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096966	TG(a-13/a-13/14)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096965	TG(i-13/a-13/14)[rac]	C43H82O6	M-H20-H	675.5928	-1.3

HMDB0096964	TG(13/a-13/14)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096969	TG(13/i-13/14)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096971	TG(a-13/13/i-14)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096968	TG(a-13/a-13/i-14)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096970	TG(a-13/13/14)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096972	TG(a-13/i-13/i-14)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096974	TG(i-13/13/i-14)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096973	TG(a-13/i-13/14)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096975	TG(13/i-13/i-14)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096806	TG(i-13/i-12/i-15)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096807	TG(i-13/12/15)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096698	TG(13/i-17)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096696	TG(i-13//17)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096697	TG(13//17)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096793	TG(a-13/12/a-15)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096794	TG(13/i-12/15)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096795	TG(a-13/12/15)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096799	TG(i-13/12/i-15)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096798	TG(a-13/i-12/15)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096796	TG(a-13/12/i-15)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096797	TG(a-13/i-12/i-15)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096801	TG(13/i-12/a-15)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096800	TG(i-13/i-12/a-15)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096802	TG(a-13/i-12/a-15)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096803	TG(13/i-12/i-15)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096804	TG(i-13/i-12/15)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096805	TG(i-13/12/a-15)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096979	TG(13/13/14)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096977	TG(i-13/i-13/i-14)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097365	TG(a-13/a-15/12)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097366	TG(13/a-15/i-12)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097367	TG(a-13/a-15/i-12)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097371	TG(a-13/i-15/i-12)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097368	TG(13/i-15/12)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097369	TG(a-13/15/12)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097370	TG(a-13/15/i-12)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097374	TG(13/i-15/i-12)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097375	TG(i-13/i-15/12)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097372	TG(a-13/i-15/12)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097373	TG(i-13/15/i-12)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097379	TG(13/15/i-12)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097378	TG(13/15/12)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097376	TG(i-13/i-15/i-12)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097377	TG(i-13/15/12)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097788	TG(13/a-17/)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097364	TG(i-13/a-15/12)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097363	TG(13/a-15/12)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096978	TG(i-13/13/14)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096976	TG(i-13/i-13/14)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0096980	TG(13/13/i-14)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097195	TG(a-13/14/i-13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097194	TG(a-13/14/13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097196	TG(a-13/i-14/i-13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097199	TG(13/i-14/a-13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097197	TG(a-13/i-14/13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097198	TG(i-13/i-14/a-13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097201	TG(i-13/i-14/13)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097203	TG(i-13/14/13)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097200	TG(13/i-14/i-13)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097202	TG(i-13/14/a-13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097204	TG(13/14/i-13)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097205	TG(13/14/a-13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097362	TG(i-13/a-15/i-12)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0097791	TG(13/i-17/)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0101005	TG(i-15//a-15)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3

HMDB0103896	TG(16/i-14/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105302	TG(17//13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105299	TG(i-17//i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105304	TG(17//a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105303	TG(17//i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105563	TG(17/a-13/)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105566	TG(17/i-13/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105565	TG(a-17/a-13/)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105564	TG(i-17/a-13/)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105568	TG(a-17/i-13/)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105570	TG(i-17/13/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105569	TG(i-17/i-13/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105567	TG(a-17/13/)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105571	TG(17/13/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0106006	TG(a-17/a-15/8)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0106005	TG(i-17/a-15/8)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0106004	TG(17/a-15/8)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105300	TG(i-17//a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105301	TG(i-17//13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103898	TG(i-16/14/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103899	TG(16/14/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0104186	TG(i-16/16/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0104185	TG(16/i-16/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105222	TG(a-17/8/15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105221	TG(a-17/8/a-15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105225	TG(i-17/8/a-15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105223	TG(a-17/8/i-15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105224	TG(i-17/8/i-15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105226	TG(i-17/8/15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105228	TG(17/8/i-15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105229	TG(17/8/a-15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105227	TG(17/8/15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105297	TG(a-17//13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105296	TG(a-17//a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0105298	TG(a-17//i-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0106009	TG(a-17/i-15/8)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0106008	TG(a-17/15/8)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0108229	TG(18/14/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0108228	TG(i-18/14/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0109544	TG(i-19/8/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0109546	TG(19/8/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0109545	TG(i-19/8/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0109543	TG(i-19/8/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0109547	TG(19/8/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0109548	TG(19/8/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0109777	TG(19/i-13/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0109775	TG(19/a-13/8)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0109776	TG(i-19/a-13/8)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0109778	TG(i-19/i-13/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0109779	TG(i-19/13/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0109780	TG(19/13/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0108227	TG(i-18/i-14/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0108226	TG(18/i-14/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0106010	TG(i-17/i-15/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0106007	TG(17/i-15/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0106011	TG(i-17/15/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0106012	TG(17/15/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0107822	TG(18/8/14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0107820	TG(i-18/8/i-14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0107821	TG(i-18/8/14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0107823	TG(18/8/i-14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0107870	TG(i-18//i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0107873	TG(18//i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0107871	TG(i-18//12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0107872	TG(18//12)	C43H82O6	M-H20-H	675.5928	-1.3

675.5919

HMDB0107930	TG(18/i-12/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0107933	TG(18/12/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0107931	TG(i-18/i-12/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0107932	TG(i-18/12/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103897	TG(i-16/i-14/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101003	TG(a-15//i-15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101105	TG(15/12/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101102	TG(i-15/12/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101104	TG(15/12/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101103	TG(15/12/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101263	TG(15/a-13/12)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101262	TG(i-15/a-13/i-12)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101264	TG(i-15/a-13/12)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101266	TG(15/a-13/i-12)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101265	TG(a-15/a-13/12)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101269	TG(a-15/13/12)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101267	TG(a-15/a-13/i-12)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101270	TG(a-15/13/i-12)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101268	TG(15/i-13/12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101273	TG(i-15/13/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101272	TG(a-15/i-13/12)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101271	TG(a-15/i-13/i-12)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101101	TG(i-15/i-12/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101100	TG(i-15/12/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101008	TG(15//i-15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101007	TG(15/15/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101009	TG(15//a-15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101006	TG(i-15//15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101090	TG(a-15/12/13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101089	TG(15/i-12/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101088	TG(a-15/12/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101092	TG(a-15/i-12/i-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101093	TG(a-15/i-12/13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101094	TG(i-15/12/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101091	TG(a-15/12/i-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101097	TG(a-15/i-12/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101096	TG(15/i-12/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101095	TG(i-15/i-12/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101098	TG(15/i-12/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101099	TG(i-15/i-12/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101274	TG(15/i-13/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101276	TG(i-15/i-13/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0102100	TG(15/17/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103497	TG(i-16/8/16)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103496	TG(i-16/i-16/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103498	TG(16/16/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103499	TG(16/8/i-16)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103548	TG(16//14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103549	TG(16//i-14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103547	TG(i-16//14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103546	TG(i-16//i-14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103600	TG(16/i-12/12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103601	TG(i-16/12/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103604	TG(i-16/i-12/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103602	TG(16/i-12/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103603	TG(i-16/i-12/12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103607	TG(16/12/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103606	TG(16/12/12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0102097	TG(a-15/i-17/8)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0102098	TG(i-15/i-17/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101275	TG(i-15/i-13/12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101278	TG(15/13/12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101277	TG(i-15/13/12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101279	TG(15/13/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101697	TG(i-15/a-15/)[rac]	C43H82O6	M-H20-H	675.5928	-1.3

HMDB0101696	TG(15/a-15/)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101698	TG(15/i-15/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101699	TG(a-15/15/)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101700	TG(a-15/i-15/)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0101701	TG(i-15/15/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0102092	TG(15/a-17/8)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0102093	TG(i-15/a-17/8)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0102094	TG(a-15/a-17/8)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0102095	TG(15/i-17/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0102096	TG(a-15/17/8)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0102099	TG(i-15/17/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0103605	TG(i-16/12/12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071650	TG(/17/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071964	TG(8/17/i-15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071974	TG(8/15/17)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071981	TG(8/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072000	TG(i-18/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072046	TG(8/i-19/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072067	TG(8/i-22/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072070	TG(8/i-18/i-14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072068	TG(8/a-17/15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072073	TG(/22/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072086	TG(/i-15/15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072097	TG(8/17/15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072100	TG(/i-17/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071922	TG(8/i-17/a-15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071914	TG(8/16/16)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071668	TG(/a-17/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071702	TG(8/12/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071730	TG(8/i-15/17)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071739	TG(/a-15/i-15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071761	TG(/a-17/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071780	TG(8/a-15/17)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071799	TG(/i-)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071803	TG(/i-15/a-15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071818	TG(/14/i-16)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071840	TG(/i-16/i-14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071896	TG(8/13/19)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071906	TG(/13/17)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072106	TG(/15/i-15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072111	TG(8/14/18)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072110	TG(8/19/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072393	TG(/i-15/i-15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072403	TG(8/i-12/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072412	TG(8/a-15/a-17)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072447	TG(/13/a-17)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072444	TG(/16/i-14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072465	TG(8/i-13/i-19)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072528	TG(/a-15/15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072571	TG(8/18/14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072589	TG(8/i-16/i-16)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072630	TG(/8/22)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072657	TG(/i-18/12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072665	TG(8/i-15/i-17)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072384	TG(/a-13/i-17)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072378	TG(8/i-17/i-15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072120	TG(8/8/i-24)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072187	TG(/i-14/i-16)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072196	TG(/i-14/16)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072200	TG(/i-22/8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072219	TG(/a-17/a-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072225	TG(8/i-/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072257	TG(8/a-17/i-15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072275	TG(8/12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072304	TG(/17/a-13)	C43H82O6	M-H20-H	675.5928	-1.3

HMDB0072307	TG(/a-13/a-17)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0072311	TG(8/i-18/14)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0072347	TG(8/18/i-14)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0072681	TG(8/13/i-19)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0063111	TG(i-/8/12)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0063139	TG(/i-12/8)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0063151	TG(/12/8)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0063745	TG(8/i-12)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0064061	TG(8/12)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0064323	TG(i-/12/8)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0064417	TG(/)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0064431	TG(i-/8/i-12)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0067667	TG(i-22/8)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0067895	TG(22/8/)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0067980	TG(22/8)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0068389	TG(i-22/8/)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0063052	TG(i-/i-12/8)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0062996	TG(i-/)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0072096	TG(/i-17/a-13)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0072323	TG(/)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0094986	TG(12/12/16)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071634	TG(/14/16)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071576	TG(/15/15)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0072613	TG(/12/18)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0095256	TG(12/14/14)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0069359	TG(i-24/8/8)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071137	TG(/i-12/i-18)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071141	TG(8/i-16/16)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071367	TG(8/a-15/i-17)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071385	TG(/i-13/i-17)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071399	TG(8/i-14/i-18)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071427	TG(/a-15/a-15)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071460	TG(8/i-/12)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071459	TG(/i-13/17)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071474	TG(/16/14)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071487	TG(/13/i-17)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071517	TG(8/a-13/19)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071587	TG(8/15/a-17)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071590	TG(8/14/i-18)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071602	TG(8/i-17/15)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071360	TG(8/a-17/a-15)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071338	TG(8/22/)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071158	TG(8/17/a-15)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071163	TG(8/i-13/19)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071175	TG(8/16/i-16)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071191	TG(/i-12/18)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071204	TG(/a-13/17)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071205	TG(8/i-12/i-)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071219	TG(8/12/i-)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071232	TG(/17/13)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071236	TG(8/19/a-13)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071287	TG(8/i-19/a-13)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071308	TG(8/i-19/13)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071319	TG(/i-13/a-17)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0071610	TG(/i-16/14)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0095110	TG(12/i-13/i-15)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0095257	TG(12/14/i-14)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0095360	TG(12/a-15/a-13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0095361	TG(i-12/a-15/a-13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0095363	TG(12/a-15/13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0095362	TG(i-12/a-15/i-13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0095364	TG(i-12/a-15/13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0095365	TG(12/a-15/i-13)[rac]	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0095366	TG(12/i-15/13)	C43H82O6	M-H2O-H	675.5928	-1.3
HMDB0095367	TG(i-12/15/i-13)	C43H82O6	M-H2O-H	675.5928	-1.3

HMDB0095368	TG(i-12/i-15/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095372	TG(i-12/15/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095371	TG(i-12/i-15/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095252	TG(12/i-14/i-14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095254	TG(i-12/i-14/i-14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095109	TG(12/i-13/a-15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095108	TG(i-12/i-13/a-15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095114	TG(i-12/13/15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095115	TG(12/13/15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095113	TG(i-12/i-13/i-15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095112	TG(i-12/13/a-15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095117	TG(12/13/a-15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095116	TG(12/13/i-15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095250	TG(12/i-14/14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095251	TG(i-12/14/i-14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095255	TG(i-12/14/14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095253	TG(i-12/i-14/14)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095369	TG(12/i-15/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095370	TG(12/i-15/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095375	TG(12/15/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096038	TG(i-12/i-8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096040	TG(12//8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096619	TG(i-13/8/19)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096618	TG(i-13/8/i-19)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096617	TG(a-13/8/i-19)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096616	TG(a-13/8/19)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096620	TG(13/8/19)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096621	TG(13/8/i-19)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096691	TG(a-13//a-17)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096692	TG(a-13//17)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096693	TG(a-13//i-17)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096694	TG(i-13/i-17)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096037	TG(12/i-8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096039	TG(i-12//8)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095376	TG(12/15/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095374	TG(i-12/15/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095373	TG(i-12/i-15/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095377	TG(12/15/a-13)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095524	TG(12/i-16/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095525	TG(i-12/i-16/12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095526	TG(i-12/16/12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095527	TG(12/16/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095813	TG(12/18/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095810	TG(12/i-18/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095811	TG(i-12/i-18/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095812	TG(i-12/18/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0096695	TG(i-13//a-17)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0095111	TG(i-12/i-13/15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072833	TG(8/19/13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0094864	TG(12/8/i-)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0094863	TG(12/8/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0094861	TG(i-12/8/i-)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0094862	TG(i-12/8/)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072759	TG(/i-17/i-13)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0071837	TG(/18/12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072768	TG(/8/i-22)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072790	TG(8/i-14/18)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072801	TG(8/i-15/a-17)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072812	TG(8/15/i-17)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072828	TG(8/a-13/i-19)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0094983	TG(i-12/i-12/16)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072724	TG(/15/a-15)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072702	TG(/18/i-12)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0072838	TG(8//22)	C43H82O6	M-H20-H	675.5928	-1.3
HMDB0094913	TG(i-12//i-18)	C43H82O6	M-H20-H	675.5928	-1.3

	HMDB0094914	TG(i-12//18)	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0094916	TG(12//i-18)	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0095104	TG(i-12/a-13/15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0095106	TG(12/i-13/15)	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0095105	TG(12/a-13/i-15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0095107	TG(i-12/13/i-15)	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0095100	TG(12/a-13/a-15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0095103	TG(12/a-13/15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0095101	TG(i-12/a-13/a-15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0095102	TG(i-12/a-13/i-15)[rac]	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0094984	TG(i-12/i-12/i-16)	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0094987	TG(12/12/i-16)	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0094980	TG(12/i-12/16)	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0094982	TG(12/i-12/i-16)	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0094915	TG(12//18)	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0094981	TG(i-12/12/i-16)	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0094985	TG(i-12/12/16)	C43H82O6	M-H20-H	675.5928	-1.3
	HMDB0056216	DG(:1n9/:1n9)	C43H80O5	M-H	675.5933	-2.1
	HMDB0007624	DG(22:1(13Z)/18:1(9Z))	C43H80O5	M-H	675.5933	-2.1
	HMDB0007623	DG(22:1(13Z)/18:1(11Z))	C43H80O5	M-H	675.5933	-2.1
	HMDB0007596	DG(22/18:2(9Z,12Z))	C43H80O5	M-H	675.5933	-2.1
	HMDB0007426	DG(:2(11Z,14Z)/)	C43H80O5	M-H	675.5933	-2.1
	HMDB0007398	DG(:1(11Z)/:1(11Z))	C43H80O5	M-H	675.5933	-2.1
	HMDB0007370	DG(/:2(11Z,14Z))	C43H80O5	M-H	675.5933	-2.1
	HMDB0007260	DG(18:2(9Z,12Z)/22)	C43H80O5	M-H	675.5933	-2.1
	HMDB0007232	DG(18:1(9Z)/22:1(13Z))	C43H80O5	M-H	675.5933	-2.1
	HMDB0007203	DG(18:1(11Z)/22:1(13Z))	C43H80O5	M-H	675.5933	-2.1
	HMDB0007175	DG(18/22:2(13Z,16Z))	C43H80O5	M-H	675.5933	-2.1
	HMDB0007651	DG(22:2(13Z,16Z)/18)	C43H80O5	M-H	675.5933	-2.1
	HMDB0007824	DG(24:1(15Z)/16:1(9Z))	C43H80O5	M-H	675.5933	-2.1
	HMDB0056200	DG(18:1n9/22:1n9)	C43H80O5	M-H	675.5933	-2.1
	HMDB0056075	DG(/:2n6)	C43H80O5	M-H	675.5933	-2.1
	HMDB0007152	DG(16:1(9Z)/24:1(15Z))	C43H80O5	M-H	675.5933	-2.1
	HMDB0056181	DG(18:1n7/22:1n9)	C43H80O5	M-H	675.5933	-2.1
	HMDB0056162	DG(16:1n7/24:1n9)	C43H80O5	M-H	675.5933	-2.1
	HMDB0056053	DG(18/22:2n6)	C43H80O5	M-H	675.5933	-2.1
676.1816	HMDB0138785	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{4-(3,5-dihydroxyphenyl)-12-hydroxy-12-methyl-3,-dioxatricyclo[7.5,tetradeca-1(9),2(6),4,7-tetraen-13-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H33N3O11S	M+FA-H	676.1818	-0.3
	HMDB0138784	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{{4-(3,5-dihydroxyphenyl)-13-hydroxy-12-methyl-3,-dioxatricyclo[7.5,tetradeca-1(9),2(6),4,7-tetraen-12-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H33N3O11S	M+FA-H	676.1818	-0.3
676.4355	HMDB0113003	PE-NMe(14:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C38H66NO8P	M-H20-H	676.4342	1.9
	HMDB0113251	PE-NMe(18:4(6Z,9Z,12Z,15Z)/14:1(9Z))	C38H66NO8P	M-H20-H	676.4342	1.9
677.0736	HMDB0147503	[3-(2,4-dihydroxyphenyl)-9,17-dihydroxy-7-(6-hydroxy-1-benzofuran-2-yl)-13-methyl-4,14-dioxapentacyclo[11.7.1,??癩henicosa-2,5,7,9,11,15(),16,18-octaen-21-yl]oxidanesulfonic acid	C34H24O12S	M+Na-2H	677.0735	0.1
	HMDB0031994	Licorice glycoside D1	C35H36O15	M-H20-H	677.1870	-1.1
	HMDB0126439	6-[2-(6-carboxy-5-{3-[3-(2,4-dihydroxyphenyl)propanoyl]-2,6-dihydroxyphenyl}-3-methylcyclohex-3-en-1-yl)-5-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C35H36O15	M-H20-H	677.1870	-1.1
	HMDB0126435	6-[4-(3-{3-[6-carboxy-5-(2,4-dihydroxyphenyl)-3-methylcyclohex-2-en-1-yl]-2,4-dihydroxyphenyl}-3-oxopropyl)-3-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C35H36O15	M-H20-H	677.1870	-1.1

677.1863	HMDB0126438	6-[4-(6-carboxy-5-{3-[3-(2,4-dihydroxyphenyl)propanoyl]-2,6-dihydroxyphenyl}-3-methylcyclohex-3-en-1-yl)-3-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C35H36O15	M-H2O-H	677.1870	-1.1
	HMDB0126436	6-[2-(3-{3-[6-carboxy-5-(2,4-dihydroxyphenyl)-3-methylcyclohex-2-en-1-yl]-2,4-dihydroxyphenyl}-3-oxopropyl)-5-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C35H36O15	M-H2O-H	677.1870	-1.1
	HMDB0126437	6-{2-[6-carboxy-5-(2,4-dihydroxyphenyl)-3-methylcyclohex-2-en-1-yl]-4-[3-(2,4-dihydroxyphenyl)propanoyl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C35H36O15	M-H2O-H	677.1870	-1.1
	HMDB0126434	6-{2-[6-carboxy-5-(2,4-dihydroxyphenyl)-3-methylcyclohex-2-en-1-yl]-6-[3-(2,4-dihydroxyphenyl)propanoyl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C35H36O15	M-H2O-H	677.1870	-1.1
	HMDB0126440	6-[6-(2,4-dihydroxyphenyl)-2-{3-[3-(2,4-dihydroxyphenyl)propanoyl]-2,6-dihydroxyphenyl}-4-methylcyclohex-3-ene-1-carboxyloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C35H36O15	M-H2O-H	677.1870	-1.1
	HMDB0031988	Licorice glycoside B	C35H36O15	M-H2O-H	677.1870	-1.1
677.6252	HMDB0005193	CE(:1(11Z))	C47H82O2	M-H	677.6242	1.5
	HMDB0172585	2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.,heptadec-7-en-5-yl (11E)-icos-11-enoate	C47H82O2	M-H	677.6242	1.5
	HMDB0030508	Cyclolaudenyl palmitate	C47H82O2	M-H	677.6242	1.5
678.3990	HMDB0015616	Telaprevir	C36H53N7O6	M-H	678.3985	0.8
679.2435	HMDB0161051	3-[-(2-carboxyethyl)-15-(1-hydroxyethyl)-5,9,14,19-tetramethyl--[1-(sulfooxy)ethyl]-21,22,23,24-tetraazapentacyclo[16.2.1.1,?1?.1,tetracos-1(21),2,4,6,8,,12,14,16(22),17,19-undecaen-4-yl]propanoic acid	C34H38N4O9S	M-H	679.2432	0.4
	HMDB0161050	3-[-(2-carboxyethyl)--(1-hydroxyethyl)-5,9,14,19-tetramethyl-15-[1-(sulfooxy)ethyl]-21,22,23,24-tetraazapentacyclo[16.2.1.1,?1?.1,tetracos-1(21),2,4,6,8,,12,14,16(22),17,19-undecaen-4-yl]propanoic acid	C34H38N4O9S	M-H	679.2432	0.4
	HMDB0035944	Cyclopasifloside I	C37H62O12	M-H2O-H	679.4057	-0.5
	HMDB0164867	4,6,14-trihydroxy-15-[5-hydroxy-6-methyl-5-({3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}methyl)heptan-2-yl]-7,12,16-trimethylpentacyclo[9.7,,,octadecane-7-carboxylic acid	C37H62O12	M-H2O-H	679.4057	-0.5
	HMDB0035946	Cyclopasifloside IV	C37H62O12	M-H2O-H	679.4057	-0.5
	HMDB0036365	trans-delta-Viniferin 3'''-glucoside	C37H62O12	M-H2O-H	679.4057	-0.5
	HMDB0165736	6-{[6a-(hydroxymethyl)-1,2,4a,6b,9,9,12a-heptamethyl--oxo-docosahydricen-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
	HMDB0165729	3,4,5-trihydroxy-6-[(2-hydroxy-1,4a,6a,6b,9,9,12a-heptamethyl--oxo-docosahydricen-2-yl)methoxy]oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
	HMDB0165739	6-{[6b-(hydroxymethyl)-1,2,4a,6a,9,9,12a-heptamethyl--oxo-docosahydricen-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
	HMDB0165730	3,4,5-trihydroxy-6-{[2-(hydroxymethyl)-1,4a,6a,6b,9,9,12a-heptamethyl--oxo-docosahydricen-2-yl]oxy}oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
	HMDB0165732	3,4,5-trihydroxy-6-[(2-hydroxy-1,2,6a,6b,9,9,12a-heptamethyl--oxo-docosahydricen-4a-yl)methoxy]oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
	HMDB0165733	6-{[4a-(hydroxymethyl)-1,2,6a,6b,9,9,12a-heptamethyl--oxo-docosahydricen-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3

HMDB0165735	3,4,5-trihydroxy-6-[(2-hydroxy-1,2,4a,6b,9,9,12a-heptamethyl--oxo-docosahdropicen-6a-yl)methoxy]oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0165738	3,4,5-trihydroxy-6-[(11-hydroxy-4,4,6b,8a,11,12,14b-heptamethyl-3-oxo-docosahdropicen-6a-yl)methoxy]oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0177829	3,4,5-trihydroxy-6-{[8-hydroxy-8a-(hydroxymethyl)-4,4,6a,6b,11,11,14b-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahdropicen-3-yl]oxy} oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0165741	3,4,5-trihydroxy-6-[(11-hydroxy-4,4a,6b,8a,11,12,14b-heptamethyl-3-oxo-docosahdropicen-4-yl)methoxy]oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0165744	3,4,5-trihydroxy-6-[(2-hydroxy-1,2,4a,6a,6b,9,9-heptamethyl--oxo-docosahdropicen-12a-yl)methoxy]oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0165745	6-{[12a-(hydroxymethyl)-1,2,4a,6a,6b,9,9-heptamethyl--oxo-docosahdropicen-2-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0177830	3,4,5-trihydroxy-6-{[-hydroxy-4a-(hydroxymethyl)-2,2,6a,6b,9,9,12a-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahdropicen-5-yl]oxy} oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0177831	6-[(5,-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahdropicen-4a-yl)methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0177856	3,4,5-trihydroxy-6-{[-hydroxy-9-(hydroxymethyl)-2,2,4a,6a,6b,9,12a-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahdropicen-4-yl]oxy} oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0177855	6-[(3,9-dihydroxy-4,6a,6b,8a,11,11,14b-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahdropicen-4-yl)methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0177892	6-[(8,-dihydroxy-4,4,6a,6b,8a,11,12,14b-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahdropicen-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0177893	6-[(3,-dihydroxy-1,2,4a,6a,6b,9,9,12a-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahdropicen-5-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0177894	6-[(5,-dihydroxy-1,2,4a,6a,6b,9,9,12a-octamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahdropicen-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0176181	3,4,5-trihydroxy-6-{[-hydroxy-4a-(hydroxymethyl)-2,2,6a,6b,9,9,12a-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahdropicen-4-yl]oxy} oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0176180	6-[(4,-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahdropicen-4a-yl)methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0176179	3,4,5-trihydroxy-6-{[9-hydroxy-8a-(hydroxymethyl)-4,4,6a,6b,11,11,14b-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahdropicen-3-yl]oxy} oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0165748	3,4,5-trihydroxy-6-{[1-(hydroxymethyl)-2,4a,6a,6b,9,9,12a-heptamethyl--oxo-docosahdropicen-2-yl]oxy} oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0165747	3,4,5-trihydroxy-6-[(2-hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl--oxo-docosahdropicen-1-yl)methoxy]oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3

HMDB0165750	3,4,5-trihydroxy-6-[(2-hydroxy-1,2,4a,6a,6b,9,9,12a-octamethyl--oxo-docosahdropicen-1-yl)oxy]oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0165753	3,4,5-trihydroxy-6-[(11-hydroxy-1,2,4a,6a,6b,9,9,12a-octamethyl--oxo-docosahdropicen-2-yl)oxy]oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0165751	3,4,5-trihydroxy-6-[(1-hydroxy-1,2,4a,6a,6b,9,9,12a-octamethyl--oxo-docosahdropicen-2-yl)oxy]oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0165752	3,4,5-trihydroxy-6-[(11-hydroxy-4,4,6a,6b,8a,11,12,14b-octamethyl-3-oxo-docosahdropicen-2-yl)oxy]oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0175905	3,4,5-trihydroxy-6-[(3-hydroxy-4,4,6a,6b,8a,11,11,14b-octamethyl-14-oxo-docosahdropicen-12b-yl)oxy]oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0175906	6-[(12b-hydroxy-4,4,6a,6b,8a,11,11,14b-octamethyl-14-oxo-docosahdropicen-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0183061	6-{[14-(3,4-dihydroxy-6-methylhept-5-en-2-yl)-1,6,6,11,15-pentamethyltetracyclo[8.7.,heptadec-7-en-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0035917	Momordicoside L	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0035966	Momordicin II	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0029606	Maslinic acid 3-O-b-D-glucoside	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0039329	Soyasapogenol B 3-O-b-D-glucuronide	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0038452	28-Glucosylpomolate	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0029621	Lucyoside Q	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0165742	3,4,5-trihydroxy-6-{[9-(hydroxymethyl)-1,2,4a,6a,6b,9,12a-heptamethyl--oxo-docosahdropicen-2-yl]oxy} oxane-2-carboxylic acid	C36H58O9	M+FA-H	679.4063	-1.3
HMDB0186682	{[(6E,E,12E,14E,16E,18E,E,22E,24E,26E)-2,6,,14,19,23,27,31-octamethyldotriaconta-2,6,,12,14,16,18,,22,24,26,-dodecaen-1-yl]oxy} sulfonic acid	C40H58O4S	M+FA-H	679.4038	2.4
HMDB0186680	{[(2Z,6E,8E,E,12E,14E,16E,18E,E,22E)-6,,15,19,23,27-hexamethyl-2-(4-methylpent-3-en-1-yl)octacosa-2,6,8,,12,14,16,18,,22,26-undecaen-1-yl]oxy} sulfonic acid	C40H58O4S	M+FA-H	679.4038	2.4
HMDB0186684	{[(2E,6E,E,12E,14E,16E,18E,E,22E,24E,26E)-2,6,,14,19,23,27,31-octamethyldotriaconta-2,6,,12,14,16,18,,22,24,26,-dodecaen-1-yl]oxy} sulfonic acid	C40H58O4S	M+FA-H	679.4038	2.4
HMDB0186686	{[(6E,8E,E,12E,14E,16E,18E,E,22E,26E)-2,6,,14,19,23,27,31-octamethyldotriaconta-2,6,8,,12,14,16,18,,22,26,-dodecaen-4-yl]oxy} sulfonic acid	C40H58O4S	M+FA-H	679.4038	2.4
HMDB0186688	{[(6E,E,12E,14E,16E,18E,E,22E,24E,26E)-2,6,,14,19,23,27,31-octamethyldotriaconta-2,6,,12,14,16,18,,22,24,26,-dodecaen-8-yl]oxy} sulfonic acid	C40H58O4S	M+FA-H	679.4038	2.4
HMDB0186690	{[(6E,E,12E,14E,16E,18E,E,22E,24E,26E)-2,6,,14,19,23,27,31-octamethyldotriaconta-2,6,,12,14,16,18,,22,24,26,-dodecaen-4-yl]oxy} sulfonic acid	C40H58O4S	M+FA-H	679.4038	2.4
HMDB0186676	{[(2Z,4E,6E,8E,E,12E,14E,16E,18E)-2-[(3E)-4,8-dimethylnona-3,7-dien-1-yl]-6,11,15,19,23-pentamethyltetracosa-2,4,6,8,,12,14,16,18,22-decaen-1-yl]oxy} sulfonic acid	C40H58O4S	M+FA-H	679.4038	2.4
HMDB0186678	{[(6E,E,12E,14E,16E,18E,E,22E,24E,26E)-2,6,,14,19,23,27,31-octamethyldotriaconta-2,6,,12,14,16,18,,22,24,26,-dodecaen-5-yl]oxy} sulfonic acid	C40H58O4S	M+FA-H	679.4038	2.4

	HMDB0186674	{[(6E,E,12E,14E,16E,18E,E,22E,24E,26E)-2,6,,14,19,23,27,31-octamethyldotriaconta-2,6,,12,14,16,18,,22,24,26,-dodecaen-9-yl]oxy} sulfonic acid	C40H58O4S	M+FA-H	679.4038	2.4
	HMDB0186672	{[(2Z,4E,6E,8E,E,12E,14E)-7,11,15,19-tetramethyl-2-[(1E,3E,7E)-4,8,12-trimethyltrideca-1,3,7,11-tetraen-1-yl]icosa-2,4,6,8,,12,14,18-octaen-1-yl]oxy} sulfonic acid	C40H58O4S	M+FA-H	679.4038	2.4
	HMDB0186668	{[(2Z,4E,6E,8E,E,12E,14E,18E)-2-[(1E,3E)-4,8-dimethylnona-1,3,7-trien-1-yl]-6,11,15,19,23-pentamethyltetracosa-2,4,6,8,,12,14,18,22-nonaen-1-yl]oxy} sulfonic acid	C40H58O4S	M+FA-H	679.4038	2.4
	HMDB0186664	{[(2Z,4E,6E,8E,E,12E,14E,16E,18E,22E)-6,,15,19,23,27-hexamethyl-2-(4-methylpent-3-en-1-yl)octacosa-2,4,6,8,,12,14,16,18,22,26-undecaen-1-yl]oxy} sulfonic acid	C40H58O4S	M+FA-H	679.4038	2.4
	HMDB0186666	{[(6E,8E,E,12E,14E,16E,18E,E,22E,26E)-2,6,,14,19,23,27,31-octamethyldotriaconta-2,6,8,,12,14,16,18,,22,26,-dodecaen-5-yl]oxy} sulfonic acid	C40H58O4S	M+FA-H	679.4038	2.4
	HMDB0186662	{[(6E,8E,E,12E,14E,16E,18E,E,22E,26E)-2,6,,14,19,23,27,31-octamethyldotriaconta-2,6,8,,12,14,16,18,,22,26,-dodecaen-1-yl]oxy} sulfonic acid	C40H58O4S	M+FA-H	679.4038	2.4
	HMDB0186670	{[(2Z,4E,6E,8E,E,14E)-7,11,15,19-tetramethyl-2-[(1E,3E,5E,7E)-4,8,12-trimethyltrideca-1,3,5,7,11-pentaen-1-yl]icosa-2,4,6,8,,14,18-heptaen-1-yl]oxy} sulfonic acid	C40H58O4S	M+FA-H	679.4038	2.4
679.5453	HMDB0030129	Plastoquinone 8	C48H72O2	M-H	679.5460	-1.0
680.1797	HMDB0155308	2-[(4-{[(5-carbamimidamido-6-{[(6-carboxy-3,4,5-trihydroxyoxan-2-yl]oxy}carbonyl]-4,5-dihydropyrazin-2-yl)methyl]amino}phenyl)formamido]pentanedioic acid	C25H29N7O13	M+FA-H	680.1805	-1.2
	HMDB0125481	2-amino-4-(1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(4-{3-[2-(2,4-dihydroxyphenyl)-2-oxoethyl]-4,6-dihydroxy-2-methoxyphenyl]-3-hydroxy-2-methylbutan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C30H39N3O13S	M-H	680.2131	1.9
	HMDB0150572	2-amino-4-(1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(4-{3-[2-(2,4-dihydroxyphenyl)propanoyl]-2,4,6-trihydroxyphenyl]-3-hydroxy-2-methylbutan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C30H39N3O13S	M-H	680.2131	1.9
	HMDB0148655	2-amino-4-(1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(4-{2,6-dihydroxy-3-[1-oxo-1-(2,4,6-trihydroxyphenyl)propan-2-yl]phenyl]-3-hydroxy-2-methylbutan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C30H39N3O13S	M-H	680.2131	1.9
	HMDB0148654	2-amino-4-(1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1-{2,6-dihydroxy-3-[1-oxo-1-(2,4,6-trihydroxyphenyl)propan-2-yl]phenyl]-3-hydroxy-3-methylbutan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C30H39N3O13S	M-H	680.2131	1.9
	HMDB0150571	2-amino-4-(1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1-{3-[2-(2,4-dihydroxyphenyl)propanoyl]-2,4,6-trihydroxyphenyl]-3-hydroxy-3-methylbutan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C30H39N3O13S	M-H	680.2131	1.9
	HMDB0129069	2-amino-4-(1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(2-{3,5-dihydroxy-4-[(1E)-3-methylbut-1-en-1-yl]phenyl]-1-(3,4-dihydroxyphenyl)-2-hydroxyethyl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H37N3O11S	M+FA-H	680.2131	1.9

680.2144	HMDB0125575	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-({1-[3,5-dihydroxy-4-(3-methylbut-2-en-1-yl)phenyl]-2-(2,4-dihydroxyphenyl)-2-hydroxyethyl}sulfanyl)ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H37N3O1 1S	M+FA-H	680.2131	1.9
	HMDB0125574	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-({2-[3,5-dihydroxy-4-(3-methylbut-2-en-1-yl)phenyl]-1-(2,4-dihydroxyphenyl)-2-hydroxyethyl}sulfanyl)ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H37N3O1 1S	M+FA-H	680.2131	1.9
	HMDB0125579	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1-{4-(E)-2-(2,4-dihydroxyphenyl)ethenyl}-2,6-dihydroxyphenyl)-3-hydroxy-3-methylbutan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H37N3O1 1S	M+FA-H	680.2131	1.9
	HMDB0140129	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-({[5,-dihydroxy-8,8-dimethyl-6-(3-methylbut-2-en-1-yl)-2-oxo-2H,8H,9H,H-pyrano[2,3-h]chromen-9-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H37N3O1 1S	M+FA-H	680.2131	1.9
	HMDB0140128	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-({[5,9-dihydroxy-8,8-dimethyl-6-(3-methylbut-2-en-1-yl)-2-oxo-2H,8H,9H,H-pyrano[2,3-h]chromen--yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H37N3O1 1S	M+FA-H	680.2131	1.9
	HMDB0140126	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(3-hydroxy-4-{5-hydroxy-8,8-dimethyl-2-oxo-2H,8H-pyrano[2,3-h]chromen-6-yl}-2-methylbutan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H37N3O1 1S	M+FA-H	680.2131	1.9
	HMDB0140125	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(3-hydroxy-1-{5-hydroxy-8,8-dimethyl-2-oxo-2H,8H-pyrano[2,3-h]chromen-6-yl}-3-methylbutan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H37N3O1 1S	M+FA-H	680.2131	1.9
	HMDB0125580	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(4-{4-(E)-2-(2,4-dihydroxyphenyl)ethenyl}-2,6-dihydroxyphenyl)-3-hydroxy-2-methylbutan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H37N3O1 1S	M+FA-H	680.2131	1.9
	HMDB0129077	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1-{4-(E)-2-(3,4-dihydroxyphenyl)ethenyl}-2,6-dihydroxyphenyl)-1-hydroxy-3-methylbutan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H37N3O1 1S	M+FA-H	680.2131	1.9
680.2144	HMDB0129070	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1-{3,5-dihydroxy-4-[(1E)-3-methylbut-1-en-1-yl]phenyl]-2-(3,4-dihydroxyphenyl)-2-hydroxyethyl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H37N3O1 1S	M+FA-H	680.2131	1.9
	HMDB0129076	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1-{4-(E)-2-(3,4-dihydroxyphenyl)ethenyl}-2,6-dihydroxyphenyl)-2-hydroxy-3-methylbutyl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H37N3O1 1S	M+FA-H	680.2131	1.9
	HMDB0156311	3,4,5-trihydroxy-6-({[4-hydroxy-2-({[hydroxy({[hydroxy(phosphonoxy)phosphoryl]oxy})phosphoryl]oxy}methyl)-5-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)oxolan-3-yl]oxy}oxane-2-carboxylic acid	C15H23N2O2 1P3	M+Na-2H	680.9753	-1.6

000.7142	HMDB0156310	3,4,5-trihydroxy-6-([4-hydroxy-5-([hydroxy([hydroxy(phosphonooxy)phosphoryl]oxy)phosphoryl]oxy)methyl]-2-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)oxolan-3-yl]oxy)oxane-2-carboxylic acid	C15H23N2O21P3	M+Na-2H	680.9753	-1.6
681.1445	HMDB0128743	3,4,5-trihydroxy-6-{4-[3-hydroxy-2-oxo-8-(3,5,7-trihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)-4-oxatricyclo[4.3.1,decan-yl]-2-methoxyphenoxy]oxane-2-carboxylic acid	C31H32O16	M+Na-2H	681.1437	1.2
	HMDB0128742	6-([3,5-dihydroxy-2-[3-hydroxy--(4-hydroxy-3-methoxyphenyl)-2-oxo-4-oxatricyclo[4.3.1,decan-8-yl]-4-oxo-3,4-dihydro-2H-1-benzopyran-7-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H32O16	M+Na-2H	681.1437	1.2
	HMDB0128741	6-([3,7-dihydroxy-2-[3-hydroxy--(4-hydroxy-3-methoxyphenyl)-2-oxo-4-oxatricyclo[4.3.1,decan-8-yl]-4-oxo-3,4-dihydro-2H-1-benzopyran-5-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H32O16	M+Na-2H	681.1437	1.2
	HMDB0001957	Pentacarboxyl porphyrinogen III	C37H40N4O10	M-H2O-H	681.2561	1.8
	HMDB0129768	6-{[2-(2,4-dihydroxyphenyl)-3-(3,7-dimethylocta-2,6-dien-1-yl)-6-[(3,3-dimethyloxiran-2-yl)methyl]-5-hydroxy-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
	HMDB0129767	6-{2-[3-(3,7-dimethylocta-2,6-dien-1-yl)-6-[(3,3-dimethyloxiran-2-yl)methyl]-5,7-dihydroxy-4-oxo-4H-chromen-2-yl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
	HMDB0129769	6-{[2-(2,4-dihydroxyphenyl)-3-(3,7-dimethylocta-2,6-dien-1-yl)-6-[(3,3-dimethyloxiran-2-yl)methyl]-7-hydroxy-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
	HMDB0129763	6-{[2-(2,4-dihydroxyphenyl)-5-hydroxy-3-(5-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
	HMDB0129766	6-{4-[3-(3,7-dimethylocta-2,6-dien-1-yl)-6-[(3,3-dimethyloxiran-2-yl)methyl]-5,7-dihydroxy-4-oxo-4H-chromen-2-yl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
	HMDB0129764	6-{[2-(2,4-dihydroxyphenyl)-7-hydroxy-3-(5-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
	HMDB0129761	6-{4-[5,7-dihydroxy-3-(5-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
	HMDB0129762	6-{2-[5,7-dihydroxy-3-(5-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
	HMDB0129759	6-{[2-(2,4-dihydroxyphenyl)-7-hydroxy-3-[(6E)-8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl]-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
	HMDB0129757	6-(2-{5,7-dihydroxy-3-[(6E)-8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl]-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl}-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
	HMDB0129770	6-[4-(5,7-dihydroxy-3-{[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]methyl}-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl]-3-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0

681.2573

HMDB0129774	6-(4-{3-[5-(3,3-dimethyloxiran-2-yl)-3-methylpent-2-en-1-yl]-5,7-dihydroxy-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl}-3-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129771	6-[2-(5,7-dihydroxy-3-{[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]methyl}-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl)-5-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129781	6-{[3-(3,7-dimethylocta-2,6-dien-1-yl)-5-hydroxy-6-(3-methylbut-2-en-1-yl)-4-oxo-2-(2,4,5-trihydroxyphenyl)-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129780	6-{2-[3-(3,7-dimethylocta-2,6-dien-1-yl)-5,7-dihydroxy-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl]-4,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129779	6-{4-[3-(3,7-dimethylocta-2,6-dien-1-yl)-5,7-dihydroxy-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl]-2,5-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129782	6-{[3-(3,7-dimethylocta-2,6-dien-1-yl)-7-hydroxy-6-(3-methylbut-2-en-1-yl)-4-oxo-2-(2,4,5-trihydroxyphenyl)-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129778	6-{5-[3-(3,7-dimethylocta-2,6-dien-1-yl)-5,7-dihydroxy-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl]-2,4-dihydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129776	6-{[2-(2,4-dihydroxyphenyl)-3-[5-(3,3-dimethyloxiran-2-yl)-3-methylpent-2-en-1-yl]-5-hydroxy-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129775	6-(2-{3-[5-(3,3-dimethyloxiran-2-yl)-3-methylpent-2-en-1-yl]-5,7-dihydroxy-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl}-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129777	6-{[2-(2,4-dihydroxyphenyl)-3-[5-(3,3-dimethyloxiran-2-yl)-3-methylpent-2-en-1-yl]-7-hydroxy-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129773	6-{[2-(2,4-dihydroxyphenyl)-7-hydroxy-3-{[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]methyl}-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129772	6-{[2-(2,4-dihydroxyphenyl)-5-hydroxy-3-{[3-methyl-3-(4-methylpent-3-en-1-yl)oxiran-2-yl]methyl}-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129758	6-{[2-(2,4-dihydroxyphenyl)-5-hydroxy-3-[(6E)-8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl]-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129756	6-(4-{5,7-dihydroxy-3-[(6E)-8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl]-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl}-3-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129738	6-{[2-(2,4-dihydroxyphenyl)-3-(3,7-dimethylocta-2,6-dien-1-yl)-5-hydroxy-6-(4-hydroxy-3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129737	6-{2-[3-(3,7-dimethylocta-2,6-dien-1-yl)-5,7-dihydroxy-6-(4-hydroxy-3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0

HMDB0129736	6-{4-[3-(3,7-dimethylocta-2,6-dien-1-yl)-5,7-dihydroxy-6-(4-hydroxy-3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129741	6-{4-[5,7-dihydroxy-3-(4-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129739	6-{[2-(2,4-dihydroxyphenyl)-3-(3,7-dimethylocta-2,6-dien-1-yl)-7-hydroxy-6-(4-hydroxy-3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129742	6-{2-[5,7-dihydroxy-3-(4-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129746	6-(4-{5,7-dihydroxy-3-[(2Z)-4-hydroxy-3-(4-methylpent-3-en-1-yl)but-2-en-1-yl]-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl]-3-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129744	6-{[2-(2,4-dihydroxyphenyl)-7-hydroxy-3-(4-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129743	6-{[2-(2,4-dihydroxyphenyl)-5-hydroxy-3-(4-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129752	6-{2-[5,7-dihydroxy-3-(8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl]-5-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129754	6-{[2-(2,4-dihydroxyphenyl)-7-hydroxy-3-(8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129751	6-{4-[5,7-dihydroxy-3-(8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl]-3-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129747	6-(2-{5,7-dihydroxy-3-[(2Z)-4-hydroxy-3-(4-methylpent-3-en-1-yl)but-2-en-1-yl]-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-2-yl]-5-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129749	6-{[2-(2,4-dihydroxyphenyl)-7-hydroxy-3-[(2Z)-4-hydroxy-3-(4-methylpent-3-en-1-yl)but-2-en-1-yl]-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129748	6-{[2-(2,4-dihydroxyphenyl)-5-hydroxy-3-[4-hydroxy-3-(4-methylpent-3-en-1-yl)but-2-en-1-yl]-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0129753	6-{[2-(2,4-dihydroxyphenyl)-5-hydroxy-3-(8-hydroxy-3,7-dimethylocta-2,6-dien-1-yl)-6-(3-methylbut-2-en-1-yl)-4-oxo-4H-chromen-7-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H42O13	M-H	681.2553	3.0
HMDB0175972	6-[(8a-carboxy-3-hydroxy-4,6a,6b,11,11,14b-hexamethyl-2-oxo-1,2,3,4,6,6a,6b,7,8,8a,9,11,12,12a,14,14a,14b-octadecahydricen-4-yl)methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H52O11	M+Na-2H	681.3256	-3.0

681.3236	HMDB0175973	6-{{[8a-carboxy-4-(hydroxymethyl)-4,6a,6b,11,11,14b-hexamethyl-2-oxo-1,2,3,4,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-octadecahydricen-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H52O11	M+Na-2H	681.3256	-3.0
	HMDB0175741	(3S,4R,12S,17S,19R,22S)-9-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-3,4,8,8,12,19,22-heptamethyl-14-oxo-23-oxahexacyclo[18.2.1.??]tricos-15-ene-19-carboxylic acid	C36H52O11	M+Na-2H	681.3256	-3.0
	HMDB0175742	3,4,5-trihydroxy-6-[(3S,4R,12S,17S,19R,22S)-9-hydroxy-3,4,8,8,12,19,22-heptamethyl-14-oxo-23-oxahexacyclo[18.2.1.??]tricos-15-ene-19-carbonyloxy]oxane-2-carboxylic acid	C36H52O11	M+Na-2H	681.3256	-3.0
	HMDB0175974	3,4,5-trihydroxy-6-[-hydroxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-11-oxo-1,2,3,4,4a,5,6,6a,6b,7,9,,11,12,12a,12b,13,14b-octadecahydricen-4a-carbonyloxy]oxane-2-carboxylic acid	C36H52O11	M+Na-2H	681.3256	-3.0
681.4187	HMDB0186413	{{[(2Z,6Z,8E,E,12E,14E,16E,18Z,22E)-6,,15,19,23,27-hexamethyl-2-(4-methylpent-3-en-1-yl)octacos-2,6,8,,12,14,16,18,22,26-decaen-1-yl]oxy} sulfonic acid	C40H60O4S	M+FA-H	681.4194	-1.1
	HMDB0186411	{{[(6E,Z,12E,14E,16E,18E,E,22Z,26E)-2,6,,14,19,23,27,31-octamethyldotriaconta-2,6,,12,14,16,18,,22,26,-undecaen-1-yl]oxy} sulfonic acid	C40H60O4S	M+FA-H	681.4194	-1.1
	HMDB0186417	{{[(2E,4E,6E,8E,E,12E,14Z,18E)-2-[(3E)-4,8-dimethylnona-3,7-dien-1-yl]-6,11,15,19,23-pentamethyltetracos-2,4,6,8,,12,14,18,22-nonaen-1-yl]oxy} sulfonic acid	C40H60O4S	M+FA-H	681.4194	-1.1
	HMDB0186415	{{[(6E,Z,12E,14E,16E,18E,E,22Z,26E)-2,6,,14,19,23,27,31-octamethyldotriaconta-2,6,,12,14,16,18,,22,26,-undecaen-5-yl]oxy} sulfonic acid	C40H60O4S	M+FA-H	681.4194	-1.1
	HMDB0186419	{{[(6E,Z,14E,16E,18E,E,22Z,26E)-2,6,,14,19,23,27,31-octamethyldotriaconta-2,6,,12,14,16,18,,22,26,-undecaen-9-yl]oxy} sulfonic acid	C40H60O4S	M+FA-H	681.4194	-1.1
	HMDB0186421	{{[(2Z,4E,6E,8E,Z,14E)-7,11,15,19-tetramethyl-2-[(1E,3Z,7E)-4,8,12-trimethyltrideca-1,3,7,11-tetraen-1-yl]icosa-2,4,6,8,,14,18-heptaen-1-yl]oxy} sulfonic acid	C40H60O4S	M+FA-H	681.4194	-1.1
	HMDB0186425	{{[(6E,Z,12E,14E,16E,18E,E,22Z,26E)-2,6,,14,19,23,27,31-octamethyldotriaconta-2,6,,12,14,16,18,,22,26,-undecaen-4-yl]oxy} sulfonic acid	C40H60O4S	M+FA-H	681.4194	-1.1
	HMDB0186423	{{[(2E,6E,Z,12E,14E,16E,18E,E,22Z,26E)-2,6,,14,19,23,27,31-octamethyldotriaconta-2,6,,12,14,16,18,,22,26,-undecaen-1-yl]oxy} sulfonic acid	C40H60O4S	M+FA-H	681.4194	-1.1
	HMDB0186427	{{[(6E,Z,12E,14E,16E,18E,E,22Z,26E)-2,6,,14,19,23,27,31-octamethyldotriaconta-2,6,,12,14,16,18,,22,26,-undecaen-8-yl]oxy} sulfonic acid	C40H60O4S	M+FA-H	681.4194	-1.1
681.5691	HMDB0007087	DG(15/22:1(13Z))	C40H76O5	M+FA-H	681.5675	2.4
	HMDB0055993	DG(15/22:1n9)	C40H76O5	M+FA-H	681.5675	2.4
	HMDB0007619	DG(22:1(13Z)/15)	C40H76O5	M+FA-H	681.5675	2.4
682.4430	HMDB0008825	PE(14/16:1(9Z))	C35H68NO8P	M+Na-2H	682.4429	0.1
	HMDB0113839	PE-NMe2(14/14:1(9Z))	C35H68NO8P	M+Na-2H	682.4429	0.1
	HMDB0113018	PE-NMe(15/14:1(9Z))	C35H68NO8P	M+Na-2H	682.4429	0.1
	HMDB0112938	PE-NMe(14:1(9Z)/15)	C35H68NO8P	M+Na-2H	682.4429	0.1

HMDB0008857	PE(14:1(9Z)/16)	C35H68NO8P	M+Na-2H	682.4429	0.1
HMDB0008921	PE(16/14:1(9Z))	C35H68NO8P	M+Na-2H	682.4429	0.1
HMDB0008953	PE(16:1(9Z)/14)	C35H68NO8P	M+Na-2H	682.4429	0.1
HMDB0113899	PE-NMe2(14:1(9Z)/14)	C35H68NO8P	M+Na-2H	682.4429	0.1
HMDB0099297	TG(i-14/12/)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0097349	TG(a-13/i-15/8)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0097348	TG(a-13/15/8)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0097351	TG(i-13/15/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0097347	TG(13/i-15/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0097344	TG(13/a-15/8)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0097346	TG(a-13/a-15/8)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0097345	TG(i-13/a-15/8)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096930	TG(i-13/13/)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0097350	TG(i-13/i-15/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0097352	TG(13/15/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0099185	TG(i-14/i-14/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0099295	TG(14/i-12/)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0099237	TG(14//12)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0099236	TG(i-14//12)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0099238	TG(14//i-12)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0099235	TG(i-14//i-12)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0099188	TG(14/8/i-14)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0099187	TG(14/14/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0099186	TG(i-14/8/14)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096929	TG(a-13/i-13/)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096928	TG(a-13/13/)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096926	TG(i-13/a-13/)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096594	TG(13/8/a-15)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096592	TG(13/8/15)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096593	TG(13/8/i-15)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096590	TG(i-13/8/a-15)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096588	TG(a-13/8/i-15)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096589	TG(i-13/8/i-15)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096591	TG(i-13/8/15)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096587	TG(a-13/8/15)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096662	TG(a-13//13)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096661	TG(a-13/a-13/)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096663	TG(a-13//i-13)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096925	TG(13/a-13/)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096927	TG(13/i-13/)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096668	TG(13//i-13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096669	TG(13//a-13)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096664	TG(i-13/i-13/)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096667	TG(13/13/)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096665	TG(i-13//a-13)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096666	TG(i-13//13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0096586	TG(a-13/8/a-15)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0099298	TG(14/12/)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0103595	TG(16/12/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0103593	TG(i-16/i-12/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0103594	TG(i-16/12/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0103592	TG(16/i-12/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0103535	TG(16//)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0103534	TG(i-16//)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0103479	TG(16/8/i-12)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0103478	TG(16/8/12)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0107809	TG(18/8/)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0107808	TG(i-18/8/)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0107866	TG(i-18//8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0107867	TG(18//8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0103476	TG(i-16/8/i-12)	C39H74O6	M+FA-H	683.5467	-1.7

683.5456

HMDB0103477	TG(i-16/8/12)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0101252	TG(15/13/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0100903	TG(15/8/i-13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0100898	TG(a-15/8/i-13)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0100897	TG(a-15/8/13)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0100899	TG(i-15/8/i-13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0100900	TG(i-15/8/a-13)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0100896	TG(a-15/8/a-13)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0099592	TG(i-14/14/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0099591	TG(14/i-14/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0100901	TG(i-15/8/13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0100902	TG(15/8/13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0100904	TG(15/8/a-13)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0101250	TG(i-15/i-13/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0101251	TG(i-15/13/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0101249	TG(a-15/i-13/8)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0101248	TG(a-15/13/8)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0101244	TG(15/a-13/8)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0101247	TG(15/i-13/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0101246	TG(a-15/a-13/8)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0101245	TG(i-15/a-13/8)[rac]	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0099296	TG(i-14/i-12/)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0095519	TG(12/16/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0072051	TG(8//18)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071640	TG(8/16/i-12)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071622	TG(/i-12/14)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071617	TG(/8/i-18)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071607	TG(/i-14/i-12)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071563	TG(8//i-18)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071551	TG(8/a-15/i-13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071482	TG(8/a-13/i-15)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071477	TG(8/i-15/13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071718	TG(8/16/12)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071778	TG(/a-13/i-13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071784	TG(8/12/i-16)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071998	TG(8/13/a-15)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071986	TG(8/i-12/16)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071976	TG(8/a-13/a-15)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071958	TG(/i-16)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071935	TG(8/8/i-)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071916	TG(/i-13/i-13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071908	TG(/13/a-13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071902	TG(8/13/i-15)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071467	TG(8/a-15/a-13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071444	TG(8/i-15/a-13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071397	TG(8/i-14/i-14)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0063783	TG(i-8/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071114	TG(/12/14)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071608	TG(/16)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0064269	TG(/8/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071110	TG(8/13/15)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071131	TG(/i-13/13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071390	TG(/18/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071389	TG(/13/i-13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071342	TG(8/15/a-13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071320	TG(/13/13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071315	TG(8/i-13/i-15)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071305	TG(/a-13/a-13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071254	TG(8/i-15/i-13)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0071162	TG(8/12/16)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0011188	TG(12/12/12)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0072056	TG(8/18/)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0095518	TG(i-12/16/8)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0094895	TG(12//14)	C39H74O6	M+FA-H	683.5467	-1.7
HMDB0094896	TG(12//i-14)	C39H74O6	M+FA-H	683.5467	-1.7

	HMDB0094893	TG(i-12//i-14)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0094894	TG(i-12//14)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0094846	TG(12/8/i-16)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0094845	TG(12/8/16)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0094843	TG(i-12/8/i-16)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0094844	TG(i-12/8/16)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0094945	TG(12/i-12/i-12)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0094943	TG(12/12/i-12)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0094946	TG(i-12/i-12/i-12)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0095516	TG(12/i-16/8)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0095517	TG(i-12/i-16/8)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0095233	TG(12/14/)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0095232	TG(i-12/14/)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0095231	TG(i-12/i-14/)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0095230	TG(12/i-14/)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0094947	TG(i-12/12/12)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0094944	TG(i-12/i-12/12)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072835	TG(8/i-12/i-16)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072814	TG(/a-13/13)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072778	TG(8/8/)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072346	TG(/i-18/8)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072344	TG(/14/i-12)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072303	TG(8/a-15/13)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072296	TG(8/i-16/i-12)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072236	TG(8/i-16/12)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072215	TG(8/a-13/15)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072208	TG(/14/12)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072173	TG(8/i-18/)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072357	TG(/i-12/i-14)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072396	TG(8/14/i-14)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072405	TG(8/i-13/a-15)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072774	TG(/12/i-14)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072770	TG(/8/18)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072737	TG(8/i-14/14)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072556	TG(8/14/14)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072542	TG(/i-13/a-13)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072502	TG(8/i-13/15)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072491	TG(8/15/13)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072479	TG(8/15/i-13)	C39H74O6	M+FA-H	683.5467	-1.7
	HMDB0072131	TG(/i-14/12)	C39H74O6	M+FA-H	683.5467	-1.7
684.4037	HMDB0034610	Zucchini factor B	C44H57NO4	M+Na-2H	684.4034	0.4
685.3843	HMDB0114803	PA(14:1(9Z):5(5Z,8Z,11Z,14Z,17Z))	C37H61O8P	M+Na-2H	685.3851	-1.1
	HMDB0115199	PA(:5(5Z,8Z,11Z,14Z,17Z)/14:1(9Z))	C37H61O8P	M+Na-2H	685.3851	-1.1
685.5187	HMDB0115835	PA(i-16)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115852	PA(i-i-16)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115864	PA(i-21/15)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115874	PA(i-21/a-15)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115881	PA(i-21/i-15)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115893	PA(i-22/14)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115910	PA(i-22/i-14)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115921	PA(i-24/12)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115938	PA(i-24/i-12)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115792	PA(i-12/i-24)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115736	PA(a-21/i-15)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115729	PA(a-21/a-15)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0114788	PA(14/22)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0114839	PA(16/)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115064	PA(/16)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115228	PA(21/15)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115240	PA(22/14)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115638	PA(/i-16)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115647	PA(21/a-15)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115654	PA(21/i-15)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115670	PA(22/i-14)	C39H77O8P	M-H20-H	685.5172	2.2
	HMDB0115719	PA(a-21/15)	C39H77O8P	M-H20-H	685.5172	2.2

686.1414	HMDB0001373	Dephospho Coenzyme A	C21H35N7O13P2S	M-H	686.1416	-0.3
686.2193	HMDB0187508	6-([3-(2-((2Z)-3-(2-carboxyethyl)-5-hydroxy-4-methyl-2H-pyrrol-2-ylidene)methyl)-5-((2Z)-3-ethenyl-5-hydroxy-4-methyl-2H-pyrrol-2-ylidene)methyl)-4-methyl-1H-pyrrol-3-yl]propanoyl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H35N3O12	M+FA-H	686.2203	-1.4
	HMDB0187509	6-([3-[(2E)-2-([3-(2-carboxyethyl)-5-((2E)-3-ethenyl-5-hydroxy-4-methyl-2H-pyrrol-2-ylidene)methyl)-4-methyl-1H-pyrrol-2-yl]methylidene)-5-hydroxy-4-methyl-2H-pyrrol-3-yl]propanoyl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H35N3O12	M+FA-H	686.2203	-1.4
	HMDB0187520	6-([3-[(2Z)-2-([3-(2-carboxyethyl)-5-((2E)-4-ethenyl-5-hydroxy-3-methyl-2H-pyrrol-2-ylidene)methyl)-4-methyl-1H-pyrrol-2-yl]methylidene)-5-hydroxy-4-methyl-2H-pyrrol-3-yl]propanoyl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H35N3O12	M+FA-H	686.2203	-1.4
	HMDB0187521	6-([3-(2-([3-(2-carboxyethyl)-5-hydroxy-4-methyl-2H-pyrrol-2-ylidene)methyl)-5-((2E)-4-ethenyl-5-hydroxy-3-methyl-2H-pyrrol-2-ylidene)methyl)-4-methyl-1H-pyrrol-3-yl]propanoyl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C31H35N3O12	M+FA-H	686.2203	-1.4
686.4757	HMDB0113844	PE-NMe2(14:1(9Z)/16:1(9Z))	C37H70NO8P	M-H	686.4766	-1.4
	HMDB0113963	PE-NMe2(16:1(9Z)/14:1(9Z))	C37H70NO8P	M-H	686.4766	-1.4
	HMDB0009085	PE(18:2(9Z,12Z)/14)	C37H70NO8P	M-H	686.4766	-1.4
	HMDB0009053	PE(18:1(9Z)/14:1(9Z))	C37H70NO8P	M-H	686.4766	-1.4
	HMDB0009020	PE(18:1(11Z)/14:1(9Z))	C37H70NO8P	M-H	686.4766	-1.4
	HMDB0008957	PE(16:1(9Z)/16:1(9Z))	C37H70NO8P	M-H	686.4766	-1.4
	HMDB0008861	PE(14:1(9Z)/18:1(9Z))	C37H70NO8P	M-H	686.4766	-1.4
	HMDB0008860	PE(14:1(9Z)/18:1(11Z))	C37H70NO8P	M-H	686.4766	-1.4
	HMDB0008829	PE(14/18:2(9Z,12Z))	C37H70NO8P	M-H	686.4766	-1.4
687.0652	HMDB0140604	[4-(7-([3,4-dihydroxy-6-(hydroxymethyl)-5-(3,4,5-trihydroxybenzoyloxy)oxan-2-yl]oxy)-5-hydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl]phenyl]oxidanesulfonic acid	C28H26O17S	M+Na-2H	687.0637	2.1
	HMDB0140605	(4-([4,5-dihydroxy-6-([5-hydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro-2H-1-benzopyran-7-yl]oxy)-2-(hydroxymethyl)oxan-3-yl]oxy]carbonyl)-2,6-dihydroxyphenyl)oxidanesulfonic acid	C28H26O17S	M+Na-2H	687.0637	2.1
	HMDB0140610	{4-[5-hydroxy-4-oxo-7-([3,4,5-trihydroxy-6-([3,4,5-trihydroxybenzoyloxy)methyl]oxan-2-yl]oxy)-3,4-dihydro-2H-1-benzopyran-2-yl]phenyl]oxidanesulfonic acid	C28H26O17S	M+Na-2H	687.0637	2.1
	HMDB0140611	(2,6-dihydroxy-4-([3,4,5-trihydroxy-6-([5-hydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro-2H-1-benzopyran-7-yl]oxy)oxan-2-yl]methoxy]carbonyl]phenyl)oxidanesulfonic acid	C28H26O17S	M+Na-2H	687.0637	2.1
	HMDB0113842	PE-NMe2(14/16:1(9Z))	C37H72NO8P	M-H	688.4923	-2.0
	HMDB0112945	PE-NMe(15/16:1(9Z))	C37H72NO8P	M-H	688.4923	-2.0
	HMDB0113962	PE-NMe2(16:1(9Z)/14)	C37H72NO8P	M-H	688.4923	-2.0

688.4909	HMDB0113941	PE-NMe2(16/14:1(9Z))	C37H72NO8P	M-H	688.4923	-2.0
	HMDB0113063	PE-NMe(16:1(9Z)/15)	C37H72NO8P	M-H	688.4923	-2.0
	HMDB0113843	PE-NMe2(14:1(9Z)/16)	C37H72NO8P	M-H	688.4923	-2.0
	HMDB0009052	PE(18:1(9Z)/14)	C37H72NO8P	M-H	688.4923	-2.0
	HMDB0009019	PE(18:1(11Z)/14)	C37H72NO8P	M-H	688.4923	-2.0
	HMDB0008987	PE(18/14:1(9Z))	C37H72NO8P	M-H	688.4923	-2.0
	HMDB0008956	PE(16:1(9Z)/16)	C37H72NO8P	M-H	688.4923	-2.0
	HMDB0008924	PE(16/16:1(9Z))	C37H72NO8P	M-H	688.4923	-2.0
	HMDB0008859	PE(14:1(9Z)/18)	C37H72NO8P	M-H	688.4923	-2.0
	HMDB0008828	PE(14/18:1(9Z))	C37H72NO8P	M-H	688.4923	-2.0
	HMDB0008827	PE(14/18:1(11Z))	C37H72NO8P	M-H	688.4923	-2.0
	HMDB0007933	PC(15/14:1(9Z))	C37H72NO8P	M-H	688.4923	-2.0
	HMDB0007901	PC(14:1(9Z)/15)	C37H72NO8P	M-H	688.4923	-2.0
689.3361	HMDB0176078	-{[3,5-dihydroxy-4-(sulfooxy)oxan-2-yl]oxy}-2,2,6a,6b,9,9,12a-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C35H56O10S	M+Na-2H	689.3341	2.9
	HMDB0176080	-{[3,4-dihydroxy-5-(sulfooxy)oxan-2-yl]oxy}-2,2,6a,6b,9,9,12a-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C35H56O10S	M+Na-2H	689.3341	2.9
	HMDB0176079	-{[4,5-dihydroxy-3-(sulfooxy)oxan-2-yl]oxy}-2,2,6a,6b,9,9,12a-heptamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carboxylic acid	C35H56O10S	M+Na-2H	689.3341	2.9
689.5351	HMDB0056282	DG(18:2n6/18:2n6)	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0056221	DG(:1n9/18:3n6)	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0056228	DG(:1n9/18:3n3)	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0056205	DG(18:1n9/:3n6)	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0056199	DG(18:1n9/:3n9)	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0056186	DG(18:1n7/:3n6)	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0056028	DG(16/22:4n6)	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0056052	DG(18/:4n6)	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0056058	DG(18/:4n3)	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0056082	DG(/18:4n3)	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0056180	DG(18:1n7/:3n9)	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007118	DG(16/22:4(7Z,Z,13Z,16Z))	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007449	DG(:3(5Z,8Z,11Z)/18:1(11Z))	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007450	DG(:3(5Z,8Z,11Z)/18:1(9Z))	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007479	DG(:3(8Z,11Z,14Z)/18:1(9Z))	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007478	DG(:3(8Z,11Z,14Z)/18:1(11Z))	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007506	DG(:4(5Z,8Z,11Z,14Z)/18)	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007535	DG(:4(8Z,11Z,14Z,17Z)/18)	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007678	DG(22:4(7Z,Z,13Z,16Z)/16)	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007422	DG(:2(11Z,14Z)/18:2(9Z,12Z))	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007394	DG(:1(11Z)/18:3(6Z,9Z,12Z))	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007395	DG(:1(11Z)/18:3(9Z,12Z,15Z))	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007170	DG(18/:4(5Z,8Z,11Z,14Z))	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007171	DG(18/:4(8Z,11Z,14Z,17Z))	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007198	DG(18:1(11Z)/:3(8Z,11Z,14Z))	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007227	DG(18:1(9Z)/:3(8Z,11Z,14Z))	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007226	DG(18:1(9Z)/:3(5Z,8Z,11Z))	C41H72O5	M+FA-H	689.5362	-1.6

	HMDB0007254	DG(18:2(9Z,12Z)/:2(11Z,14Z))	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007282	DG(18:3(6Z,9Z,12Z)/:1(11Z))	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007311	DG(18:3(9Z,12Z,15Z)/:1(11Z))	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007339	DG(18:4(6Z,9Z,12Z,15Z)/)	C41H72O5	M+FA-H	689.5362	-1.6
	HMDB0007367	DG(/18:4(6Z,9Z,12Z,15Z))	C41H72O5	M+FA-H	689.5362	-1.6
690.3257	HMDB0013055	S-(11-hydroxy-9-deoxy-delta12-PGD2)-glutathione	C30H51N3O10S	M+FA-H	690.3277	-2.9
	HMDB0013059	S-(9-hydroxy-PGA1)-glutathione	C30H51N3O10S	M+FA-H	690.3277	-2.9
691.0086	HMDB0156328	[4-hydroxy-2-({[hydroxy({[hydroxy({[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})phosphoryl]oxy})phosphoryl]oxy}methyl)-5-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)oxolan-3-yl]oxidanesulfonic acid	C15H24N2O20P2S	M+FA-H	691.0100	-2.1
	HMDB0156329	[4-hydroxy-5-({[hydroxy({[hydroxy({[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})phosphoryl]oxy})phosphoryl]oxy}methyl)-2-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)oxolan-3-yl]oxidanesulfonic acid	C15H24N2O20P2S	M+FA-H	691.0100	-2.1
691.0963	HMDB0154433	(2,6-dihydroxy-4-{3,5,7-trihydroxy-8-[2-hydroxy-1-(2,4,6-trihydroxyphenyl)-3-(3,4,5-trihydroxyphenyl)propyl]-3,4-dihydro-2H-1-benzopyran-2-yl}phenyl)oxidanesulfonic acid	C30H28O17S	M-H	691.0974	-1.7
	HMDB0154434	({1-[3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-8-yl]-1-(2,4,6-trihydroxyphenyl)-3-(3,4,5-trihydroxyphenyl)propan-2-yl}oxy)sulfonic acid	C30H28O17S	M-H	691.0974	-1.7
	HMDB0154432	(2,6-dihydroxy-4-{2-hydroxy-3-[3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-8-yl]-3-(2,4,6-trihydroxyphenyl)propyl}phenyl)oxidanesulfonic acid	C30H28O17S	M-H	691.0974	-1.7
691.1945	HMDB0162585	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(2-{1,5-dihydroxy-11-methyl-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-2-yl}-1-hydroxypropan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H34N4O11S	M+FA-H	691.1927	2.6
	HMDB0162608	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(1,3-dihydroxy-2-{5-hydroxy-11-methyl-6-oxo-1H,2H,6H,11H-furo[2,3-c]acridin-2-yl}propan-2-yl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C29H34N4O11S	M+FA-H	691.1927	2.6
	HMDB0177799	3,4,5-trihydroxy-6-[4-hydroxy-9-(hydroxymethyl)-2-(methoxycarbonyl)-2,6a,6b,9,12a-pentamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carbonyloxy]oxane-2-carboxylic acid	C37H56O12	M-H	691.3699	2.3
	HMDB0177798	6-{{8a-carboxy-4-(hydroxymethyl)-11-(methoxycarbonyl)-4,6a,6b,11,14b-pentamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricene-3-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C37H56O12	M-H	691.3699	2.3
	HMDB0177797	6-{{8a-carboxy-3-hydroxy-11-(methoxycarbonyl)-4,6a,6b,11,14b-pentamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricene-4-yl]methoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C37H56O12	M-H	691.3699	2.3
	HMDB0177879	6-[1,1-dihydroxy-2-(methoxycarbonyl)-2,6a,6b,9,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carbonyloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C37H56O12	M-H	691.3699	2.3

691.3715	HMDB0177877	6-[[8a-carboxy-2-hydroxy-11-(methoxycarbonyl)-4,4,6a,6b,11,14b-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-3-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C37H56O12	M-H	691.3699	2.3
	HMDB0177878	6-[[8a-carboxy-3-hydroxy-11-(methoxycarbonyl)-4,4,6a,6b,11,14b-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-2-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C37H56O12	M-H	691.3699	2.3
	HMDB0175947	6-[(11-carboxy-14b-formyl-4,4,6a,6b,8a,11-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12b,13,14,14a,14b-icosahydricen-3-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H54O10	M+FA-H	691.3699	2.3
	HMDB0175889	6-(9-formyl--hydroxy-2,2,6a,6b,9,12a-hexamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carbonyloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H54O10	M+FA-H	691.3699	2.3
	HMDB0034520	Gypsogenin 3-O-b-D-glucuronide	C36H54O10	M+FA-H	691.3699	2.3
	HMDB0184129	6-[[6aS,6bR,8aR,14bS)-8a-carboxy-4,4,6a,6b,11,11,14b-heptamethyl-2-oxo-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-3-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H54O10	M+FA-H	691.3699	2.3
	HMDB0175809	6-[[4aR,6aR,6bS,8aS,11S,12aS,14aR,14bS)-11-carboxy-4,4,6a,6b,8a,11,14b-heptamethyl-14-oxo-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-3-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H54O10	M+FA-H	691.3699	2.3
	HMDB0175810	6-[(2S,4aS,6aS,6bR,8aR,12aS,12bR,14bS)--hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-13-oxo-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-2-carbonyloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H54O10	M+FA-H	691.3699	2.3
	HMDB0175798	3,4,5-trihydroxy-6-(-hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-13-oxo-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-2-carbonyloxy)oxane-2-carboxylic acid	C36H54O10	M+FA-H	691.3699	2.3
	HMDB0037827	Monoglucuronylglycyrrhetic acid	C36H54O10	M+FA-H	691.3699	2.3
691.4253	HMDB0175692	6-[[8a-carboxy-4,4,6a,6b,11,11,14b-heptamethyl-3-oxo-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,14,14a,14b-icosahydricen-5-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H54O10	M+FA-H	691.3699	2.3
	HMDB0175693	3,4,5-trihydroxy-6-(8-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl--oxo-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carbonyloxy)oxane-2-carboxylic acid	C36H54O10	M+FA-H	691.3699	2.3
	HMDB0184130	6-[(4aS,6aS,6bR,12aR)--hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-11-oxo-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-4a-carbonyloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C36H54O10	M+FA-H	691.3699	2.3
691.4253	HMDB0172618	{[(9Z)-18-[(8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraen-1-yl]oxy]-18-oxooctadec-9-en-7-yl]oxy} sulfonic acid	C38H62O6S	M+FA-H	691.4249	0.6
692.2303	HMDB0143655	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-(4-[4-(2-oxoethoxy)phenyl]-3,4-diphenylbut-3-en-1-yl] sulfanyl)ethyl}-C-hydroxycarbonimidoyl)butanoic	C34H37N3O8S	M+FA-H	692.2283	2.8

692.3039	HMDB0164603	4-({2-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1-hydroxy-4-methylpentylidene} amino)-5,8-dihydroxy-7-(2-methylprop-2-en-1-yl)-3-(propan-2-yl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H47N3O13	M-H	692.3036	0.4
	HMDB0164605	4-({2-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1-hydroxy-4-methylpent-4-en-1-ylidene} amino)-5,8-dihydroxy-7-(2-methylpropyl)-3-(propan-2-yl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H47N3O13	M-H	692.3036	0.4
	HMDB0164601	4-({2-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1-hydroxy-4-methylpentylidene} amino)-5,8-dihydroxy-7-(2-methylpropyl)-3-(prop-1-en-2-yl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H47N3O13	M-H	692.3036	0.4
	HMDB0164598	4-({2-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1,5-dihydroxy-4-methylpentylidene} amino)-5,8-dihydroxy-7-(2-methylpropyl)-3-(propan-2-yl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H49N3O14	M-H2O-H	692.3031	1.2
	HMDB0164597	4-({5-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1,2-dihydroxy-4-methylpentylidene} amino)-5,8-dihydroxy-7-(2-methylpropyl)-3-(propan-2-yl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H49N3O14	M-H2O-H	692.3031	1.2
	HMDB0164593	7-{3-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-2-methylpropyl}-4-[(1,2-dihydroxy-4-methylpentylidene)amino]-5,8-dihydroxy-3-(propan-2-yl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H49N3O14	M-H2O-H	692.3031	1.2
	HMDB0164594	4-({2-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1-hydroxy-4-methylpentylidene} amino)-5,8-dihydroxy-7-(3-hydroxy-2-methylpropyl)-3-(propan-2-yl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H49N3O14	M-H2O-H	692.3031	1.2
	HMDB0164590	4-({2-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1-hydroxy-4-methylpentylidene} amino)-5,8-dihydroxy-3-(1-hydroxypropan-2-yl)-7-(2-methylpropyl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H49N3O14	M-H2O-H	692.3031	1.2
	HMDB0164589	3-{1-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]propan-2-yl}-4-[(1,2-dihydroxy-4-methylpentylidene)amino]-5,8-dihydroxy-7-(2-methylpropyl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H49N3O14	M-H2O-H	692.3031	1.2
	HMDB0164587	4-({2-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1,4-dihydroxy-4-methylpentylidene} amino)-5,8-dihydroxy-7-(2-methylpropyl)-3-(propan-2-yl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H49N3O14	M-H2O-H	692.3031	1.2
	HMDB0164583	7-{2-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-2-methylpropyl}-4-[(1,2-dihydroxy-4-methylpentylidene)amino]-5,8-dihydroxy-3-(propan-2-yl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H49N3O14	M-H2O-H	692.3031	1.2
	HMDB0164586	4-({4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1,2-dihydroxy-4-methylpentylidene} amino)-5,8-dihydroxy-7-(2-methylpropyl)-3-(propan-2-yl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H49N3O14	M-H2O-H	692.3031	1.2
	HMDB0164584	4-({2-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1-hydroxy-4-methylpentylidene} amino)-5,8-dihydroxy-7-(2-hydroxy-2-methylpropyl)-3-(propan-2-yl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H49N3O14	M-H2O-H	692.3031	1.2

	HMDB0164580	3-{2-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]propan-2-yl}-4-[(1,2-dihydroxy-4-methylpentylidene)amino]-5,8-dihydroxy-7-(2-methylpropyl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H49N3O14	M-H2O-H	692.3031	1.2
	HMDB0164581	4-({2-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1-hydroxy-4-methylpentylidene}amino)-5,8-dihydroxy-3-(2-hydroxypropan-2-yl)-7-(2-methylpropyl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H49N3O14	M-H2O-H	692.3031	1.2
	HMDB0164577	4-({2-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-1-hydroxy-4-methylpentylidene}amino)-5,8,11-trihydroxy-7-(2-methylpropyl)-3-(propan-2-yl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H49N3O14	M-H2O-H	692.3031	1.2
	HMDB0164576	11-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-4-[(1,2-dihydroxy-4-methylpentylidene)amino]-5,8-dihydroxy-7-(2-methylpropyl)-3-(propan-2-yl)-2-oxa-6,9-diazabicyclo[.2.2]hexadeca-1(14),5,8,12,15-pentaene--carboxylic acid	C33H49N3O14	M-H2O-H	692.3031	1.2
692.6184	HMDB0004953	Cer(d18:1/24:1(15Z))	C42H81NO3	M+FA-H	692.6198	-2.1
693.1132	HMDB0148308	3-{3-[3,4-dihydroxy-6-(hydroxymethyl)-5-(sulfooxy)oxan-2-yl]-2,3-dihydroxy-5-[(2E)-3-(4-hydroxyphenyl)prop-2-enoyl]-4,6-dioxocyclohex-1-en-1-yl}-3-(4-hydroxyphenyl)propanoic acid	C30H30O17S	M-H	693.1131	0.2
	HMDB0148310	3-{3-[4,5-dihydroxy-6-(hydroxymethyl)-3-(sulfooxy)oxan-2-yl]-2,3-dihydroxy-5-[3-(4-hydroxyphenyl)prop-2-enoyl]-4,6-dioxocyclohex-1-en-1-yl]-3-(4-hydroxyphenyl)propanoic acid	C30H30O17S	M-H	693.1131	0.2
	HMDB0148307	3-{2,3-dihydroxy-5-[(2E)-3-(4-hydroxyphenyl)prop-2-enoyl]-4,6-dioxo-3-{3,4,5-trihydroxy-6-[(sulfooxy)methyl]oxan-2-yl}cyclohex-1-en-1-yl}-3-(4-hydroxyphenyl)propanoic acid	C30H30O17S	M-H	693.1131	0.2
	HMDB0148314	3-(2,5-dihydroxy-4,6-dioxo-3-{3-[4-(sulfooxy)phenyl]prop-2-enoyl}-5-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]cyclohex-2-en-1-yl)-3-(4-hydroxyphenyl)propanoic acid	C30H30O17S	M-H	693.1131	0.2
	HMDB0148318	3-{5-[3,5-dihydroxy-6-(hydroxymethyl)-4-(sulfooxy)oxan-2-yl]-2,5-dihydroxy-3-[3-(4-hydroxyphenyl)prop-2-enoyl]-4,6-dioxocyclohex-2-en-1-yl]-3-(4-hydroxyphenyl)propanoic acid	C30H30O17S	M-H	693.1131	0.2
	HMDB0148316	3-{2,5-dihydroxy-3-[(2E)-3-(4-hydroxyphenyl)prop-2-enoyl]-4,6-dioxo-5-{3,4,5-trihydroxy-6-[(sulfooxy)methyl]oxan-2-yl}cyclohex-2-en-1-yl}-3-(4-hydroxyphenyl)propanoic acid	C30H30O17S	M-H	693.1131	0.2
	HMDB0148315	3-{2,5-dihydroxy-3-[3-(4-hydroxyphenyl)prop-2-enoyl]-4,6-dioxo-5-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]cyclohex-2-en-1-yl}-3-[4-(sulfooxy)phenyl]propanoic acid	C30H30O17S	M-H	693.1131	0.2
	HMDB0148317	3-{5-[3,4-dihydroxy-6-(hydroxymethyl)-5-(sulfooxy)oxan-2-yl]-2,5-dihydroxy-3-[(2E)-3-(4-hydroxyphenyl)prop-2-enoyl]-4,6-dioxocyclohex-2-en-1-yl}-3-(4-hydroxyphenyl)propanoic acid	C30H30O17S	M-H	693.1131	0.2
	HMDB0148309	3-{3-[3,5-dihydroxy-6-(hydroxymethyl)-4-(sulfooxy)oxan-2-yl]-2,3-dihydroxy-5-[3-(4-hydroxyphenyl)prop-2-enoyl]-4,6-dioxocyclohex-1-en-1-yl}-3-(4-hydroxyphenyl)propanoic acid	C30H30O17S	M-H	693.1131	0.2
	HMDB0148306	3-{2,3-dihydroxy-5-[3-(4-hydroxyphenyl)prop-2-enoyl]-4,6-dioxo-3-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]cyclohex-1-en-1-yl}-3-[4-(sulfooxy)phenyl]propanoic acid	C30H30O17S	M-H	693.1131	0.2
	HMDB0148305	3-(2,3-dihydroxy-4,6-dioxo-5-{3-[4-(sulfooxy)phenyl]prop-2-enoyl}-3-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]cyclohex-1-en-1-yl)-3-(4-hydroxyphenyl)propanoic acid	C30H30O17S	M-H	693.1131	0.2

HMDB0124845	{5-[6-(3,4-dihydroxyphenyl)-13-hydroxy-4-oxo-8- {[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}- 3,11-dioxatricyclo[8.4,tetradeca-1,7,9-trien-12-yl]-2- hydroxyphenyl}oxidanesulfonic acid	C30H30O17S	M-H	693.1131	0.2
HMDB0124846	[6,12-bis(3,4-dihydroxyphenyl)-4-oxo-8- {[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-3,11- dioxatricyclo[8.4,tetradeca-1,7,9-trien-13- yl]oxidanesulfonic acid	C30H30O17S	M-H	693.1131	0.2
HMDB0148270	3-(4-hydroxyphenyl)-3-(2,3,6-trihydroxy-4-oxo-5- {3-[4-(sulfooxy)phenyl]prop-2-enoyl}-3-[3,4,5- trihydroxy-6-(hydroxymethyl)oxan-2-yl]cyclohexa-1,5- dien-1-yl}propanoic acid	C30H30O17S	M-H	693.1131	0.2
HMDB0148274	3-{3-[3,5-dihydroxy-6-(hydroxymethyl)-4- (sulfooxy)oxan-2-yl]-2,3,6-trihydroxy-5-[3-(4- hydroxyphenyl)prop-2-enoyl]-4-oxocyclohexa-1,5- dien-1-yl}-3-(4-hydroxyphenyl)propanoic acid	C30H30O17S	M-H	693.1131	0.2
HMDB0148273	3-{3-[3,4-dihydroxy-6-(hydroxymethyl)-5- (sulfooxy)oxan-2-yl]-2,3,6-trihydroxy-5-[(2E)-3-(4- hydroxyphenyl)prop-2-enoyl]-4-oxocyclohexa-1,5- dien-1-yl}-3-(4-hydroxyphenyl)propanoic acid	C30H30O17S	M-H	693.1131	0.2
HMDB0148271	3-[4-(sulfooxy)phenyl]-3-{2,3,6-trihydroxy-5-[3-(4- hydroxyphenyl)prop-2-enoyl]-4-oxo-3-[3,4,5- trihydroxy-6-(hydroxymethyl)oxan-2-yl]cyclohexa-1,5- dien-1-yl}propanoic acid	C30H30O17S	M-H	693.1131	0.2
HMDB0148272	3-(4-hydroxyphenyl)-3-{2,3,6-trihydroxy-5-[(2E)-3-(4- hydroxyphenyl)prop-2-enoyl]-4-oxo-3-{3,4,5- trihydroxy-6-[(sulfooxy)methyl]oxan-2-yl}cyclohexa- 1,5-dien-1-yl}propanoic acid	C30H30O17S	M-H	693.1131	0.2
HMDB0148275	3-{3-[4,5-dihydroxy-6-(hydroxymethyl)-3- (sulfooxy)oxan-2-yl]-2,3,6-trihydroxy-5-[3-(4- hydroxyphenyl)prop-2-enoyl]-4-oxocyclohexa-1,5- dien-1-yl}-3-(4-hydroxyphenyl)propanoic acid	C30H30O17S	M-H	693.1131	0.2
HMDB0148319	3-{5-[4,5-dihydroxy-6-(hydroxymethyl)-3- (sulfooxy)oxan-2-yl]-2,5-dihydroxy-3-[3-(4- hydroxyphenyl)prop-2-enoyl]-4,6-dioxocyclohex-2-en- 1-yl}-3-(4-hydroxyphenyl)propanoic acid	C30H30O17S	M-H	693.1131	0.2
HMDB0116639	PG(a-13/a-17)	C36H71O10P	M-H	693.4712	0.6
HMDB0116666	PG(i-12/i-18)	C36H71O10P	M-H	693.4712	0.6
HMDB0116675	PG(i-13/a-17)	C36H71O10P	M-H	693.4712	0.6
HMDB0116683	PG(i-13/i-17)	C36H71O10P	M-H	693.4712	0.6
HMDB0116697	PG(i-14/i-16)	C36H71O10P	M-H	693.4712	0.6
HMDB0116647	PG(a-13/i-17)	C36H71O10P	M-H	693.4712	0.6
HMDB0115696	PA(8/i-24)	C35H69O8P	M+FA-H	693.4712	0.6
HMDB0115710	PA(a-13/i-19)	C35H69O8P	M+FA-H	693.4712	0.6
HMDB0115789	PA(i-12/i-)	C35H69O8P	M+FA-H	693.4712	0.6
HMDB0115806	PA(i-13/i-19)	C35H69O8P	M+FA-H	693.4712	0.6
HMDB0115848	PA(i-/i-12)	C35H69O8P	M+FA-H	693.4712	0.6
HMDB0115890	PA(i-22/)	C35H69O8P	M+FA-H	693.4712	0.6
HMDB0115932	PA(i-24/8)	C35H69O8P	M+FA-H	693.4712	0.6
HMDB0115831	PA(i-/12)	C35H69O8P	M+FA-H	693.4712	0.6
HMDB0115621	PA(/i-22)	C35H69O8P	M+FA-H	693.4712	0.6
HMDB0115059	PA(/12)	C35H69O8P	M+FA-H	693.4712	0.6
HMDB0000674	PA(16/16)	C35H69O8P	M+FA-H	693.4712	0.6
HMDB0115634	PA(i-12)	C35H69O8P	M+FA-H	693.4712	0.6
HMDB0114777	PA(/22)	C35H69O8P	M+FA-H	693.4712	0.6
HMDB0114873	PA(18/14)	C35H69O8P	M+FA-H	693.4712	0.6
HMDB0115237	PA(22/)	C35H69O8P	M+FA-H	693.4712	0.6

	HMDB0116437	(2S)-1- {[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoate	C41H68O7	M+Na-2H	693.4712	0.6
	HMDB0116375	(2S)-2- {[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropyl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate	C41H68O7	M+Na-2H	693.4712	0.6
	HMDB0116442	(2S)-1-hydroxy-3- {[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propan-2-yl 11-(3-methyl-5-propylfuran-2-yl)undecanoate	C41H68O7	M+Na-2H	693.4712	0.6
	HMDB0116448	(2S)-1-hydroxy-3- {[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propan-2-yl 9-(3-methyl-5-pentylfuran-2-yl)nonanoate	C41H68O7	M+Na-2H	693.4712	0.6
	HMDB0116429	(2S)-1- {[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoate	C41H68O7	M+Na-2H	693.4712	0.6
	HMDB0116422	(2S)-1- {[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate	C41H68O7	M+Na-2H	693.4712	0.6
	HMDB0116395	(2S)-3-hydroxy-2- {[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propyl 11-(3-methyl-5-propylfuran-2-yl)undecanoate	C41H68O7	M+Na-2H	693.4712	0.6
	HMDB0116389	(2S)-1-hydroxy-3- {[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propan-2-yl 11-(3-methyl-5-propylfuran-2-yl)undecanoate	C41H68O7	M+Na-2H	693.4712	0.6
694.6353	HMDB0000831	N-Lignoceroylsphingosine	C42H83NO3	M+FA-H	694.6355	-0.3
	HMDB0011769	Cer(d18/24:1(15Z))	C42H83NO3	M+FA-H	694.6355	-0.3
	HMDB0004956	Ceramide (d18:1/24)	C42H83NO3	M+FA-H	694.6355	-0.3
695.3088	HMDB0177825	2,6a,6b,9,12a-pentamethyl-9-[(sulfooxy)methyl]--[(3,4,5-trihydroxyoxan-2-yl)oxy]-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-2,4a-dicarboxylic acid	C35H54O13S	M-H2O-H	695.3101	-1.9
	HMDB0177826	-{[4,5-dihydroxy-3-(sulfooxy)oxan-2-yl]oxy}-9-(hydroxymethyl)-2,6a,6b,9,12a-pentamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-2,4a-dicarboxylic acid	C35H54O13S	M-H2O-H	695.3101	-1.9
	HMDB0177828	-{[3,4-dihydroxy-5-(sulfooxy)oxan-2-yl]oxy}-9-(hydroxymethyl)-2,6a,6b,9,12a-pentamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-2,4a-dicarboxylic acid	C35H54O13S	M-H2O-H	695.3101	-1.9
	HMDB0177827	-{[3,5-dihydroxy-4-(sulfooxy)oxan-2-yl]oxy}-9-(hydroxymethyl)-2,6a,6b,9,12a-pentamethyl-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,,11,12,12a,12b,13,14b-icosahydricene-2,4a-dicarboxylic acid	C35H54O13S	M-H2O-H	695.3101	-1.9
695.4620	HMDB0007858	PA(16/18:1(11Z))	C37H71O8P	M+Na-2H	695.4633	-1.9
	HMDB0114899	PA(18:1(11Z)/16)	C37H71O8P	M+Na-2H	695.4633	-1.9
	HMDB0114924	PA(18:1(9Z)/16)	C37H71O8P	M+Na-2H	695.4633	-1.9
	HMDB0115062	PA(/14:1(9Z))	C37H71O8P	M+Na-2H	695.4633	-1.9
	HMDB0115091	PA(:1(11Z)/14)	C37H71O8P	M+Na-2H	695.4633	-1.9
	HMDB0007859	PA(16/18:1(9Z))	C37H71O8P	M+Na-2H	695.4633	-1.9
	HMDB0031130	9-Octadecenoic acid 1-[[[(1-oxohexadecyl)oxy]methyl]-2-(phosphonoxy)ethyl ester	C37H71O8P	M+Na-2H	695.4633	-1.9
	HMDB0114877	PA(18/16:1(9Z))	C37H71O8P	M+Na-2H	695.4633	-1.9
	HMDB0186373	(6E,8E)-4-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-5-hydroxy-9-(4-methoxy-2,3,6-trimethylphenyl)-3,7-dimethylnona-6,8-dienoic acid	C31H45N3O10S	M+FA-H	696.2808	1.3
	HMDB0186376	(4E,8E)-6-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-7-hydroxy-9-(4-methoxy-2,3,6-trimethylphenyl)-3,7-dimethylnona-4,8-dienoic acid	C31H45N3O10S	M+FA-H	696.2808	1.3

696.2817	HMDB0186377	(4E,8E)-7-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-6-hydroxy-9-(4-methoxy-2,3,6-trimethylphenyl)-3,7-dimethylnona-4,8-dienoic acid	C31H45N3O10S	M+FA-H	696.2808	1.3
	HMDB0186374	(6E,8E)-5-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-4-hydroxy-9-(4-methoxy-2,3,6-trimethylphenyl)-3,7-dimethylnona-6,8-dienoic acid	C31H45N3O10S	M+FA-H	696.2808	1.3
	HMDB0186379	(4E,6E)-8-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-9-hydroxy-9-(4-methoxy-2,3,6-trimethylphenyl)-3,7-dimethylnona-4,6-dienoic acid	C31H45N3O10S	M+FA-H	696.2808	1.3
	HMDB0186380	(4E,6E)-9-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-8-hydroxy-9-(4-methoxy-2,3,6-trimethylphenyl)-3,7-dimethylnona-4,6-dienoic acid	C31H45N3O10S	M+FA-H	696.2808	1.3
696.3856	HMDB0012342	PS(14:1(9Z)/14:1(9Z))	C34H62NO10P	M+Na-2H	696.3858	-0.3
696.4944	HMDB0008851	PE(14/P-18)	C37H74NO7P	M+Na-2H	696.4950	-0.8
	HMDB0011368	PE(P-18/14)	C37H74NO7P	M+Na-2H	696.4950	-0.8
	HMDB0011158	PE(P-16/16)	C37H74NO7P	M+Na-2H	696.4950	-0.8
	HMDB0008949	PE(16/P-16)	C37H74NO7P	M+Na-2H	696.4950	-0.8
697.2524	HMDB0000789	Pentacarboxylporphyrin I	C37H38N4O10	M-H	697.2515	1.3
	HMDB0002242	Dehydroisocoproprophyrinogen	C36H36N4O8	M+FA-H	697.2515	1.3
	HMDB0038229	Bn-NCC-1	C37H40N4O11	M-H20-H	697.2510	2.1
697.4790	HMDB0115791	PA(i-12/i-22)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115797	PA(i-13/a-21)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115808	PA(i-13/i-21)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115833	PA(i-/14)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115850	PA(i-/i-14)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115862	PA(i-21/13)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115873	PA(i-21/a-13)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115879	PA(i-21/i-13)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115891	PA(i-22/12)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115908	PA(i-22/i-12)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115920	PA(i-24/)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115734	PA(a-21/i-13)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115728	PA(a-21/a-13)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115717	PA(a-21/13)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0114783	PA(14/)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0114876	PA(18/16)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115061	PA(/14)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115226	PA(21/13)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115238	PA(22/12)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115622	PA(i-24)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115636	PA(i-/14)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115646	PA(21/a-13)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115652	PA(21/i-13)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115668	PA(22/i-12)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115701	PA(a-13/a-21)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0115712	PA(a-13/i-21)	C37H73O8P	M+Na-2H	697.4790	0.0
	HMDB0113850	PE-NMe2(16/16:1(9Z))	C39H76NO8P	M-H20-H	698.5125	-1.2

698.5116	HMDB0113851	PE-NMe2(14/18:1(9Z))	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0113852	PE-NMe2(14/18:1(11Z))	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0113853	PE-NMe2(14:1(9Z)/18)	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0112953	PE-NMe(15/18:1(9Z))	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0112954	PE-NMe(15/18:1(11Z))	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0114011	PE-NMe2(18:1(11Z)/14)	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0114038	PE-NMe2(18:1(9Z)/14)	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0113986	PE-NMe2(18/14:1(9Z))	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0113965	PE-NMe2(16:1(9Z)/16)	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0113139	PE-NMe(18:1(9Z)/15)	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0113112	PE-NMe(18:1(11Z)/15)	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0007936	PC(15/16:1(9Z))	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0009218	PE(/14:1(9Z))	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0009250	PE(:1(11Z)/14)	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0009055	PE(18:1(9Z)/16)	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0008000	PC(16:1(9Z)/15)	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0008834	PE(14/:1(11Z))	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0008866	PE(14:1(9Z)/)	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0008926	PE(16/18:1(11Z))	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0008927	PE(16/18:1(9Z))	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0008958	PE(16:1(9Z)/18)	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0008990	PE(18/16:1(9Z))	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0009022	PE(18:1(11Z)/16)	C39H76NO8P	M-H20-H	698.5125	-1.2
	HMDB0008984	PE(16:1(9Z)/P-18:1(11Z))	C39H74NO7P	M-H	698.5130	-2.0
	HMDB0008985	PE(16:1(9Z)/P-18:1(9Z))	C39H74NO7P	M-H	698.5130	-2.0
	HMDB0011343	PE(P-16/18:2(9Z,12Z))	C39H74NO7P	M-H	698.5130	-2.0
	HMDB0011438	PE(P-18:1(9Z)/16:1(9Z))	C39H74NO7P	M-H	698.5130	-2.0
	HMDB0011405	PE(P-18:1(11Z)/16:1(9Z))	C39H74NO7P	M-H	698.5130	-2.0
	HMDB0009114	PE(18:2(9Z,12Z)/P-16)	C39H74NO7P	M-H	698.5130	-2.0
699.0970	HMDB0173483	(2Z)-5-{9-[(3Z)-1,4-dicarboxy-2,3-dihydroxy-4-(4-hydroxyphenyl)but-3-en-1-yl]-11-hydroxy-3-oxo-2-oxatricyclo[6.3.1?]dodeca-1(11),4,6,8(12),9-pentaen-6-yl}-3,4-dihydroxy-2-(4-hydroxyphenyl)hex-2-enedioic acid	C35H26O17	M-H20-H	699.0986	-2.3

699.1919	HMDB0173015	3,4,5-trihydroxy-6-({5-hydroxy-2,9,26-trimethyl-4,,16,22,29-pentaoxo-3,19,23,28-tetraoxaocetacyclo[16.9.1.1?,,,??,nonacos-11-en-14-yl}oxy)oxane-2-carboxylic acid	C34H38O17	M-H2O-H	699.1925	-0.9
	HMDB0173016	3,4,5-trihydroxy-6-({14-hydroxy-2,9,26-trimethyl-4,,16,22,29-pentaoxo-3,19,23,28-tetraoxaocetacyclo[16.9.1.1?,,,??,nonacos-11-en-5-yl}oxy)oxane-2-carboxylic acid	C34H38O17	M-H2O-H	699.1925	-0.9
	HMDB0166238	3,4,5-trihydroxy-6-({5-hydroxy-1,14,21-trimethyl-25-methylidene-7,13,19,24,27-pentaoxo-4,,23-trioxaheptacyclo[.3.1.1.,,,??heptacos-8,11-dien-18-yl}oxy)oxane-2-carboxylic acid	C34H36O16	M-H	699.1931	-1.7
699.4049	HMDB0060814	Descladinose roxithromycin	C33H62N2O12	M+Na-2H	699.4049	-0.1
699.4955	HMDB0056295	DG(18:2n6/22:6n3)	C44H70O5	M+Na-2H	699.4970	-2.1
	HMDB0116699	PA(14/22:2(13Z,16Z))	C39H73O8P	M-H	699.4970	-2.2
	HMDB0115535	PA(:2(11Z,14Z)/16)	C39H73O8P	M-H	699.4970	-2.2
	HMDB0115510	PA(16/:2(11Z,14Z))	C39H73O8P	M-H	699.4970	-2.2
	HMDB0115296	PA(22:2(13Z,16Z)/14)	C39H73O8P	M-H	699.4970	-2.2
	HMDB0115271	PA(22:1(13Z)/14:1(9Z))	C39H73O8P	M-H	699.4970	-2.2
	HMDB0115095	PA(:1(11Z)/16:1(9Z))	C39H73O8P	M-H	699.4970	-2.2
	HMDB0114951	PA(18:2(9Z,12Z)/18)	C39H73O8P	M-H	699.4970	-2.2
	HMDB0114804	PA(14:1(9Z)/22:1(13Z))	C39H73O8P	M-H	699.4970	-2.2
	HMDB0007862	PA(18:1(11Z)/18:1(11Z))	C39H73O8P	M-H	699.4970	-2.2
	HMDB0007863	PA(18:1(11Z)/18:1(9Z))	C39H73O8P	M-H	699.4970	-2.2
	HMDB0007864	PA(18:1(9Z)/18:1(11Z))	C39H73O8P	M-H	699.4970	-2.2
	HMDB0007865	PA(18:1(9Z)/18:1(9Z))	C39H73O8P	M-H	699.4970	-2.2
	HMDB0031129	9-Octadecenoic acid 1-[(phosphonoxy)methyl]-1,2-ethanediyl ester	C39H73O8P	M-H	699.4970	-2.2
	HMDB0007861	PA(18/18:2(9Z,12Z))	C39H73O8P	M-H	699.4970	-2.2
699.5895	HMDB0056021	DG(16/24:1n9)	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0056046	DG(18/22:1n9)	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0056069	DG(/:1n9)	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0056091	DG(22/18:1n7)	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0056092	DG(22/18:1n9)	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0056113	DG(24/16:1n7)	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0007123	DG(16/24:1(15Z))	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0007823	DG(24:1(15Z)/16)	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0007795	DG(24/16:1(9Z))	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0007622	DG(22:1(13Z)/18)	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0007151	DG(16:1(9Z)/24)	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0007174	DG(18/22:1(13Z))	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0007202	DG(18:1(11Z)/22)	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0007231	DG(18:1(9Z)/22)	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0007369	DG(/:1(11Z))	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0007397	DG(:1(11Z)/)	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0007594	DG(22/18:1(11Z))	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0007595	DG(22/18:1(9Z))	C43H82O5	M+Na-2H	699.5909	-2.0
	HMDB0007935	PC(15/16)	C39H78NO8P	M-H2O-H	700.5281	-1.0
	HMDB0113985	PE-NMe2(18/14)	C39H78NO8P	M-H2O-H	700.5281	-1.0
	HMDB0113086	PE-NMe(18/15)	C39H78NO8P	M-H2O-H	700.5281	-1.0
	HMDB0113019	PE-NMe(15/18)	C39H78NO8P	M-H2O-H	700.5281	-1.0
	HMDB0113860	PE-NMe2(14/18)	C39H78NO8P	M-H2O-H	700.5281	-1.0
	HMDB0007967	PC(16/15)	C39H78NO8P	M-H2O-H	700.5281	-1.0
	HMDB0008833	PE(14/)	C39H78NO8P	M-H2O-H	700.5281	-1.0
	HMDB0008925	PE(16/18)	C39H78NO8P	M-H2O-H	700.5281	-1.0

700.5274	HMDB0008989	PE(18/16)	C39H78NO8P	M-H20-H	700.5281	-1.0
	HMDB0009217	PE(/14)	C39H78NO8P	M-H20-H	700.5281	-1.0
	HMDB0010566	PE-NMe2(16/16)	C39H78NO8P	M-H20-H	700.5281	-1.0
	HMDB0008951	PE(16/P-18:1(11Z))	C39H76NO7P	M-H	700.5287	-1.8
	HMDB0011437	PE(P-18:1(9Z)/16)	C39H76NO7P	M-H	700.5287	-1.8
	HMDB0011404	PE(P-18:1(11Z)/16)	C39H76NO7P	M-H	700.5287	-1.8
	HMDB0011372	PE(P-18/16:1(9Z))	C39H76NO7P	M-H	700.5287	-1.8
	HMDB0011341	PEP-16/18:1(11Z))	C39H76NO7P	M-H	700.5287	-1.8
	HMDB0011342	PE(P-16/18:1(9Z))	C39H76NO7P	M-H	700.5287	-1.8
	HMDB0009081	PE(18:1(9Z)/P-16)	C39H76NO7P	M-H	700.5287	-1.8
	HMDB0008983	PE(16:1(9Z)/P-18)	C39H76NO7P	M-H	700.5287	-1.8
	HMDB0008952	PE(16/P-18:1(9Z))	C39H76NO7P	M-H	700.5287	-1.8
	HMDB0009048	PE(18:1(11Z)/P-16)	C39H76NO7P	M-H	700.5287	-1.8
701.5299	HMDB0030129	Plastoquinone 8	C48H72O2	M+Na-2H	701.5279	2.9
714.5068	HMDB0113849	PE-NMe2(16:1(9Z)/16:1(9Z))	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0113848	PE-NMe2(14:1(9Z)/18:1(11Z))	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0113847	PE-NMe2(14:1(9Z)/18:1(9Z))	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0114065	PE-NMe2(18:2(9Z,12Z)/14)	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0114039	PE-NMe2(18:1(9Z)/14:1(9Z))	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0114012	PE-NMe2(18:1(11Z)/14:1(9Z))	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0113879	PE-NMe2(14/18:2(9Z,12Z))	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0113166	PE-NMe(18:2(9Z,12Z)/15)	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0113020	PE-NMe(15/18:2(9Z,12Z))	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0009283	PE(:2(11Z,14Z)/14)	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0009251	PE(:1(11Z)/14:1(9Z))	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0009088	PE(18:2(9Z,12Z)/16)	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0009056	PE(18:1(9Z)/16:1(9Z))	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0009023	PE(18:1(11Z)/16:1(9Z))	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0008960	PE(16:1(9Z)/18:1(9Z))	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0008959	PE(16:1(9Z)/18:1(11Z))	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0008928	PE(16/18:2(9Z,12Z))	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0008867	PE(14:1(9Z):1(11Z))	C39H74NO8P	M-H	714.5079	-1.6
	HMDB0008835	PE(14/:2(11Z,14Z))	C39H74NO8P	M-H	714.5079	-1.6

716.5225	HMDB0113852	PE-NMe2(14/18:1(11Z))	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0113853	PE-NMe2(14:1(9Z)/18)	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0113851	PE-NMe2(14/18:1(9Z))	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0112954	PE-NMe(15/18:1(11Z))	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0113850	PE-NMe2(16/16:1(9Z))	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0114038	PE-NMe2(18:1(9Z)/14)	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0114011	PE-NMe2(18:1(11Z)/14)	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0113986	PE-NMe2(18/14:1(9Z))	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0113965	PE-NMe2(16:1(9Z)/16)	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0113139	PE-NMe(18:1(9Z)/15)	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0113112	PE-NMe(18:1(11Z)/15)	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0112953	PE-NMe(15/18:1(9Z))	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0009250	PE(:1(11Z)/14)	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0009218	PE(/14:1(9Z))	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0009055	PE(18:1(9Z)/16)	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0008000	PC(16:1(9Z)/15)	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0008834	PE(14/:1(11Z))	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0008866	PE(14:1(9Z)/)	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0008926	PE(16/18:1(11Z))	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0008927	PE(16/18:1(9Z))	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0008958	PE(16:1(9Z)/18)	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0008990	PE(18/16:1(9Z))	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0009022	PE(18:1(11Z)/16)	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0007936	PC(15/16:1(9Z))	C39H76NO8P	M-H	716.5236	-1.5
	HMDB0114127	PE-NMe2(18:3(9Z,12Z,15Z)/16:1(9Z))	C41H74NO8P	M-H20-H	720.4968	0.1
	HMDB0114297	PE-NMe2(:3(8Z,11Z,14Z)/14:1(9Z))	C41H74NO8P	M-H20-H	720.4968	0.1
	HMDB0114324	PE-NMe2(:4(5Z,8Z,11Z,14Z)/14)	C41H74NO8P	M-H20-H	720.4968	0.1
	HMDB0114352	PE-NMe2(:4(8Z,11Z,14Z,17Z)/14)	C41H74NO8P	M-H20-H	720.4968	0.1
	HMDB0114269	PE-NMe2(:3(5Z,8Z,11Z)/14:1(9Z))	C41H74NO8P	M-H20-H	720.4968	0.1
	HMDB0114155	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/16)	C41H74NO8P	M-H20-H	720.4968	0.1
	HMDB0114098	PE-NMe2(18:3(6Z,9Z,12Z)/16:1(9Z))	C41H74NO8P	M-H20-H	720.4968	0.1
	HMDB0113028	PE-NMe(15/:4(5Z,8Z,11Z,14Z))	C41H74NO8P	M-H20-H	720.4968	0.1

720.4969

HMDB0113029	PE-NMe(15/:4(8Z,11Z,14Z,17Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0113424	PE-NMe(:4(5Z,8Z,11Z,14Z)/15)	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0113452	PE-NMe(:4(8Z,11Z,14Z,17Z)/15)	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0113887	PE-NMe2(14/:4(5Z,8Z,11Z,14Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0113888	PE-NMe2(14/:4(8Z,11Z,14Z,17Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0113906	PE-NMe2(14:1(9Z)/:3(8Z,11Z,14Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0113905	PE-NMe2(14:1(9Z)/:3(5Z,8Z,11Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0113946	PE-NMe2(16/18:4(6Z,9Z,12Z,15Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0113967	PE-NMe2(16:1(9Z)/18:3(6Z,9Z,12Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0113968	PE-NMe2(16:1(9Z)/18:3(9Z,12Z,15Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0007943	PC(15/18:4(6Z,9Z,12Z,15Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0009158	PE(18:3(9Z,12Z,15Z)/18:1(9Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0009157	PE(18:3(9Z,12Z,15Z)/18:1(11Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0009189	PE(18:4(6Z,9Z,12Z,15Z)/18)	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0009320	PE(:3(5Z,8Z,11Z)/16:1(9Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0009353	PE(:3(8Z,11Z,14Z)/16:1(9Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0009385	PE(:4(5Z,8Z,11Z,14Z)/16)	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0009580	PE(22:4(7Z,Z,13Z,16Z)/14)	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0009418	PE(:4(8Z,11Z,14Z,17Z)/16)	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0009125	PE(18:3(6Z,9Z,12Z)/18:1(9Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0009124	PE(18:3(6Z,9Z,12Z)/18:1(11Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0009093	PE(18:2(9Z,12Z)/18:2(9Z,12Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0008231	PC(18:4(6Z,9Z,12Z,15Z)/15)	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0008844	PE(14/22:4(7Z,Z,13Z,16Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0008937	PE(16/:4(5Z,8Z,11Z,14Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0008938	PE(16/:4(8Z,11Z,14Z,17Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0008968	PE(16:1(9Z)/:3(5Z,8Z,11Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0008997	PE(18/18:4(6Z,9Z,12Z,15Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0009028	PE(18:1(11Z)/18:3(6Z,9Z,12Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0009029	PE(18:1(11Z)/18:3(9Z,12Z,15Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0009062	PE(18:1(9Z)/18:3(9Z,12Z,15Z))	C41H74NO8P	M-H20-H	720.4968	0.1
HMDB0009061	PE(18:1(9Z)/18:3(6Z,9Z,12Z))	C41H74NO8P	M-H20-H	720.4968	0.1

	HMDB0009477	PE(:5(5Z,8Z,11Z,14Z,17Z)/P-16)	C41H72NO7P	M-H	720.4974	-0.6
	HMDB0011354	PE(P-16/:5(5Z,8Z,11Z,14Z,17Z))	C41H72NO7P	M-H	720.4974	-0.6
	HMDB0011412	PE(P-18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO7P	M-H	720.4974	-0.6
	HMDB0009215	PE(18:4(6Z,9Z,12Z,15Z)/P-18:1(11Z))	C41H72NO7P	M-H	720.4974	-0.6
	HMDB0009216	PE(18:4(6Z,9Z,12Z,15Z)/P-18:1(9Z))	C41H72NO7P	M-H	720.4974	-0.6
	HMDB0011445	PE(P-18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO7P	M-H	720.4974	-0.6
	HMDB0011438	PE(P-18:1(9Z)/16:1(9Z))	C39H74NO7P	M+Na-2H	720.4950	2.7
	HMDB0011405	PE(P-18:1(11Z)/16:1(9Z))	C39H74NO7P	M+Na-2H	720.4950	2.7
	HMDB0008984	PE(16:1(9Z)/P-18:1(11Z))	C39H74NO7P	M+Na-2H	720.4950	2.7
	HMDB0008985	PE(16:1(9Z)/P-18:1(9Z))	C39H74NO7P	M+Na-2H	720.4950	2.7
	HMDB0009114	PE(18:2(9Z,12Z)/P-16)	C39H74NO7P	M+Na-2H	720.4950	2.7
	HMDB0011343	PE(P-16/18:2(9Z,12Z))	C39H74NO7P	M+Na-2H	720.4950	2.7
721.5010	HMDB0116369	(2S)-1- {[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate	C43H72O7	M+Na-2H	721.5025	-2.0
	HMDB0116376	(2S)-2- {[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropyl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate	C43H72O7	M+Na-2H	721.5025	-2.0
	HMDB0116384	(2S)-2- {[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropyl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C43H72O7	M+Na-2H	721.5025	-2.0
	HMDB0116390	(2S)-1-hydroxy-3- {[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propan-2-yl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate	C43H72O7	M+Na-2H	721.5025	-2.0
	HMDB0116398	(2S)-1-hydroxy-3- {[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propan-2-yl 11-(3-methyl-5-propylfuran-2-yl)undecanoate	C43H72O7	M+Na-2H	721.5025	-2.0
	HMDB0116404	(2S)-3-hydroxy-2- {[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propyl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate	C43H72O7	M+Na-2H	721.5025	-2.0
	HMDB0116423	(2S)-1- {[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C43H72O7	M+Na-2H	721.5025	-2.0
	HMDB0116431	(2S)-1- {[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate	C43H72O7	M+Na-2H	721.5025	-2.0
	HMDB0116438	(2S)-1- {[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoate	C43H72O7	M+Na-2H	721.5025	-2.0
	HMDB0116443	(2S)-1-hydroxy-3- {[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propan-2-yl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate	C43H72O7	M+Na-2H	721.5025	-2.0
	HMDB0115728	PA(a-21/a-13)	C37H73O8P	M+FA-H	721.5025	-2.1
	HMDB0115717	PA(a-21/13)	C37H73O8P	M+FA-H	721.5025	-2.1
	HMDB0115712	PA(a-13/i-21)	C37H73O8P	M+FA-H	721.5025	-2.1
	HMDB0115734	PA(a-21/i-13)	C37H73O8P	M+FA-H	721.5025	-2.1
	HMDB0115908	PA(i-22/i-12)	C37H73O8P	M+FA-H	721.5025	-2.1
	HMDB0115891	PA(i-22/12)	C37H73O8P	M+FA-H	721.5025	-2.1
	HMDB0115879	PA(i-21/i-13)	C37H73O8P	M+FA-H	721.5025	-2.1
	HMDB0115873	PA(i-21/a-13)	C37H73O8P	M+FA-H	721.5025	-2.1
	HMDB0115862	PA(i-21/13)	C37H73O8P	M+FA-H	721.5025	-2.1
	HMDB0115850	PA(i-/i-14)	C37H73O8P	M+FA-H	721.5025	-2.1
	HMDB0115833	PA(i-/14)	C37H73O8P	M+FA-H	721.5025	-2.1

HMDB0115808	PA(i-13/i-21)	C37H73O8P	M+FA-H	721.5025	-2.1
HMDB0115797	PA(i-13/a-21)	C37H73O8P	M+FA-H	721.5025	-2.1
HMDB0115791	PA(i-12/i-22)	C37H73O8P	M+FA-H	721.5025	-2.1
HMDB0115701	PA(a-13/a-21)	C37H73O8P	M+FA-H	721.5025	-2.1
HMDB0115668	PA(22/i-12)	C37H73O8P	M+FA-H	721.5025	-2.1
HMDB0115652	PA(21/i-13)	C37H73O8P	M+FA-H	721.5025	-2.1
HMDB0115920	PA(i-24/)	C37H73O8P	M+FA-H	721.5025	-2.1
HMDB0114783	PA(14/)	C37H73O8P	M+FA-H	721.5025	-2.1
HMDB0114876	PA(18/16)	C37H73O8P	M+FA-H	721.5025	-2.1
HMDB0115061	PA(/14)	C37H73O8P	M+FA-H	721.5025	-2.1
HMDB0115226	PA(21/13)	C37H73O8P	M+FA-H	721.5025	-2.1
HMDB0115646	PA(21/a-13)	C37H73O8P	M+FA-H	721.5025	-2.1
HMDB0115636	PA(/i-14)	C37H73O8P	M+FA-H	721.5025	-2.1
HMDB0115622	PA(/i-24)	C37H73O8P	M+FA-H	721.5025	-2.1
HMDB0115238	PA(22/12)	C37H73O8P	M+FA-H	721.5025	-2.1
HMDB0010570	PG(16/16)	C38H75O10P	M-H	721.5025	-2.1
HMDB0116685	PG(i-13/i-19)	C38H75O10P	M-H	721.5025	-2.1
HMDB0116668	PG(i-12/i-)	C38H75O10P	M-H	721.5025	-2.1
HMDB0116649	PG(a-13/i-19)	C38H75O10P	M-H	721.5025	-2.1
HMDB0113886	PE-NMe2(14/:3(8Z,11Z,14Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0114069	PE-NMe2(18:2(9Z,12Z)/16:1(9Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0114097	PE-NMe2(18:3(6Z,9Z,12Z)/16)	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0114126	PE-NMe2(18:3(9Z,12Z,15Z)/16)	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0114268	PE-NMe2(:3(5Z,8Z,11Z)/14)	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0114296	PE-NMe2(:3(8Z,11Z,14Z)/14)	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0113904	PE-NMe2(14:1(9Z)/:2(11Z,14Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0114240	PE-NMe2(:2(11Z,14Z)/14:1(9Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0113966	PE-NMe2(16:1(9Z)/18:2(9Z,12Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0113945	PE-NMe2(16/18:3(9Z,12Z,15Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0113944	PE-NMe2(16/18:3(6Z,9Z,12Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0113027	PE-NMe(15/:3(8Z,11Z,14Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0113026	PE-NMe(15/:3(5Z,8Z,11Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0113368	PE-NMe(:3(5Z,8Z,11Z)/15)	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0113396	PE-NMe(:3(8Z,11Z,14Z)/15)	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0113885	PE-NMe2(14/:3(5Z,8Z,11Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0009548	PE(22:2(13Z,16Z)/14:1(9Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0008995	PE(18/18:3(6Z,9Z,12Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0009027	PE(18:1(11Z)/18:2(9Z,12Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0009060	PE(18:1(9Z)/18:2(9Z,12Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0009156	PE(18:3(9Z,12Z,15Z)/18)	C41H76NO8P	M-H20-H	722.5125	-1.1

722.5117

HMDB0009091	PE(18:2(9Z,12Z)/18:1(11Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0009092	PE(18:2(9Z,12Z)/18:1(9Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0009123	PE(18:3(6Z,9Z,12Z)/18)	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0007942	PC(15/18:3(9Z,12Z,15Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0009287	PE(:2(11Z,14Z)/16:1(9Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0009319	PE(:3(5Z,8Z,11Z)/16)	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0009352	PE(:3(8Z,11Z,14Z)/16)	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0008996	PE(18/18:3(9Z,12Z,15Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0008967	PE(16:1(9Z):2(11Z,14Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0008876	PE(14:1(9Z)/22:2(13Z,16Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0008936	PE(16/:3(8Z,11Z,14Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0008935	PE(16/:3(5Z,8Z,11Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0008165	PC(18:3(6Z,9Z,12Z)/15)	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0007941	PC(15/18:3(6Z,9Z,12Z))	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0008198	PC(18:3(9Z,12Z,15Z)/15)	C41H76NO8P	M-H20-H	722.5125	-1.1
HMDB0008983	PE(16:1(9Z)/P-18)	C39H76NO7P	M+Na-2H	722.5106	1.5
HMDB0009081	PE(18:1(9Z)/P-16)	C39H76NO7P	M+Na-2H	722.5106	1.5
HMDB0008951	PE(16/P-18:1(11Z))	C39H76NO7P	M+Na-2H	722.5106	1.5
HMDB0009048	PE(18:1(11Z)/P-16)	C39H76NO7P	M+Na-2H	722.5106	1.5
HMDB0008952	PE(16/P-18:1(9Z))	C39H76NO7P	M+Na-2H	722.5106	1.5
HMDB0011342	PE(P-16/18:1(9Z))	C39H76NO7P	M+Na-2H	722.5106	1.5
HMDB0011341	PEP-16/18:1(11Z))	C39H76NO7P	M+Na-2H	722.5106	1.5
HMDB0011404	PE(P-18:1(11Z)/16)	C39H76NO7P	M+Na-2H	722.5106	1.5
HMDB0011372	PE(P-18/16:1(9Z))	C39H76NO7P	M+Na-2H	722.5106	1.5
HMDB0011437	PE(P-18:1(9Z)/16)	C39H76NO7P	M+Na-2H	722.5106	1.5
HMDB0009150	PE(18:3(6Z,9Z,12Z)/P-18:1(9Z))	C41H74NO7P	M-H	722.5130	-1.8
HMDB0009149	PE(18:3(6Z,9Z,12Z)/P-18:1(11Z))	C41H74NO7P	M-H	722.5130	-1.8
HMDB0011444	PE(P-18:1(9Z)/18:3(9Z,12Z,15Z))	C41H74NO7P	M-H	722.5130	-1.8
HMDB0009214	PE(18:4(6Z,9Z,12Z,15Z)/P-18)	C41H74NO7P	M-H	722.5130	-1.8
HMDB0009183	PE(18:3(9Z,12Z,15Z)/P-18:1(9Z))	C41H74NO7P	M-H	722.5130	-1.8
HMDB0009182	PE(18:3(9Z,12Z,15Z)/P-18:1(11Z))	C41H74NO7P	M-H	722.5130	-1.8
HMDB0011379	PE(P-18/18:4(6Z,9Z,12Z,15Z))	C41H74NO7P	M-H	722.5130	-1.8

	HMDB0011410	PE(P-18:1(11Z)/18:3(6Z,9Z,12Z))	C41H74NO7P	M-H	722.5130	-1.8
	HMDB0009411	PE(:4(5Z,8Z,11Z,14Z)/P-16)	C41H74NO7P	M-H	722.5130	-1.8
	HMDB0009444	PE(:4(8Z,11Z,14Z,17Z)/P-16)	C41H74NO7P	M-H	722.5130	-1.8
	HMDB0011352	PE(P-16/:4(5Z,8Z,11Z,14Z))	C41H74NO7P	M-H	722.5130	-1.8
	HMDB0011411	PE(P-18:1(11Z)/18:3(9Z,12Z,15Z))	C41H74NO7P	M-H	722.5130	-1.8
	HMDB0011353	PE(P-16/:4(8Z,11Z,14Z,17Z))	C41H74NO7P	M-H	722.5130	-1.8
	HMDB0011443	PE(P-18:1(9Z)/18:3(6Z,9Z,12Z))	C41H74NO7P	M-H	722.5130	-1.8
724.5274	HMDB0113857	PE-NMe2(16:1(9Z)/18:1(9Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0113856	PE-NMe2(14:1(9Z)/:1(11Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0113943	PE-NMe2(16/18:2(9Z,12Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0114015	PE-NMe2(18:1(11Z)/16:1(9Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0114042	PE-NMe2(18:1(9Z)/16:1(9Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0114068	PE-NMe2(18:2(9Z,12Z)/16)	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0114211	PE-NMe2(:1(11Z)/14:1(9Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0113025	PE-NMe(15/:2(11Z,14Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0113339	PE-NMe(:2(11Z,14Z)/15)	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0113884	PE-NMe2(14/:2(11Z,14Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0114239	PE-NMe2(:2(11Z,14Z)/14)	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0113858	PE-NMe2(16:1(9Z)/18:1(11Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0009058	PE(18:1(9Z)/18:1(11Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0009025	PE(18:1(11Z)/18:1(11Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0009026	PE(18:1(11Z)/18:1(9Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0009059	PE(18:1(9Z)/18:1(9Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0009286	PE(:2(11Z,14Z)/16)	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0009090	PE(18:2(9Z,12Z)/18)	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0009254	PE(:1(11Z)/16:1(9Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0007940	PC(15/18:2(9Z,12Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0008875	PE(14:1(9Z)/22:1(13Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0008843	PE(14/22:2(13Z,16Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0008132	PC(18:2(9Z,12Z)/15)	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0008934	PE(16/:2(11Z,14Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
	HMDB0009515	PE(22:1(13Z)/14:1(9Z))	C41H78NO8P	M-H20-H	724.5281	-1.0

HMDB0008994	PE(18/18:2(9Z,12Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
HMDB0008966	PE(16:1(9Z):1(11Z))	C41H78NO8P	M-H20-H	724.5281	-1.0
HMDB0009547	PE(22:2(13Z,16Z)/14)	C41H78NO8P	M-H20-H	724.5281	-1.0
HMDB0011157	PE(O-16/18:1(9Z))	C39H78NO7P	M+Na-2H	724.5263	1.6
HMDB0011371	PE(P-18/16)	C39H78NO7P	M+Na-2H	724.5263	1.6
HMDB0011205	PC(P-16/15)	C39H78NO7P	M+Na-2H	724.5263	1.6
HMDB0011340	PE(P-16/18)	C39H78NO7P	M+Na-2H	724.5263	1.6
HMDB0008950	PE(16/P-18)	C39H78NO7P	M+Na-2H	724.5263	1.6
HMDB0009015	PE(18/P-16)	C39H78NO7P	M+Na-2H	724.5263	1.6
HMDB0007961	PC(15/P-16)	C39H78NO7P	M+Na-2H	724.5263	1.6
HMDB0009181	PE(18:3(9Z,12Z,15Z)/P-18)	C41H76NO7P	M-H	724.5287	-1.7
HMDB0009378	PE(:3(8Z,11Z,14Z)/P-16)	C41H76NO7P	M-H	724.5287	-1.7
HMDB0009117	PE(18:2(9Z,12Z)/P-18:1(9Z))	C41H76NO7P	M-H	724.5287	-1.7
HMDB0009345	PE(:3(5Z,8Z,11Z)/P-16)	C41H76NO7P	M-H	724.5287	-1.7
HMDB0009116	PE(18:2(9Z,12Z)/P-18:1(11Z))	C41H76NO7P	M-H	724.5287	-1.7
HMDB0009148	PE(18:3(6Z,9Z,12Z)/P-18)	C41H76NO7P	M-H	724.5287	-1.7
HMDB0011350	PE(P-16/:3(5Z,8Z,11Z))	C41H76NO7P	M-H	724.5287	-1.7
HMDB0011351	PE(P-16/:3(8Z,11Z,14Z))	C41H76NO7P	M-H	724.5287	-1.7
HMDB0011442	PE(P-18:1(9Z)/18:2(9Z,12Z))	C41H76NO7P	M-H	724.5287	-1.7
HMDB0011378	PE(P-18/18:3(9Z,12Z,15Z))	C41H76NO7P	M-H	724.5287	-1.7
HMDB0011377	PE(P-18/18:3(6Z,9Z,12Z))	C41H76NO7P	M-H	724.5287	-1.7
HMDB0011409	PE(P-18:1(11Z)/18:2(9Z,12Z))	C41H76NO7P	M-H	724.5287	-1.7
HMDB0010568	PE-NMe2(16/18:1(9Z))	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0009514	PE(22:1(13Z)/14)	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0009482	PE(22/14:1(9Z))	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0007939	PC(15/18:1(9Z))	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0008992	PE(18/18:1(11Z))	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0008965	PE(16:1(9Z)/)	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0008933	PE(16/:1(11Z))	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0008874	PE(14:1(9Z)/22)	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0008842	PE(14/22:1(13Z))	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0008099	PC(18:1(9Z)/15)	C41H80NO8P	M-H20-H	726.5438	-1.1

726.5430

HMDB0007938	PC(15/18:1(11Z))	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0008066	PC(18:1(11Z)/15)	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0009024	PE(18:1(11Z)/18)	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0009253	PE(:1(11Z)/16)	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0009221	PE(/16:1(9Z))	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0113863	PE-NMe2(16:1(9Z)/18)	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0113862	PE-NMe2(16/18:1(11Z))	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0112963	PE-NMe(15/:1(11Z))	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0113859	PE-NMe2(14/:1(11Z))	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0113861	PE-NMe2(14:1(9Z)/)	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0113989	PE-NMe2(18/16:1(9Z))	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0114014	PE-NMe2(18:1(11Z)/16)	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0114041	PE-NMe2(18:1(9Z)/16)	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0114182	PE-NMe2(/14:1(9Z))	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0114210	PE-NMe2(:1(11Z)/14)	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0113310	PE-NMe(:1(11Z)/15)	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0008993	PE(18/18:1(9Z))	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0009057	PE(18:1(9Z)/18)	C41H80NO8P	M-H20-H	726.5438	-1.1
HMDB0011441	PE(P-18:1(9Z)/18:1(9Z))	C41H78NO7P	M-H	726.5443	-1.8
HMDB0009051	PE(18:1(11Z)/P-18:1(9Z))	C41H78NO7P	M-H	726.5443	-1.8
HMDB0011407	PE(P-18:1(11Z)/18:1(11Z))	C41H78NO7P	M-H	726.5443	-1.8
HMDB0009050	PE(18:1(11Z)/P-18:1(11Z))	C41H78NO7P	M-H	726.5443	-1.8
HMDB0011440	PE(P-18:1(9Z)/18:1(11Z))	C41H78NO7P	M-H	726.5443	-1.8
HMDB0009083	PE(18:1(9Z)/P-18:1(11Z))	C41H78NO7P	M-H	726.5443	-1.8
HMDB0009084	PE(18:1(9Z)/P-18:1(9Z))	C41H78NO7P	M-H	726.5443	-1.8
HMDB0009115	PE(18:2(9Z,12Z)/P-18)	C41H78NO7P	M-H	726.5443	-1.8
HMDB0011349	PE(P-16/:2(11Z,14Z))	C41H78NO7P	M-H	726.5443	-1.8
HMDB0011376	PE(P-18/18:2(9Z,12Z))	C41H78NO7P	M-H	726.5443	-1.8
HMDB0011408	PE(P-18:1(11Z)/18:1(9Z))	C41H78NO7P	M-H	726.5443	-1.8
HMDB0009312	PE(:2(11Z,14Z)/P-16)	C41H78NO7P	M-H	726.5443	-1.8
HMDB0060501	Phosphatidylethanolamine	C41H82NO8P	M-H20-H	728.5594	-0.8
HMDB0009481	PE(22/14)	C41H82NO8P	M-H20-H	728.5594	-0.8

728.5588	HMDB0008932	PE(16/)	C41H82NO8P	M-H2O-H	728.5594	-0.8
	HMDB0008841	PE(14/22)	C41H82NO8P	M-H2O-H	728.5594	-0.8
	HMDB0008033	PC(18/15)	C41H82NO8P	M-H2O-H	728.5594	-0.8
	HMDB0007937	PC(15/18)	C41H82NO8P	M-H2O-H	728.5594	-0.8
	HMDB0009220	PE(/16)	C41H82NO8P	M-H2O-H	728.5594	-0.8
	HMDB0114181	PE-NMe2(/14)	C41H82NO8P	M-H2O-H	728.5594	-0.8
	HMDB0113988	PE-NMe2(18/16)	C41H82NO8P	M-H2O-H	728.5594	-0.8
	HMDB0113883	PE-NMe2(14/)	C41H82NO8P	M-H2O-H	728.5594	-0.8
	HMDB0113281	PE-NMe(/15)	C41H82NO8P	M-H2O-H	728.5594	-0.8
	HMDB0113024	PE-NMe(15/)	C41H82NO8P	M-H2O-H	728.5594	-0.8
	HMDB0113866	PE-NMe2(16/18)	C41H82NO8P	M-H2O-H	728.5594	-0.8
	HMDB0008991	PE(18/18)	C41H82NO8P	M-H2O-H	728.5594	-0.8
	HMDB0009017	PE(18/P-18:1(11Z))	C41H80NO7P	M-H	728.5600	-1.6
	HMDB0011439	PE(P-18:1(9Z)/18)	C41H80NO7P	M-H	728.5600	-1.6
	HMDB0011406	PE(P-18:1(11Z)/18)	C41H80NO7P	M-H	728.5600	-1.6
	HMDB0011375	PE(P-18/18:1(9Z))	C41H80NO7P	M-H	728.5600	-1.6
	HMDB0011374	PE(P-18/18:1(11Z))	C41H80NO7P	M-H	728.5600	-1.6
	HMDB0011348	PE(P-16/:1(11Z))	C41H80NO7P	M-H	728.5600	-1.6
	HMDB0011304	PC(P-18:1(9Z)/15)	C41H80NO7P	M-H	728.5600	-1.6
	HMDB0011271	PC(P-18:1(11Z)/15)	C41H80NO7P	M-H	728.5600	-1.6
	HMDB0009279	PE(:1(11Z)/P-16)	C41H80NO7P	M-H	728.5600	-1.6
	HMDB0009082	PE(18:1(9Z)/P-18)	C41H80NO7P	M-H	728.5600	-1.6
	HMDB0009049	PE(18:1(11Z)/P-18)	C41H80NO7P	M-H	728.5600	-1.6
	HMDB0009018	PE(18/P-18:1(9Z))	C41H80NO7P	M-H	728.5600	-1.6
	HMDB0007963	PC(15/P-18:1(11Z))	C41H80NO7P	M-H	728.5600	-1.6
	HMDB0007964	PC(15/P-18:1(9Z))	C41H80NO7P	M-H	728.5600	-1.6
	HMDB0113844	PE-NMe2(14:1(9Z)/16:1(9Z))	C37H70NO8P	M+FA-H	732.4821	-2.3
	HMDB0008829	PE(14/18:2(9Z,12Z))	C37H70NO8P	M+FA-H	732.4821	-2.3
	HMDB0009085	PE(18:2(9Z,12Z)/14)	C37H70NO8P	M+FA-H	732.4821	-2.3
	HMDB0009053	PE(18:1(9Z)/14:1(9Z))	C37H70NO8P	M+FA-H	732.4821	-2.3
	HMDB0009020	PE(18:1(11Z)/14:1(9Z))	C37H70NO8P	M+FA-H	732.4821	-2.3
	HMDB0008957	PE(16:1(9Z)/16:1(9Z))	C37H70NO8P	M+FA-H	732.4821	-2.3

732.4804	HMDB0008861	PE(14:1(9Z)/18:1(9Z))	C37H70NO8P	M+FA-H	732.4821	-2.3
	HMDB0113963	PE-NMe2(16:1(9Z)/14:1(9Z))	C37H70NO8P	M+FA-H	732.4821	-2.3
	HMDB0008860	PE(14:1(9Z)/18:1(11Z))	C37H70NO8P	M+FA-H	732.4821	-2.3
	HMDB0012375	PS(18/14:1(9Z))	C38H72NO10P	M-H	732.4821	-2.3
	HMDB0012345	PS(14:1(9Z)/18)	C38H72NO10P	M-H	732.4821	-2.3
	HMDB0112266	PS(14/18:1(11Z))	C38H72NO10P	M-H	732.4821	-2.3
	HMDB0112269	PS(18:1(11Z)/14)	C38H72NO10P	M-H	732.4821	-2.3
	HMDB0012365	PS(16:1(9Z)/16)	C38H72NO10P	M-H	732.4821	-2.3
	HMDB0012385	PS(18:1(9Z)/14)	C38H72NO10P	M-H	732.4821	-2.3
	HMDB0012355	PS(16/16:1(9Z))	C38H72NO10P	M-H	732.4821	-2.3
	HMDB0012335	PS(14/18:1(9Z))	C38H72NO10P	M-H	732.4821	-2.3
733.4830	HMDB0180968	(25Z)-N-[2-(1H-indol-3-yl)ethyl]-2-(sulfooxy)triacont-25-enimidic acid	C40H68N2O5S	M+FA-H	733.4831	-0.1
	HMDB0180970	(25Z)-N-[2-(1H-indol-3-yl)-2-(sulfooxy)ethyl]triacont-25-enimidic acid	C40H68N2O5S	M+FA-H	733.4831	-0.1
	HMDB0180966	(25Z)-N-[2-(1H-indol-3-yl)ethyl]--(sulfooxy)triacont-25-enimidic acid	C40H68N2O5S	M+FA-H	733.4831	-0.1
	HMDB0180960	(25Z)-N-[2-(1H-indol-3-yl)ethyl]-29-(sulfooxy)triacont-25-enimidic acid	C40H68N2O5S	M+FA-H	733.4831	-0.1
	HMDB0180956	(25Z)-N-[2-(1H-indol-3-yl)ethyl]-27-(sulfooxy)triacont-25-enimidic acid	C40H68N2O5S	M+FA-H	733.4831	-0.1
	HMDB0180958	(25Z)-N-[2-(1H-indol-3-yl)ethyl]-24-(sulfooxy)triacont-25-enimidic acid	C40H68N2O5S	M+FA-H	733.4831	-0.1
	HMDB0056386	DG(22:6n3/22:6n3)	C47H68O5	M+Na-2H	733.4813	2.3
	HMDB0007788	DG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C47H68O5	M+Na-2H	733.4813	2.3
734.4958	HMDB0113842	PE-NMe2(14/16:1(9Z))	C37H72NO8P	M+FA-H	734.4978	-2.7
	HMDB0112945	PE-NMe(15/16:1(9Z))	C37H72NO8P	M+FA-H	734.4978	-2.7
	HMDB0113962	PE-NMe2(16:1(9Z)/14)	C37H72NO8P	M+FA-H	734.4978	-2.7
	HMDB0113941	PE-NMe2(16/14:1(9Z))	C37H72NO8P	M+FA-H	734.4978	-2.7
	HMDB0113063	PE-NMe(16:1(9Z)/15)	C37H72NO8P	M+FA-H	734.4978	-2.7
	HMDB0113843	PE-NMe2(14:1(9Z)/16)	C37H72NO8P	M+FA-H	734.4978	-2.7
	HMDB0008827	PE(14/18:1(11Z))	C37H72NO8P	M+FA-H	734.4978	-2.7
	HMDB0008828	PE(14/18:1(9Z))	C37H72NO8P	M+FA-H	734.4978	-2.7
	HMDB0008859	PE(14:1(9Z)/18)	C37H72NO8P	M+FA-H	734.4978	-2.7
	HMDB0008924	PE(16/16:1(9Z))	C37H72NO8P	M+FA-H	734.4978	-2.7
	HMDB0009052	PE(18:1(9Z)/14)	C37H72NO8P	M+FA-H	734.4978	-2.7
	HMDB0009019	PE(18:1(11Z)/14)	C37H72NO8P	M+FA-H	734.4978	-2.7
	HMDB0008987	PE(18/14:1(9Z))	C37H72NO8P	M+FA-H	734.4978	-2.7
	HMDB0007901	PC(14:1(9Z)/15)	C37H72NO8P	M+FA-H	734.4978	-2.7

	HMDB0007933	PC(15/14:1(9Z))	C37H72NO8P	M+FA-H	734.4978	-2.7
	HMDB0008956	PE(16:1(9Z)/16)	C37H72NO8P	M+FA-H	734.4978	-2.7
	HMDB0012334	PS(14/18)	C38H74NO10P	M-H	734.4978	-2.7
	HMDB0012374	PS(18/14)	C38H74NO10P	M-H	734.4978	-2.7
	HMDB0000614	PS(16/16)	C38H74NO10P	M-H	734.4978	-2.7
736.5272	HMDB0113143	PE-NMe(18:1(9Z)/18:2(9Z,12Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113116	PE-NMe(18:1(11Z)/18:2(9Z,12Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113090	PE-NMe(18/18:3(6Z,9Z,12Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113091	PE-NMe(18/18:3(9Z,12Z,15Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113049	PE-NMe(16/:3(8Z,11Z,14Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113048	PE-NMe(16/:3(5Z,8Z,11Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113011	PE-NMe(14:1(9Z)/22:2(13Z,16Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113170	PE-NMe(18:2(9Z,12Z)/18:1(11Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113171	PE-NMe(18:2(9Z,12Z)/18:1(9Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113198	PE-NMe(18:3(6Z,9Z,12Z)/18)	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113341	PE-NMe(:2(11Z,14Z)/16:1(9Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113069	PE-NMe(16:1(9Z)/:2(11Z,14Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0114298	PE-NMe2(:3(8Z,11Z,14Z)/15)	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0114270	PE-NMe2(:3(5Z,8Z,11Z)/15)	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113927	PE-NMe2(15/:3(8Z,11Z,14Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113926	PE-NMe2(15/:3(5Z,8Z,11Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113564	PE-NMe(22:2(13Z,16Z)/14:1(9Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113397	PE-NMe(:3(8Z,11Z,14Z)/16)	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113369	PE-NMe(:3(5Z,8Z,11Z)/16)	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0113226	PE-NMe(18:3(9Z,12Z,15Z)/18)	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0007882	PC(14/:3(8Z,11Z,14Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0008394	PC(:3(8Z,11Z,14Z)/14)	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0007881	PC(14/:3(5Z,8Z,11Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0007913	PC(14:1(9Z)/:2(11Z,14Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0007975	PC(16/18:3(9Z,12Z,15Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0007974	PC(16/18:3(6Z,9Z,12Z))	C42H78NO8P	M-H20-H	736.5281	-1.2
	HMDB0008006	PC(16:1(9Z)/18:2(9Z,12Z))	C42H78NO8P	M-H20-H	736.5281	-1.2

HMDB0008134	PC(18:2(9Z,12Z)/16:1(9Z))	C42H78NO8P	M-H2O-H	736.5281	-1.2
HMDB0008166	PC(18:3(6Z,9Z,12Z)/16)	C42H78NO8P	M-H2O-H	736.5281	-1.2
HMDB0008199	PC(18:3(9Z,12Z,15Z)/16)	C42H78NO8P	M-H2O-H	736.5281	-1.2
HMDB0008329	PC(:2(11Z,14Z)/14:1(9Z))	C42H78NO8P	M-H2O-H	736.5281	-1.2
HMDB0008361	PC(:3(5Z,8Z,11Z)/14)	C42H78NO8P	M-H2O-H	736.5281	-1.2
HMDB0008027	PC(16:1(9Z)/P-16)	C40H78NO7P	M+Na-2H	736.5263	1.3
HMDB0013411	PC(O-16:1(9Z)/16:1(9Z))	C40H78NO7P	M+Na-2H	736.5263	1.3
HMDB0007929	PC(14:1(9Z)/P-18)	C40H78NO7P	M+Na-2H	736.5263	1.3
HMDB0007898	PC(14/P-18:1(9Z))	C40H78NO7P	M+Na-2H	736.5263	1.3
HMDB0007897	PC(14/P-18:1(11Z))	C40H78NO7P	M+Na-2H	736.5263	1.3
HMDB0011207	PC(P-16/16:1(9Z))	C40H78NO7P	M+Na-2H	736.5263	1.3
HMDB0011302	PC(P-18:1(9Z)/14)	C40H78NO7P	M+Na-2H	736.5263	1.3
HMDB0011269	PC(P-18:1(11Z)/14)	C40H78NO7P	M+Na-2H	736.5263	1.3
HMDB0011237	PC(P-18/14:1(9Z))	C40H78NO7P	M+Na-2H	736.5263	1.3
HMDB0011214	PC(P-16/18:4(6Z,9Z,12Z,15Z))	C42H76NO7P	M-H	736.5287	-2.0
HMDB0008258	PC(18:4(6Z,9Z,12Z,15Z)/P-16)	C42H76NO7P	M-H	736.5287	-2.0
HMDB0114155	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/16)	C41H74NO8P	M-H	738.5079	-1.3
HMDB0114127	PE-NMe2(18:3(9Z,12Z,15Z)/16:1(9Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0114098	PE-NMe2(18:3(6Z,9Z,12Z)/16:1(9Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0113968	PE-NMe2(16:1(9Z)/18:3(9Z,12Z,15Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0113967	PE-NMe2(16:1(9Z)/18:3(6Z,9Z,12Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0113946	PE-NMe2(16/18:4(6Z,9Z,12Z,15Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0114352	PE-NMe2(:4(8Z,11Z,14Z,17Z)/14)	C41H74NO8P	M-H	738.5079	-1.3
HMDB0114324	PE-NMe2(:4(5Z,8Z,11Z,14Z)/14)	C41H74NO8P	M-H	738.5079	-1.3
HMDB0114297	PE-NMe2(:3(8Z,11Z,14Z)/14:1(9Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0113905	PE-NMe2(14:1(9Z)/:3(5Z,8Z,11Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0113424	PE-NMe(:4(5Z,8Z,11Z,14Z)/15)	C41H74NO8P	M-H	738.5079	-1.3
HMDB0113029	PE-NMe(15/:4(8Z,11Z,14Z,17Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0113028	PE-NMe(15/:4(5Z,8Z,11Z,14Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0113906	PE-NMe2(14:1(9Z)/:3(8Z,11Z,14Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0113888	PE-NMe2(14/:4(8Z,11Z,14Z,17Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0113887	PE-NMe2(14/:4(5Z,8Z,11Z,14Z))	C41H74NO8P	M-H	738.5079	-1.3

738.5070

HMDB0113452	PE-NMe(:4(8Z,11Z,14Z,17Z)/15)	C41H74NO8P	M-H	738.5079	-1.3
HMDB0114269	PE-NMe2(:3(5Z,8Z,11Z)/14:1(9Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0009124	PE(18:3(6Z,9Z,12Z)/18:1(11Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0009061	PE(18:1(9Z)/18:3(6Z,9Z,12Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0009093	PE(18:2(9Z,12Z)/18:2(9Z,12Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0008997	PE(18/18:4(6Z,9Z,12Z,15Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0009125	PE(18:3(6Z,9Z,12Z)/18:1(9Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0009158	PE(18:3(9Z,12Z,15Z)/18:1(9Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0009157	PE(18:3(9Z,12Z,15Z)/18:1(11Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0009189	PE(18:4(6Z,9Z,12Z,15Z)/18)	C41H74NO8P	M-H	738.5079	-1.3
HMDB0009320	PE(:3(5Z,8Z,11Z)/16:1(9Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0009062	PE(18:1(9Z)/18:3(9Z,12Z,15Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0009029	PE(18:1(11Z)/18:3(9Z,12Z,15Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0007943	PC(15/18:4(6Z,9Z,12Z,15Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0008231	PC(18:4(6Z,9Z,12Z,15Z)/15)	C41H74NO8P	M-H	738.5079	-1.3
HMDB0008844	PE(14/22:4(7Z,Z,13Z,16Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0008937	PE(16/:4(5Z,8Z,11Z,14Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0008938	PE(16/:4(8Z,11Z,14Z,17Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0008968	PE(16:1(9Z)/:3(5Z,8Z,11Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0009353	PE(:3(8Z,11Z,14Z)/16:1(9Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0009028	PE(18:1(11Z)/18:3(6Z,9Z,12Z))	C41H74NO8P	M-H	738.5079	-1.3
HMDB0009385	PE(:4(5Z,8Z,11Z,14Z)/16)	C41H74NO8P	M-H	738.5079	-1.3
HMDB0009418	PE(:4(8Z,11Z,14Z,17Z)/16)	C41H74NO8P	M-H	738.5079	-1.3
HMDB0009580	PE(22:4(7Z,Z,13Z,16Z)/14)	C41H74NO8P	M-H	738.5079	-1.3
HMDB0113853	PE-NMe2(14:1(9Z)/18)	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0113112	PE-NMe(18:1(11Z)/15)	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0113986	PE-NMe2(18/14:1(9Z))	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0113965	PE-NMe2(16:1(9Z)/16)	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0114038	PE-NMe2(18:1(9Z)/14)	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0114011	PE-NMe2(18:1(11Z)/14)	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0113139	PE-NMe(18:1(9Z)/15)	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0008000	PC(16:1(9Z)/15)	C39H76NO8P	M+Na-2H	738.5055	2.0

HMDB0008834	PE(14:1(11Z))	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0008866	PE(14:1(9Z)/)	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0008926	PE(16/18:1(11Z))	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0008927	PE(16/18:1(9Z))	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0008958	PE(16:1(9Z)/18)	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0008990	PE(18/16:1(9Z))	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0009022	PE(18:1(11Z)/16)	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0009055	PE(18:1(9Z)/16)	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0007936	PC(15/16:1(9Z))	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0009218	PE(/14:1(9Z))	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0009250	PE(:1(11Z)/14)	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0112954	PE-NMe(15/18:1(11Z))	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0113850	PE-NMe2(16/16:1(9Z))	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0113851	PE-NMe2(14/18:1(9Z))	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0112953	PE-NMe(15/18:1(9Z))	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0113852	PE-NMe2(14/18:1(11Z))	C39H76NO8P	M+Na-2H	738.5055	2.0
HMDB0009217	PE(/14)	C39H78NO8P	M+Na-2H	740.5212	1.3
HMDB0010566	PE-NMe2(16/16)	C39H78NO8P	M+Na-2H	740.5212	1.3
HMDB0113860	PE-NMe2(14/18)	C39H78NO8P	M+Na-2H	740.5212	1.3
HMDB0113019	PE-NMe(15/18)	C39H78NO8P	M+Na-2H	740.5212	1.3
HMDB0113985	PE-NMe2(18/14)	C39H78NO8P	M+Na-2H	740.5212	1.3
HMDB0007935	PC(15/16)	C39H78NO8P	M+Na-2H	740.5212	1.3
HMDB0007967	PC(16/15)	C39H78NO8P	M+Na-2H	740.5212	1.3
HMDB0008833	PE(14/)	C39H78NO8P	M+Na-2H	740.5212	1.3
HMDB0008925	PE(16/18)	C39H78NO8P	M+Na-2H	740.5212	1.3
HMDB0113086	PE-NMe(18/15)	C39H78NO8P	M+Na-2H	740.5212	1.3
HMDB0008989	PE(18/16)	C39H78NO8P	M+Na-2H	740.5212	1.3
HMDB0113368	PE-NMe(:3(5Z,8Z,11Z)/15)	C41H76NO8P	M-H	740.5236	-2.0
HMDB0113026	PE-NMe(15/:3(5Z,8Z,11Z))	C41H76NO8P	M-H	740.5236	-2.0
HMDB0113027	PE-NMe(15/:3(8Z,11Z,14Z))	C41H76NO8P	M-H	740.5236	-2.0
HMDB0113396	PE-NMe(:3(8Z,11Z,14Z)/15)	C41H76NO8P	M-H	740.5236	-2.0
HMDB0113904	PE-NMe2(14:1(9Z)/:2(11Z,14Z))	C41H76NO8P	M-H	740.5236	-2.0

740.5221	HMDB0114240	PE-NMe2(:2(11Z,14Z)/14:1(9Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0009027	PE(18:1(11Z)/18:2(9Z,12Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0114296	PE-NMe2(:3(8Z,11Z,14Z)/14)	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0114268	PE-NMe2(:3(5Z,8Z,11Z)/14)	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0113886	PE-NMe2(14/:3(8Z,11Z,14Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0113885	PE-NMe2(14/:3(5Z,8Z,11Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0113944	PE-NMe2(16/18:3(6Z,9Z,12Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0113945	PE-NMe2(16/18:3(9Z,12Z,15Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0113966	PE-NMe2(16:1(9Z)/18:2(9Z,12Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0114069	PE-NMe2(18:2(9Z,12Z)/16:1(9Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0114097	PE-NMe2(18:3(6Z,9Z,12Z)/16)	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0114126	PE-NMe2(18:3(9Z,12Z,15Z)/16)	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0007942	PC(15/18:3(9Z,12Z,15Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0009156	PE(18:3(9Z,12Z,15Z)/18)	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0009287	PE(:2(11Z,14Z)/16:1(9Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0009319	PE(:3(5Z,8Z,11Z)/16)	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0009352	PE(:3(8Z,11Z,14Z)/16)	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0009548	PE(22:2(13Z,16Z)/14:1(9Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0009123	PE(18:3(6Z,9Z,12Z)/18)	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0009092	PE(18:2(9Z,12Z)/18:1(9Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0007941	PC(15/18:3(6Z,9Z,12Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0008165	PC(18:3(6Z,9Z,12Z)/15)	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0008198	PC(18:3(9Z,12Z,15Z)/15)	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0008876	PE(14:1(9Z)/22:2(13Z,16Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0008936	PE(16/:3(8Z,11Z,14Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0008935	PE(16/:3(5Z,8Z,11Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0008967	PE(16:1(9Z)/:2(11Z,14Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0008996	PE(18/18:3(9Z,12Z,15Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0008995	PE(18/18:3(6Z,9Z,12Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0009060	PE(18:1(9Z)/18:2(9Z,12Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0009091	PE(18:2(9Z,12Z)/18:1(11Z))	C41H76NO8P	M-H	740.5236	-2.0
	HMDB0113856	PE-NMe2(14:1(9Z)/:1(11Z))	C41H78NO8P	M-H	742.5392	-1.7

742.5380	HMDB0113858	PE-NMe2(16:1(9Z)/18:1(11Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0113857	PE-NMe2(16:1(9Z)/18:1(9Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0114211	PE-NMe2(:1(11Z)/14:1(9Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0113025	PE-NMe(15/:2(11Z,14Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0113339	PE-NMe(:2(11Z,14Z)/15)	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0113884	PE-NMe2(14/:2(11Z,14Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0114239	PE-NMe2(:2(11Z,14Z)/14)	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0114068	PE-NMe2(18:2(9Z,12Z)/16)	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0114042	PE-NMe2(18:1(9Z)/16:1(9Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0114015	PE-NMe2(18:1(11Z)/16:1(9Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0113943	PE-NMe2(16/18:2(9Z,12Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0007940	PC(15/18:2(9Z,12Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0009286	PE(:2(11Z,14Z)/16)	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0009515	PE(22:1(13Z)/14:1(9Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0009547	PE(22:2(13Z,16Z)/14)	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0009254	PE(:1(11Z)/16:1(9Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0009090	PE(18:2(9Z,12Z)/18)	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0009059	PE(18:1(9Z)/18:1(9Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0008132	PC(18:2(9Z,12Z)/15)	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0008843	PE(14/22:2(13Z,16Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0008875	PE(14:1(9Z)/22:1(13Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0008934	PE(16/:2(11Z,14Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0008966	PE(16:1(9Z)/:1(11Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0008994	PE(18/18:2(9Z,12Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0009025	PE(18:1(11Z)/18:1(11Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0009026	PE(18:1(11Z)/18:1(9Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0009058	PE(18:1(9Z)/18:1(11Z))	C41H78NO8P	M-H	742.5392	-1.7
	HMDB0007938	PC(15/18:1(11Z))	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0007939	PC(15/18:1(9Z))	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0008066	PC(18:1(11Z)/15)	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0008099	PC(18:1(9Z)/15)	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0008842	PE(14/22:1(13Z))	C41H80NO8P	M-H	744.5549	-1.0

744.5541	HMDB0008874	PE(14:1(9Z)/22)	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0008933	PE(16:1(11Z))	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0008965	PE(16:1(9Z)/)	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0008992	PE(18/18:1(11Z))	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0009024	PE(18:1(11Z)/18)	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0009221	PE(/16:1(9Z))	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0009253	PE(:1(11Z)/16)	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0009482	PE(22/14:1(9Z))	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0010568	PE-NMe2(16/18:1(9Z))	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0009514	PE(22:1(13Z)/14)	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0113863	PE-NMe2(16:1(9Z)/18)	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0113862	PE-NMe2(16/18:1(11Z))	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0113859	PE-NMe2(14:1(11Z))	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0113861	PE-NMe2(14:1(9Z)/)	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0113310	PE-NMe(:1(11Z)/15)	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0114210	PE-NMe2(:1(11Z)/14)	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0114182	PE-NMe2(/14:1(9Z))	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0114041	PE-NMe2(18:1(9Z)/16)	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0114014	PE-NMe2(18:1(11Z)/16)	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0113989	PE-NMe2(18/16:1(9Z))	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0009057	PE(18:1(9Z)/18)	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0112963	PE-NMe(15:1(11Z))	C41H80NO8P	M-H	744.5549	-1.0
	HMDB0008993	PE(18/18:1(9Z))	C41H80NO8P	M-H	744.5549	-1.0
745.5014	HMDB0115535	PA(:2(11Z,14Z)/16)	C39H73O8P	M+FA-H	745.5025	-1.5
	HMDB0115510	PA(16/:2(11Z,14Z))	C39H73O8P	M+FA-H	745.5025	-1.5
	HMDB0115296	PA(22:2(13Z,16Z)/14)	C39H73O8P	M+FA-H	745.5025	-1.5
	HMDB0115271	PA(22:1(13Z)/14:1(9Z))	C39H73O8P	M+FA-H	745.5025	-1.5
	HMDB0115095	PA(:1(11Z)/16:1(9Z))	C39H73O8P	M+FA-H	745.5025	-1.5
	HMDB0114951	PA(18:2(9Z,12Z)/18)	C39H73O8P	M+FA-H	745.5025	-1.5
	HMDB0116699	PA(14/22:2(13Z,16Z))	C39H73O8P	M+FA-H	745.5025	-1.5
	HMDB0031129	9-Octadecenoic acid 1-[(phosphonoxy)methyl]-1,2-ethanediyl ester	C39H73O8P	M+FA-H	745.5025	-1.5
	HMDB0114804	PA(14:1(9Z)/22:1(13Z))	C39H73O8P	M+FA-H	745.5025	-1.5
	HMDB0007864	PA(18:1(9Z)/18:1(11Z))	C39H73O8P	M+FA-H	745.5025	-1.5
	HMDB0007865	PA(18:1(9Z)/18:1(9Z))	C39H73O8P	M+FA-H	745.5025	-1.5
	HMDB0007863	PA(18:1(11Z)/18:1(9Z))	C39H73O8P	M+FA-H	745.5025	-1.5
	HMDB0007862	PA(18:1(11Z)/18:1(11Z))	C39H73O8P	M+FA-H	745.5025	-1.5
	HMDB0007861	PA(18/18:2(9Z,12Z))	C39H73O8P	M+FA-H	745.5025	-1.5
	HMDB0010575	PG(16/18:2(9Z,12Z))	C40H75O10P	M-H	745.5025	-1.5
	HMDB0010616	PG(18:1(11Z)/16:1(9Z))	C40H75O10P	M-H	745.5025	-1.5

HMDB0010645	PG(18:2(9Z,12Z)/16)	C40H75O10P	M-H	745.5025	-1.5
HMDB0010631	PG(18:1(9Z)/16:1(9Z))	C40H75O10P	M-H	745.5025	-1.5
HMDB0010589	PG(16:1(9Z)/18:1(9Z))	C40H75O10P	M-H	745.5025	-1.5
HMDB0010588	PG(16:1(9Z)/18:1(11Z))	C40H75O10P	M-H	745.5025	-1.5
HMDB0113912	PE-NMe2(14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0113895	PE-NMe2(14/22:5(7Z,Z,13Z,16Z,19Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0113894	PE-NMe2(14/22:5(4Z,7Z,Z,13Z,16Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0113648	PE-NMe2(22:5(7Z,Z,13Z,16Z,19Z)/15)	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0113622	PE-NMe2(22:5(4Z,7Z,Z,13Z,16Z)/15)	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0113952	PE-NMe2(16/:5(5Z,8Z,11Z,14Z,17Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0114074	PE-NMe2(18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0114047	PE-NMe2(18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0114020	PE-NMe2(18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0113974	PE-NMe2(16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0113973	PE-NMe2(16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0113035	PE-NMe(15/22:5(4Z,7Z,Z,13Z,16Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0112978	PE-NMe(15/22:5(7Z,Z,13Z,16Z,19Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009293	PE(:2(11Z,14Z)/18:3(9Z,12Z,15Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009165	PE(18:3(9Z,12Z,15Z)/:2(11Z,14Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009197	PE(18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009261	PE(:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009292	PE(:2(11Z,14Z)/18:3(6Z,9Z,12Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0114158	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009324	PE(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009357	PE(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009388	PE(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009389	PE(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009132	PE(18:3(6Z,9Z,12Z)/:2(11Z,14Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0007951	PC(15/:5(5Z,8Z,11Z,14Z,17Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0008494	PC(:5(5Z,8Z,11Z,14Z,17Z)/15)	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0008944	PE(16/22:5(4Z,7Z,Z,13Z,16Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0008945	PE(16/22:5(7Z,Z,13Z,16Z,19Z))	C43H76NO8P	M-H20-H	746.5125	-0.4

746.5122

HMDB0008976	PE(16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009005	PE(18/:5(5Z,8Z,11Z,14Z,17Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009036	PE(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009037	PE(18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009070	PE(18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009069	PE(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009100	PE(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009101	PE(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009422	PE(:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009421	PE(:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009453	PE(:5(5Z,8Z,11Z,14Z,17Z)/18)	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0114102	PE-NMe2(18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0114075	PE-NMe2(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0114131	PE-NMe2(18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0114159	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009584	PE(22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009616	PE(22:5(4Z,7Z,Z,13Z,16Z)/16)	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0009649	PE(22:5(7Z,Z,13Z,16Z,19Z)/16)	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0114549	PE-NMe2(22:5(7Z,Z,13Z,16Z,19Z)/14)	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0114523	PE-NMe2(22:5(4Z,7Z,Z,13Z,16Z)/14)	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0114496	PE-NMe2(22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0114384	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/16)	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0114356	PE-NMe2(:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0114328	PE-NMe2(:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C43H76NO8P	M-H20-H	746.5125	-0.4
HMDB0005780	PE(P-16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H74NO7P	M-H	746.5130	-1.1
HMDB0011420	PE(P-18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H74NO7P	M-H	746.5130	-1.1
HMDB0011453	PE(P-18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H74NO7P	M-H	746.5130	-1.1
HMDB0009708	PE(22:6(4Z,7Z,Z,13Z,16Z,19Z)/P-16)	C43H74NO7P	M-H	746.5130	-1.1
HMDB0009479	PE(:5(5Z,8Z,11Z,14Z,17Z)/P-18:1(11Z))	C43H74NO7P	M-H	746.5130	-1.1
HMDB0009480	PE(:5(5Z,8Z,11Z,14Z,17Z)/P-18:1(9Z))	C43H74NO7P	M-H	746.5130	-1.1
HMDB0009116	PE(18:2(9Z,12Z)/P-18:1(11Z))	C41H76NO7P	M+Na-2H	746.5106	2.1
HMDB0009117	PE(18:2(9Z,12Z)/P-18:1(9Z))	C41H76NO7P	M+Na-2H	746.5106	2.1

	HMDB0009148	PE(18:3(6Z,9Z,12Z)/P-18)	C41H76NO7P	M+Na-2H	746.5106	2.1
	HMDB0009378	PE(:3(8Z,11Z,14Z)/P-16)	C41H76NO7P	M+Na-2H	746.5106	2.1
	HMDB0009345	PE(:3(5Z,8Z,11Z)/P-16)	C41H76NO7P	M+Na-2H	746.5106	2.1
	HMDB0011350	PE(P-16/:3(5Z,8Z,11Z))	C41H76NO7P	M+Na-2H	746.5106	2.1
	HMDB0011351	PE(P-16/:3(8Z,11Z,14Z))	C41H76NO7P	M+Na-2H	746.5106	2.1
	HMDB0011442	PE(P-18:1(9Z)/18:2(9Z,12Z))	C41H76NO7P	M+Na-2H	746.5106	2.1
	HMDB0011409	PE(P-18:1(11Z)/18:2(9Z,12Z))	C41H76NO7P	M+Na-2H	746.5106	2.1
	HMDB0011377	PE(P-18/18:3(6Z,9Z,12Z))	C41H76NO7P	M+Na-2H	746.5106	2.1
	HMDB0011378	PE(P-18/18:3(9Z,12Z,15Z))	C41H76NO7P	M+Na-2H	746.5106	2.1
	HMDB0009181	PE(18:3(9Z,12Z,15Z)/P-18)	C41H76NO7P	M+Na-2H	746.5106	2.1
747.5161	HMDB0115270	PA(22:1(13Z)/14)	C39H75O8P	M+FA-H	747.5182	-2.8
	HMDB0115241	PA(22/14:1(9Z))	C39H75O8P	M+FA-H	747.5182	-2.8
	HMDB0115094	PA(:1(11Z)/16)	C39H75O8P	M+FA-H	747.5182	-2.8
	HMDB0115065	PA(/16:1(9Z))	C39H75O8P	M+FA-H	747.5182	-2.8
	HMDB0114926	PA(18:1(9Z)/18)	C39H75O8P	M+FA-H	747.5182	-2.8
	HMDB0114901	PA(18:1(11Z)/18)	C39H75O8P	M+FA-H	747.5182	-2.8
	HMDB0114789	PA(14/22:1(13Z))	C39H75O8P	M+FA-H	747.5182	-2.8
	HMDB0010574	PG(16/18:1(9Z))	C40H77O10P	M-H	747.5182	-2.8
	HMDB0010630	PG(18:1(9Z)/16)	C40H77O10P	M-H	747.5182	-2.8
	HMDB0010615	PG(18:1(11Z)/16)	C40H77O10P	M-H	747.5182	-2.8
	HMDB0010601	PG(18/16:1(9Z))	C40H77O10P	M-H	747.5182	-2.8
	HMDB0010587	PG(16:1(9Z)/18)	C40H77O10P	M-H	747.5182	-2.8
	HMDB0010573	PG(16/18:1(11Z))	C40H77O10P	M-H	747.5182	-2.8
	HMDB0113034	PE-NMe(15/22:4(7Z,Z,13Z,16Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
	HMDB0114327	PE-NMe2(:4(5Z,8Z,11Z,14Z)/16)	C43H78NO8P	M-H20-H	748.5281	-1.1
	HMDB0114355	PE-NMe2(:4(8Z,11Z,14Z,17Z)/16)	C43H78NO8P	M-H20-H	748.5281	-1.1
	HMDB0114495	PE-NMe2(22:4(7Z,Z,13Z,16Z)/14)	C43H78NO8P	M-H20-H	748.5281	-1.1
	HMDB0114300	PE-NMe2(:3(8Z,11Z,14Z)/16:1(9Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
	HMDB0114272	PE-NMe2(:3(5Z,8Z,11Z)/16:1(9Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
	HMDB0114130	PE-NMe2(18:3(9Z,12Z,15Z)/18:1(9Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
	HMDB0113594	PE-NMe(22:4(7Z,Z,13Z,16Z)/15)	C43H78NO8P	M-H20-H	748.5281	-1.1
	HMDB0113893	PE-NMe2(14/22:4(7Z,Z,13Z,16Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
	HMDB0113951	PE-NMe2(16/:4(5Z,8Z,11Z,14Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
	HMDB0116711	PE-NMe2(16/:4(8Z,11Z,14Z,17Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
	HMDB0113972	PE-NMe2(16:1(9Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
	HMDB0113971	PE-NMe2(16:1(9Z)/:3(5Z,8Z,11Z))	C43H78NO8P	M-H20-H	748.5281	-1.1

HMDB0113993	PE-NMe ₂ (18:18:4(6Z,9Z,12Z,15Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0114019	PE-NMe ₂ (18:1(11Z)/18:3(9Z,12Z,15Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0114018	PE-NMe ₂ (18:1(11Z)/18:3(6Z,9Z,12Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0114045	PE-NMe ₂ (18:1(9Z)/18:3(6Z,9Z,12Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0114046	PE-NMe ₂ (18:1(9Z)/18:3(9Z,12Z,15Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0114073	PE-NMe ₂ (18:2(9Z,12Z)/18:2(9Z,12Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0114100	PE-NMe ₂ (18:3(6Z,9Z,12Z)/18:1(11Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0114101	PE-NMe ₂ (18:3(6Z,9Z,12Z)/18:1(9Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0114129	PE-NMe ₂ (18:3(9Z,12Z,15Z)/18:1(11Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009067	PE(18:1(9Z)/:3(5Z,8Z,11Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009291	PE(:2(11Z,14Z)/18:2(9Z,12Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009035	PE(18:1(11Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009034	PE(18:1(11Z)/:3(5Z,8Z,11Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0114157	PE-NMe ₂ (18:4(6Z,9Z,12Z,15Z)/18)	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009323	PE(:3(5Z,8Z,11Z)/18:1(9Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009260	PE(:1(11Z)/18:3(9Z,12Z,15Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009259	PE(:1(11Z)/18:3(6Z,9Z,12Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009068	PE(18:1(9Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009099	PE(18:2(9Z,12Z)/:2(11Z,14Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009131	PE(18:3(6Z,9Z,12Z)/:1(11Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009164	PE(18:3(9Z,12Z,15Z)/:1(11Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009196	PE(18:4(6Z,9Z,12Z,15Z)/)	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009228	PE(/18:4(6Z,9Z,12Z,15Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0007950	PC(15/:4(8Z,11Z,14Z,17Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0008943	PE(16/22:4(7Z,Z,13Z,16Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0008461	PC(:4(8Z,11Z,14Z,17Z)/15)	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009355	PE(:3(8Z,11Z,14Z)/18:1(11Z))	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009387	PE(:4(5Z,8Z,11Z,14Z)/18)	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0008428	PC(:4(5Z,8Z,11Z,14Z)/15)	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009420	PE(:4(8Z,11Z,14Z,17Z)/18)	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0009583	PE(22:4(7Z,Z,13Z,16Z)/16)	C43H78NO8P	M-H20-H	748.5281	-1.1
HMDB0007949	PC(15/:4(5Z,8Z,11Z,14Z))	C43H78NO8P	M-H20-H	748.5281	-1.1

HMDB0008969	PE(16:1(9Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M-H2O-H	748.5281	-1.1
HMDB0009003	PE(18/:4(5Z,8Z,11Z,14Z))	C43H78NO8P	M-H2O-H	748.5281	-1.1
HMDB0009322	PE(:3(5Z,8Z,11Z)/18:1(11Z))	C43H78NO8P	M-H2O-H	748.5281	-1.1
HMDB0009004	PE(18/:4(8Z,11Z,14Z,17Z))	C43H78NO8P	M-H2O-H	748.5281	-1.1
HMDB0009356	PE(:3(8Z,11Z,14Z)/18:1(9Z))	C43H78NO8P	M-H2O-H	748.5281	-1.1
HMDB0009051	PE(18:1(11Z)/P-18:1(9Z))	C41H78NO7P	M+Na-2H	748.5263	1.4
HMDB0011349	PE(P-16/:2(11Z,14Z))	C41H78NO7P	M+Na-2H	748.5263	1.4
HMDB0011440	PE(P-18:1(9Z)/18:1(11Z))	C41H78NO7P	M+Na-2H	748.5263	1.4
HMDB0009083	PE(18:1(9Z)/P-18:1(11Z))	C41H78NO7P	M+Na-2H	748.5263	1.4
HMDB0009084	PE(18:1(9Z)/P-18:1(9Z))	C41H78NO7P	M+Na-2H	748.5263	1.4
HMDB0011407	PE(P-18:1(11Z)/18:1(11Z))	C41H78NO7P	M+Na-2H	748.5263	1.4
HMDB0011408	PE(P-18:1(11Z)/18:1(9Z))	C41H78NO7P	M+Na-2H	748.5263	1.4
HMDB0011376	PE(P-18/18:2(9Z,12Z))	C41H78NO7P	M+Na-2H	748.5263	1.4
HMDB0009115	PE(18:2(9Z,12Z)/P-18)	C41H78NO7P	M+Na-2H	748.5263	1.4
HMDB0009312	PE(:2(11Z,14Z)/P-16)	C41H78NO7P	M+Na-2H	748.5263	1.4
HMDB0011441	PE(P-18:1(9Z)/18:1(9Z))	C41H78NO7P	M+Na-2H	748.5263	1.4
HMDB0009050	PE(18:1(11Z)/P-18:1(11Z))	C41H78NO7P	M+Na-2H	748.5263	1.4
HMDB0009414	PE(:4(5Z,8Z,11Z,14Z)/P-18:1(9Z))	C43H76NO7P	M-H	748.5287	-1.8
HMDB0009413	PE(:4(5Z,8Z,11Z,14Z)/P-18:1(11Z))	C43H76NO7P	M-H	748.5287	-1.8
HMDB0009446	PE(:4(8Z,11Z,14Z,17Z)/P-18:1(11Z))	C43H76NO7P	M-H	748.5287	-1.8
HMDB0009447	PE(:4(8Z,11Z,14Z,17Z)/P-18:1(9Z))	C43H76NO7P	M-H	748.5287	-1.8
HMDB0011387	PE(P-18/:5(5Z,8Z,11Z,14Z,17Z))	C43H76NO7P	M-H	748.5287	-1.8
HMDB0011418	PE(P-18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO7P	M-H	748.5287	-1.8
HMDB0011419	PE(P-18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO7P	M-H	748.5287	-1.8
HMDB0011452	PE(P-18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO7P	M-H	748.5287	-1.8
HMDB0011359	PE(P-16/22:5(4Z,7Z,Z,13Z,16Z))	C43H76NO7P	M-H	748.5287	-1.8
HMDB0011360	PE(P-16/22:5(7Z,Z,13Z,16Z,19Z))	C43H76NO7P	M-H	748.5287	-1.8
HMDB0009675	PE(22:5(7Z,Z,13Z,16Z,19Z)/P-16)	C43H76NO7P	M-H	748.5287	-1.8
HMDB0011451	PE(P-18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO7P	M-H	748.5287	-1.8
HMDB0009642	PE(22:5(4Z,7Z,Z,13Z,16Z)/P-16)	C43H76NO7P	M-H	748.5287	-1.8
HMDB0009478	PE(:5(5Z,8Z,11Z,14Z,17Z)/P-18)	C43H76NO7P	M-H	748.5287	-1.8
HMDB0116411	(2S)-2-{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na-2H	749.5338	-2.9

HMDB0116392	(2S)-1-hydroxy-3-{{[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na-2H	749.5338	-2.9
HMDB0116399	(2S)-1-hydroxy-3-{{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propan-2-yl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+Na-2H	749.5338	-2.9
HMDB0116378	(2S)-1-{{[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate	C45H76O7	M+Na-2H	749.5338	-2.9
HMDB0116432	(2S)-1-{{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+Na-2H	749.5338	-2.9
HMDB0116416	(2S)-3-hydroxy-2-{{[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na-2H	749.5338	-2.9
HMDB0116421	(2S)-3-hydroxy-2-{{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na-2H	749.5338	-2.9
HMDB0116426	(2S)-1-{{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na-2H	749.5338	-2.9
HMDB0116370	(2S)-1-{{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+Na-2H	749.5338	-2.9
HMDB0116445	(2S)-1-hydroxy-3-{{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C45H76O7	M+Na-2H	749.5338	-2.9
HMDB0116385	(2S)-2-{{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropyl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C45H76O7	M+Na-2H	749.5338	-2.9
HMDB0115670	PA(22/i-14)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115719	PA(a-21/15)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115729	PA(a-21/a-15)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115736	PA(a-21/i-15)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115938	PA(i-24/i-12)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115921	PA(i-24/12)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115910	PA(i-22/i-14)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115893	PA(i-22/14)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115881	PA(i-21/i-15)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115874	PA(i-21/a-15)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115864	PA(i-21/15)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115852	PA(i-i-16)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115835	PA(i-/16)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115792	PA(i-12/i-24)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115654	PA(21/i-15)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115647	PA(21/a-15)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115638	PA(i-/16)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0114788	PA(14/22)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0114839	PA(16/)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115064	PA(/16)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115228	PA(21/15)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0115240	PA(22/14)	C39H77O8P	M+FA-H	749.5338	-2.9
HMDB0010600	PG(18/16)	C40H79O10P	M-H	749.5338	-2.9
HMDB0010572	PG(16/18)	C40H79O10P	M-H	749.5338	-2.9
HMDB0116687	PG(i-13/i-21)	C40H79O10P	M-H	749.5338	-2.9
HMDB0116676	PG(i-13/a-21)	C40H79O10P	M-H	749.5338	-2.9
HMDB0116670	PG(i-12/i-22)	C40H79O10P	M-H	749.5338	-2.9
HMDB0116651	PG(a-13/i-21)	C40H79O10P	M-H	749.5338	-2.9

	HMDB0116640	PG(a-13/a-21)	C40H79O10P	M-H	749.5338	-2.9
	HMDB0009551	PE(22:2(13Z,16Z)/16:1(9Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0009354	PE(:3(8Z,11Z,14Z)/18)	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0009321	PE(:3(5Z,8Z,11Z)/18)	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0009289	PE(:2(11Z,14Z)/18:1(11Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0009290	PE(:2(11Z,14Z)/18:1(9Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0009258	PE(:1(11Z)/18:2(9Z,12Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0009226	PE(/18:3(6Z,9Z,12Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0009002	PE(18/:3(8Z,11Z,14Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0008975	PE(16:1(9Z)/22:2(13Z,16Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0008396	PC(:3(8Z,11Z,14Z)/15)	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0008363	PC(:3(5Z,8Z,11Z)/15)	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0009033	PE(18:1(11Z)/:2(11Z,14Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0007948	PC(15/:3(8Z,11Z,14Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0009227	PE(/18:3(9Z,12Z,15Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0009163	PE(18:3(9Z,12Z,15Z)/)	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0009130	PE(18:3(6Z,9Z,12Z)/)	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0009098	PE(18:2(9Z,12Z)/:1(11Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0009001	PE(18/:3(5Z,8Z,11Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0009066	PE(18:1(9Z)/:2(11Z,14Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0007947	PC(15/:3(5Z,8Z,11Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0113970	PE-NMe2(16:1(9Z)/:2(11Z,14Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0114243	PE-NMe2(:2(11Z,14Z)/16:1(9Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0114467	PE-NMe2(22:2(13Z,16Z)/14:1(9Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0114299	PE-NMe2(:3(8Z,11Z,14Z)/16)	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0113911	PE-NMe2(14:1(9Z)/22:2(13Z,16Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0113949	PE-NMe2(16/:3(5Z,8Z,11Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0113950	PE-NMe2(16/:3(8Z,11Z,14Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0113992	PE-NMe2(18/18:3(9Z,12Z,15Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0113991	PE-NMe2(18/18:3(6Z,9Z,12Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0114017	PE-NMe2(18:1(11Z)/18:2(9Z,12Z))	C43H80NO8P	M-H20-H	750.5438	-0.5
	HMDB0114044	PE-NMe2(18:1(9Z)/18:2(9Z,12Z))	C43H80NO8P	M-H20-H	750.5438	-0.5

750.5434

HMDB0114072	PE-NMe ₂ (18:2(9Z,12Z)/18:1(9Z))	C43H80NO8P	M-H2O-H	750.5438	-0.5
HMDB0114071	PE-NMe ₂ (18:2(9Z,12Z)/18:1(11Z))	C43H80NO8P	M-H2O-H	750.5438	-0.5
HMDB0114099	PE-NMe ₂ (18:3(6Z,9Z,12Z)/18)	C43H80NO8P	M-H2O-H	750.5438	-0.5
HMDB0114271	PE-NMe ₂ (:3(5Z,8Z,11Z)/16)	C43H80NO8P	M-H2O-H	750.5438	-0.5
HMDB0114128	PE-NMe ₂ (18:3(9Z,12Z,15Z)/18)	C43H80NO8P	M-H2O-H	750.5438	-0.5
HMDB0005779	PE(P-18/:4(5Z,8Z,11Z,14Z))	C43H78NO7P	M-H	750.5443	-1.2
HMDB0061335	PE(P-18/:4(5Z,8Z,11Z,14Z))	C43H78NO7P	M-H	750.5443	-1.2
HMDB0011386	PE(P-18/:4(8Z,11Z,14Z,17Z))	C43H78NO7P	M-H	750.5443	-1.2
HMDB0011416	PE(P-18:1(11Z)/:3(5Z,8Z,11Z))	C43H78NO7P	M-H	750.5443	-1.2
HMDB0011449	PE(P-18:1(9Z)/:3(5Z,8Z,11Z))	C43H78NO7P	M-H	750.5443	-1.2
HMDB0011417	PE(P-18:1(11Z)/:3(8Z,11Z,14Z))	C43H78NO7P	M-H	750.5443	-1.2
HMDB0011358	PE(P-16/22:4(7Z,Z,13Z,16Z))	C43H78NO7P	M-H	750.5443	-1.2
HMDB0009609	PE(22:4(7Z,Z,13Z,16Z)/P-16)	C43H78NO7P	M-H	750.5443	-1.2
HMDB0009347	PE(:3(5Z,8Z,11Z)/P-18:1(11Z))	C43H78NO7P	M-H	750.5443	-1.2
HMDB0009380	PE(:3(8Z,11Z,14Z)/P-18:1(11Z))	C43H78NO7P	M-H	750.5443	-1.2
HMDB0009381	PE(:3(8Z,11Z,14Z)/P-18:1(9Z))	C43H78NO7P	M-H	750.5443	-1.2
HMDB0009348	PE(:3(5Z,8Z,11Z)/P-18:1(9Z))	C43H78NO7P	M-H	750.5443	-1.2
HMDB0009412	PE(:4(5Z,8Z,11Z,14Z)/P-18)	C43H78NO7P	M-H	750.5443	-1.2
HMDB0009445	PE(:4(8Z,11Z,14Z,17Z)/P-18)	C43H78NO7P	M-H	750.5443	-1.2
HMDB0009017	PE(18/P-18:1(11Z))	C41H80NO7P	M+Na-2H	750.5419	2.0
HMDB0007964	PC(15/P-18:1(9Z))	C41H80NO7P	M+Na-2H	750.5419	2.0
HMDB0007963	PC(15/P-18:1(11Z))	C41H80NO7P	M+Na-2H	750.5419	2.0
HMDB0009018	PE(18/P-18:1(9Z))	C41H80NO7P	M+Na-2H	750.5419	2.0
HMDB0009082	PE(18:1(9Z)/P-18)	C41H80NO7P	M+Na-2H	750.5419	2.0
HMDB0011271	PC(P-18:1(11Z)/15)	C41H80NO7P	M+Na-2H	750.5419	2.0
HMDB0011439	PE(P-18:1(9Z)/18)	C41H80NO7P	M+Na-2H	750.5419	2.0
HMDB0009279	PE(:1(11Z)/P-16)	C41H80NO7P	M+Na-2H	750.5419	2.0
HMDB0011406	PE(P-18:1(11Z)/18)	C41H80NO7P	M+Na-2H	750.5419	2.0
HMDB0011375	PE(P-18/18:1(9Z))	C41H80NO7P	M+Na-2H	750.5419	2.0
HMDB0011374	PE(P-18/18:1(11Z))	C41H80NO7P	M+Na-2H	750.5419	2.0
HMDB0011348	PE(P-16/:1(11Z))	C41H80NO7P	M+Na-2H	750.5419	2.0
HMDB0011304	PC(P-18:1(9Z)/15)	C41H80NO7P	M+Na-2H	750.5419	2.0

	HMDB0009049	PE(18:1(11Z)/P-18)	C41H80NO7P	M+Na-2H	750.5419	2.0
752.5588	HMDB0010564	PE-NMe2(18:1(9Z)/18:1(9Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0009746	PE(24:1(15Z)/14:1(9Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0009550	PE(22:2(13Z,16Z)/16)	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0009518	PE(22:1(13Z)/16:1(9Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0007946	PC(15/:2(11Z,14Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0009097	PE(18:2(9Z,12Z)/)	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0009065	PE(18:1(9Z)/:1(11Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0009256	PE(:1(11Z)/18:1(11Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0009257	PE(:1(11Z)/18:1(9Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0009032	PE(18:1(11Z)/:1(11Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0009288	PE(:2(11Z,14Z)/18)	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0009000	PE(18/:2(11Z,14Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0008974	PE(16:1(9Z)/22:1(13Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0008942	PE(16/22:2(13Z,16Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0008882	PE(14:1(9Z)/24:1(15Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0008330	PC(:2(11Z,14Z)/15)	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0009225	PE(/18:2(9Z,12Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0113867	PE-NMe2(16:1(9Z)/:1(11Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0113868	PE-NMe2(18:1(9Z)/18:1(11Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0114070	PE-NMe2(18:2(9Z,12Z)/18)	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0114214	PE-NMe2(:1(11Z)/16:1(9Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0114438	PE-NMe2(22:1(13Z)/14:1(9Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0114466	PE-NMe2(22:2(13Z,16Z)/14)	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0113948	PE-NMe2(16/:2(11Z,14Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0114242	PE-NMe2(:2(11Z,14Z)/16)	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0113990	PE-NMe2(18/18:2(9Z,12Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0113910	PE-NMe2(14:1(9Z)/22:1(13Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0113870	PE-NMe2(18:1(11Z)/18:1(11Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0113869	PE-NMe2(18:1(11Z)/18:1(9Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0113033	PE-NMe(15/22:2(13Z,16Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0113565	PE-NMe(22:2(13Z,16Z)/15)	C43H82NO8P	M-H2O-H	752.5594	-0.8

	HMDB0113892	PE-NMe2(14/22:2(13Z,16Z))	C43H82NO8P	M-H2O-H	752.5594	-0.8
	HMDB0009379	PE(:3(8Z,11Z,14Z)/P-18)	C43H80NO7P	M-H	752.5600	-1.5
	HMDB0009315	PE(:2(11Z,14Z)/P-18:1(9Z))	C43H80NO7P	M-H	752.5600	-1.5
	HMDB0011448	PE(P-18:1(9Z):2(11Z,14Z))	C43H80NO7P	M-H	752.5600	-1.5
	HMDB0011415	PE(P-18:1(11Z):2(11Z,14Z))	C43H80NO7P	M-H	752.5600	-1.5
	HMDB0011384	PE(P-18/:3(8Z,11Z,14Z))	C43H80NO7P	M-H	752.5600	-1.5
	HMDB0011383	PE(P-18/:3(5Z,8Z,11Z))	C43H80NO7P	M-H	752.5600	-1.5
	HMDB0009346	PE(:3(5Z,8Z,11Z)/P-18)	C43H80NO7P	M-H	752.5600	-1.5
	HMDB0009314	PE(:2(11Z,14Z)/P-18:1(11Z))	C43H80NO7P	M-H	752.5600	-1.5
	HMDB0061334	1-alkyl-2-acylglycerol 3 phosphoethanolamine(18/:4)	C43H80NO7P	M-H	752.5600	-1.5
	HMDB0009246	PE(/P-16)	C41H82NO7P	M+Na-2H	752.5576	1.7
	HMDB0009016	PE(18/P-18)	C41H82NO7P	M+Na-2H	752.5576	1.7
	HMDB0011238	PC(P-18/15)	C41H82NO7P	M+Na-2H	752.5576	1.7
	HMDB0011347	PE(P-16/)	C41H82NO7P	M+Na-2H	752.5576	1.7
	HMDB0011373	PE(P-18/18)	C41H82NO7P	M+Na-2H	752.5576	1.7
	HMDB0007962	PC(15/P-18)	C41H82NO7P	M+Na-2H	752.5576	1.7
754.5032	HMDB0174781	21-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-22-hydroxytriacontanoic acid	C40H75N3O9S	M-H2O-H	754.5040	-1.1
	HMDB0174782	22-({2-[(4-amino-4-carboxy-1-hydroxybutylidene)amino]-2-[(carboxymethyl)-C-hydroxycarbonimidoyl]ethyl}sulfanyl)-21-hydroxytriacontanoic acid	C40H75N3O9S	M-H2O-H	754.5040	-1.1
	HMDB0112328	PS(15/:2(11Z,14Z))	C41H76NO10P	M-H2O-H	754.5023	1.2
	HMDB0112569	PS(:2(11Z,14Z)/15)	C41H76NO10P	M-H2O-H	754.5023	1.2
	HMDB0113900	PE-NMe2(14:1(9Z)/18:2(9Z,12Z))	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0114123	PE-NMe2(18:3(9Z,12Z,15Z)/14)	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0114094	PE-NMe2(18:3(6Z,9Z,12Z)/14)	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0114066	PE-NMe2(18:2(9Z,12Z)/14:1(9Z))	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0113881	PE-NMe2(14/18:3(9Z,12Z,15Z))	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0113880	PE-NMe2(14/18:3(6Z,9Z,12Z))	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0113223	PE-NMe(18:3(9Z,12Z,15Z)/15)	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0113195	PE-NMe(18:3(6Z,9Z,12Z)/15)	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0113021	PE-NMe(15/18:3(6Z,9Z,12Z))	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0113022	PE-NMe(15/18:3(9Z,12Z,15Z))	C39H72NO8P	M+FA-H	758.4978	-1.7

758.4965	HMDB0009284	PE(:2(11Z,14Z)/14:1(9Z))	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0009316	PE(:3(5Z,8Z,11Z)/14)	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0009349	PE(:3(8Z,11Z,14Z)/14)	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0009154	PE(18:3(9Z,12Z,15Z)/16)	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0009121	PE(18:3(6Z,9Z,12Z)/16)	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0008836	PE(14/:3(5Z,8Z,11Z))	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0008868	PE(14:1(9Z)/:2(11Z,14Z))	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0008929	PE(16/18:3(6Z,9Z,12Z))	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0008837	PE(14/:3(8Z,11Z,14Z))	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0008930	PE(16/18:3(9Z,12Z,15Z))	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0008961	PE(16:1(9Z)/18:2(9Z,12Z))	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0009089	PE(18:2(9Z,12Z)/16:1(9Z))	C39H72NO8P	M+FA-H	758.4978	-1.7
	HMDB0012358	PS(16/18:2(9Z,12Z))	C40H74NO10P	M-H	758.4978	-1.7
	HMDB0012398	PS(18:2(9Z,12Z)/16)	C40H74NO10P	M-H	758.4978	-1.7
	HMDB0112268	PS(16:1(9Z)/18:1(11Z))	C40H74NO10P	M-H	758.4978	-1.7
	HMDB0112271	PS(18:1(11Z)/16:1(9Z))	C40H74NO10P	M-H	758.4978	-1.7
	HMDB0112541	PS(:1(11Z)/14:1(9Z))	C40H74NO10P	M-H	758.4978	-1.7
	HMDB0112296	PS(14/:2(11Z,14Z))	C40H74NO10P	M-H	758.4978	-1.7
	HMDB0112567	PS(:2(11Z,14Z)/14)	C40H74NO10P	M-H	758.4978	-1.7
	HMDB0012388	PS(18:1(9Z)/16:1(9Z))	C40H74NO10P	M-H	758.4978	-1.7
	HMDB0012368	PS(16:1(9Z)/18:1(9Z))	C40H74NO10P	M-H	758.4978	-1.7
	HMDB0112278	PS(14:1(9Z)/:1(11Z))	C40H74NO10P	M-H	758.4978	-1.7
	HMDB0113847	PE-NMe2(14:1(9Z)/18:1(9Z))	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0113848	PE-NMe2(14:1(9Z)/18:1(11Z))	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0113020	PE-NMe2(15/18:2(9Z,12Z))	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0113849	PE-NMe2(16:1(9Z)/16:1(9Z))	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0113166	PE-NMe2(18:2(9Z,12Z)/15)	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0113879	PE-NMe2(14/18:2(9Z,12Z))	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0114012	PE-NMe2(18:1(11Z)/14:1(9Z))	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0114039	PE-NMe2(18:1(9Z)/14:1(9Z))	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0114065	PE-NMe2(18:2(9Z,12Z)/14)	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0009251	PE(:1(11Z)/14:1(9Z))	C39H74NO8P	M+FA-H	760.5134	-1.8

760.5120	HMDB0009283	PE(:2(11Z,14Z)/14)	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0008960	PE(16:1(9Z)/18:1(9Z))	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0009088	PE(18:2(9Z,12Z)/16)	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0009056	PE(18:1(9Z)/16:1(9Z))	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0009023	PE(18:1(11Z)/16:1(9Z))	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0008835	PE(14/:2(11Z,14Z))	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0008867	PE(14:1(9Z)/:1(11Z))	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0008928	PE(16/18:2(9Z,12Z))	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0008959	PE(16:1(9Z)/18:1(11Z))	C39H74NO8P	M+FA-H	760.5134	-1.8
	HMDB0012357	PS(16/18:1(9Z))	C40H76NO10P	M-H	760.5134	-1.9
	HMDB0112540	PS(:1(11Z)/14)	C40H76NO10P	M-H	760.5134	-1.9
	HMDB0012367	PS(16:1(9Z)/18)	C40H76NO10P	M-H	760.5134	-1.9
	HMDB0012387	PS(18:1(9Z)/16)	C40H76NO10P	M-H	760.5134	-1.9
	HMDB0112512	PS(/14:1(9Z))	C40H76NO10P	M-H	760.5134	-1.9
	HMDB0112270	PS(18:1(11Z)/16)	C40H76NO10P	M-H	760.5134	-1.9
	HMDB0112274	PS(14/:1(11Z))	C40H76NO10P	M-H	760.5134	-1.9
	HMDB0112277	PS(14:1(9Z)/)	C40H76NO10P	M-H	760.5134	-1.9
	HMDB0112267	PS(16/18:1(11Z))	C40H76NO10P	M-H	760.5134	-1.9
	HMDB0012377	PS(18/16:1(9Z))	C40H76NO10P	M-H	760.5134	-1.9
	HMDB0113648	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/15)	C43H76NO8P	M-H	764.5236	-1.0
	HMDB0112978	PE-NMe(15/22:5(7Z,Z,13Z,16Z,19Z))	C43H76NO8P	M-H	764.5236	-1.0
	HMDB0114159	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C43H76NO8P	M-H	764.5236	-1.0
	HMDB0114328	PE-NMe2(:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C43H76NO8P	M-H	764.5236	-1.0
	HMDB0114356	PE-NMe2(:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C43H76NO8P	M-H	764.5236	-1.0
	HMDB0114384	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/16)	C43H76NO8P	M-H	764.5236	-1.0
	HMDB0114496	PE-NMe2(22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C43H76NO8P	M-H	764.5236	-1.0
	HMDB0114523	PE-NMe2(22:5(4Z,7Z,Z,13Z,16Z)/14)	C43H76NO8P	M-H	764.5236	-1.0
	HMDB0114549	PE-NMe2(22:5(7Z,Z,13Z,16Z,19Z)/14)	C43H76NO8P	M-H	764.5236	-1.0
	HMDB0114131	PE-NMe2(18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C43H76NO8P	M-H	764.5236	-1.0
	HMDB0114102	PE-NMe2(18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C43H76NO8P	M-H	764.5236	-1.0
	HMDB0114075	PE-NMe2(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C43H76NO8P	M-H	764.5236	-1.0
	HMDB0113035	PE-NMe(15/22:5(4Z,7Z,Z,13Z,16Z))	C43H76NO8P	M-H	764.5236	-1.0

HMDB0114158	PE-NMe ₂ (18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0113622	PE-NMe ₂ (22:5(4Z,7Z,Z,13Z,16Z)/15)	C43H76NO8P	M-H	764.5236	-1.0
HMDB0113894	PE-NMe ₂ (14/22:5(4Z,7Z,Z,13Z,16Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0113895	PE-NMe ₂ (14/22:5(7Z,Z,13Z,16Z,19Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0113912	PE-NMe ₂ (14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0113952	PE-NMe ₂ (16/:5(5Z,8Z,11Z,14Z,17Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0113973	PE-NMe ₂ (16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0113974	PE-NMe ₂ (16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0114020	PE-NMe ₂ (18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0114047	PE-NMe ₂ (18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0114074	PE-NMe ₂ (18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009453	PE(:5(5Z,8Z,11Z,14Z,17Z)/18)	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009649	PE(22:5(7Z,Z,13Z,16Z,19Z)/16)	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009389	PE(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009069	PE(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009070	PE(18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009037	PE(18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009036	PE(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009616	PE(22:5(4Z,7Z,Z,13Z,16Z)/16)	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009100	PE(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009421	PE(:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009422	PE(:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009388	PE(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009357	PE(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009324	PE(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009293	PE(:2(11Z,14Z)/18:3(9Z,12Z,15Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009292	PE(:2(11Z,14Z)/18:3(6Z,9Z,12Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009261	PE(:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009197	PE(18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009165	PE(18:3(9Z,12Z,15Z)/:2(11Z,14Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009132	PE(18:3(6Z,9Z,12Z)/:2(11Z,14Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009101	PE(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C43H76NO8P	M-H	764.5236	-1.0

HMDB0009584	PE(22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0009005	PE(18/:5(5Z,8Z,11Z,14Z,17Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0007951	PC(15/:5(5Z,8Z,11Z,14Z,17Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0008945	PE(16/22:5(7Z,Z,13Z,16Z,19Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0008944	PE(16/22:5(4Z,7Z,Z,13Z,16Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0008494	PC(:5(5Z,8Z,11Z,14Z,17Z)/15)	C43H76NO8P	M-H	764.5236	-1.0
HMDB0008976	PE(16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C43H76NO8P	M-H	764.5236	-1.0
HMDB0113943	PE-NMe2(16/18:2(9Z,12Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0008966	PE(16:1(9Z)/:1(11Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0009254	PE(:1(11Z)/16:1(9Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0009286	PE(:2(11Z,14Z)/16)	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0008132	PC(18:2(9Z,12Z)/15)	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0008994	PE(18/18:2(9Z,12Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0009059	PE(18:1(9Z)/18:1(9Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0009058	PE(18:1(9Z)/18:1(11Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0113025	PE-NMe(15/:2(11Z,14Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0114211	PE-NMe2(:1(11Z)/14:1(9Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0009026	PE(18:1(11Z)/18:1(9Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0113339	PE-NMe(:2(11Z,14Z)/15)	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0114068	PE-NMe2(18:2(9Z,12Z)/16)	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0114015	PE-NMe2(18:1(11Z)/16:1(9Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0008843	PE(14/22:2(13Z,16Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0114042	PE-NMe2(18:1(9Z)/16:1(9Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0008875	PE(14:1(9Z)/22:1(13Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0008934	PE(16/:2(11Z,14Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0009090	PE(18:2(9Z,12Z)/18)	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0114239	PE-NMe2(:2(11Z,14Z)/14)	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0113884	PE-NMe2(14/:2(11Z,14Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0009025	PE(18:1(11Z)/18:1(11Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0007940	PC(15/18:2(9Z,12Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0113856	PE-NMe2(14:1(9Z)/:1(11Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
HMDB0113858	PE-NMe2(16:1(9Z)/18:1(11Z))	C41H78NO8P	M+Na-2H	764.5212	2.1

	HMDB0113857	PE-NMe2(16:1(9Z)/18:1(9Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
	HMDB0009547	PE(22:2(13Z,16Z)/14)	C41H78NO8P	M+Na-2H	764.5212	2.1
	HMDB0009515	PE(22:1(13Z)/14:1(9Z))	C41H78NO8P	M+Na-2H	764.5212	2.1
766.4872	HMDB0112342	PS(16/15)	C37H72NO10P	M+FA-H	766.4876	-0.5
	HMDB0112281	PS(15/16)	C37H72NO10P	M+FA-H	766.4876	-0.5
	HMDB0114157	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/18)	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0114130	PE-NMe2(18:3(9Z,12Z,15Z)/18:1(9Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0114129	PE-NMe2(18:3(9Z,12Z,15Z)/18:1(11Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0114101	PE-NMe2(18:3(6Z,9Z,12Z)/18:1(9Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0114100	PE-NMe2(18:3(6Z,9Z,12Z)/18:1(11Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0114073	PE-NMe2(18:2(9Z,12Z)/18:2(9Z,12Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0114046	PE-NMe2(18:1(9Z)/18:3(9Z,12Z,15Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0114045	PE-NMe2(18:1(9Z)/18:3(6Z,9Z,12Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0114018	PE-NMe2(18:1(11Z)/18:3(6Z,9Z,12Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0114495	PE-NMe2(22:4(7Z,Z,13Z,16Z)/14)	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0114327	PE-NMe2(:4(5Z,8Z,11Z,14Z)/16)	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0114300	PE-NMe2(:3(8Z,11Z,14Z)/16:1(9Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0114272	PE-NMe2(:3(5Z,8Z,11Z)/16:1(9Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0114019	PE-NMe2(18:1(11Z)/18:3(9Z,12Z,15Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0113893	PE-NMe2(14/22:4(7Z,Z,13Z,16Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0113594	PE-NMe2(22:4(7Z,Z,13Z,16Z)/15)	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0113034	PE-NMe2(15/22:4(7Z,Z,13Z,16Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0113951	PE-NMe2(16/:4(5Z,8Z,11Z,14Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0113993	PE-NMe2(18/18:4(6Z,9Z,12Z,15Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0113971	PE-NMe2(16:1(9Z)/:3(5Z,8Z,11Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0113972	PE-NMe2(16:1(9Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0116711	PE-NMe2(16/:4(8Z,11Z,14Z,17Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0007949	PC(15/:4(5Z,8Z,11Z,14Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0009131	PE(18:3(6Z,9Z,12Z)/:1(11Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0009164	PE(18:3(9Z,12Z,15Z)/:1(11Z))	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0009196	PE(18:4(6Z,9Z,12Z,15Z)/)	C43H78NO8P	M-H	766.5392	-1.5
	HMDB0009228	PE(/18:4(6Z,9Z,12Z,15Z))	C43H78NO8P	M-H	766.5392	-1.5

766.5381

HMDB0009259	PE(:1(11Z)/18:3(6Z,9Z,12Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009260	PE(:1(11Z)/18:3(9Z,12Z,15Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009291	PE(:2(11Z,14Z)/18:2(9Z,12Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0007950	PC(15/:4(8Z,11Z,14Z,17Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009322	PE(:3(5Z,8Z,11Z)/18:1(11Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0114355	PE-NMe2(:4(8Z,11Z,14Z,17Z)/16)	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009356	PE(:3(8Z,11Z,14Z)/18:1(9Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009099	PE(18:2(9Z,12Z)/:2(11Z,14Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009067	PE(18:1(9Z)/:3(5Z,8Z,11Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009068	PE(18:1(9Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009387	PE(:4(5Z,8Z,11Z,14Z)/18)	C43H78NO8P	M-H	766.5392	-1.5
HMDB0008428	PC(:4(5Z,8Z,11Z,14Z)/15)	C43H78NO8P	M-H	766.5392	-1.5
HMDB0008461	PC(:4(8Z,11Z,14Z,17Z)/15)	C43H78NO8P	M-H	766.5392	-1.5
HMDB0008943	PE(16/22:4(7Z,Z,13Z,16Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0008969	PE(16:1(9Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009004	PE(18/:4(8Z,11Z,14Z,17Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009003	PE(18/:4(5Z,8Z,11Z,14Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009034	PE(18:1(11Z)/:3(5Z,8Z,11Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009035	PE(18:1(11Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009355	PE(:3(8Z,11Z,14Z)/18:1(11Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009420	PE(:4(8Z,11Z,14Z,17Z)/18)	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009323	PE(:3(5Z,8Z,11Z)/18:1(9Z))	C43H78NO8P	M-H	766.5392	-1.5
HMDB0009583	PE(22:4(7Z,Z,13Z,16Z)/16)	C43H78NO8P	M-H	766.5392	-1.5
HMDB0113310	PE-NMe(:1(11Z)/15)	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0114182	PE-NMe2(/14:1(9Z))	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0114014	PE-NMe2(18:1(11Z)/16)	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0113989	PE-NMe2(18/16:1(9Z))	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0114041	PE-NMe2(18:1(9Z)/16)	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0114210	PE-NMe2(:1(11Z)/14)	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0008993	PE(18/18:1(9Z))	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0009057	PE(18:1(9Z)/18)	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0113859	PE-NMe2(14/:1(11Z))	C41H80NO8P	M+Na-2H	766.5368	1.7

HMDB0113861	PE-NMe2(14:1(9Z)/)	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0113862	PE-NMe2(16/18:1(11Z))	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0113863	PE-NMe2(16:1(9Z)/18)	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0112963	PE-NMe(15/:1(11Z))	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0009024	PE(18:1(11Z)/18)	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0009253	PE(:1(11Z)/16)	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0009482	PE(22/14:1(9Z))	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0009514	PE(22:1(13Z)/14)	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0010568	PE-NMe2(16/18:1(9Z))	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0008992	PE(18/18:1(11Z))	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0008965	PE(16:1(9Z)/)	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0008933	PE(16/:1(11Z))	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0008874	PE(14:1(9Z)/22)	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0008842	PE(14/22:1(13Z))	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0008099	PC(18:1(9Z)/15)	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0008066	PC(18:1(11Z)/15)	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0007939	PC(15/18:1(9Z))	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0007938	PC(15/18:1(11Z))	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0009221	PE(/16:1(9Z))	C41H80NO8P	M+Na-2H	766.5368	1.7
HMDB0113866	PE-NMe2(16/18)	C41H82NO8P	M+Na-2H	768.5525	0.9
HMDB0113988	PE-NMe2(18/16)	C41H82NO8P	M+Na-2H	768.5525	0.9
HMDB0008991	PE(18/18)	C41H82NO8P	M+Na-2H	768.5525	0.9
HMDB0113883	PE-NMe2(14/)	C41H82NO8P	M+Na-2H	768.5525	0.9
HMDB0113281	PE-NMe(/15)	C41H82NO8P	M+Na-2H	768.5525	0.9
HMDB0114181	PE-NMe2(/14)	C41H82NO8P	M+Na-2H	768.5525	0.9
HMDB0113024	PE-NMe(15/)	C41H82NO8P	M+Na-2H	768.5525	0.9
HMDB0008033	PC(18/15)	C41H82NO8P	M+Na-2H	768.5525	0.9
HMDB0009481	PE(22/14)	C41H82NO8P	M+Na-2H	768.5525	0.9
HMDB0008841	PE(14/22)	C41H82NO8P	M+Na-2H	768.5525	0.9
HMDB0008932	PE(16/)	C41H82NO8P	M+Na-2H	768.5525	0.9
HMDB0060501	Phosphatidylethanolamine	C41H82NO8P	M+Na-2H	768.5525	0.9
HMDB0009220	PE(/16)	C41H82NO8P	M+Na-2H	768.5525	0.9

768.5532

HMDB0007937	PC(15/18)	C41H82NO8P	M+Na-2H	768.5525	0.9
HMDB0009321	PE(:3(5Z,8Z,11Z)/18)	C43H80NO8P	M-H	768.5549	-2.2
HMDB0009289	PE(:2(11Z,14Z)/18:1(11Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0009290	PE(:2(11Z,14Z)/18:1(9Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0009258	PE(:1(11Z)/18:2(9Z,12Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0009226	PE(/18:3(6Z,9Z,12Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0009227	PE(/18:3(9Z,12Z,15Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0009163	PE(18:3(9Z,12Z,15Z)/)	C43H80NO8P	M-H	768.5549	-2.2
HMDB0009130	PE(18:3(6Z,9Z,12Z)/)	C43H80NO8P	M-H	768.5549	-2.2
HMDB0009098	PE(18:2(9Z,12Z)/:1(11Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0009066	PE(18:1(9Z)/:2(11Z,14Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0009033	PE(18:1(11Z)/:2(11Z,14Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0009002	PE(18/:3(8Z,11Z,14Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0009001	PE(18/:3(5Z,8Z,11Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0008975	PE(16:1(9Z)/22:2(13Z,16Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0008363	PC(:3(5Z,8Z,11Z)/15)	C43H80NO8P	M-H	768.5549	-2.2
HMDB0009354	PE(:3(8Z,11Z,14Z)/18)	C43H80NO8P	M-H	768.5549	-2.2
HMDB0009551	PE(22:2(13Z,16Z)/16:1(9Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0007948	PC(15/:3(8Z,11Z,14Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0008396	PC(:3(8Z,11Z,14Z)/15)	C43H80NO8P	M-H	768.5549	-2.2
HMDB0007947	PC(15/:3(5Z,8Z,11Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0113970	PE-NMe2(16:1(9Z)/:2(11Z,14Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0114467	PE-NMe2(22:2(13Z,16Z)/14:1(9Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0114299	PE-NMe2(:3(8Z,11Z,14Z)/16)	C43H80NO8P	M-H	768.5549	-2.2
HMDB0114243	PE-NMe2(:2(11Z,14Z)/16:1(9Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0114271	PE-NMe2(:3(5Z,8Z,11Z)/16)	C43H80NO8P	M-H	768.5549	-2.2
HMDB0114128	PE-NMe2(18:3(9Z,12Z,15Z)/18)	C43H80NO8P	M-H	768.5549	-2.2
HMDB0114099	PE-NMe2(18:3(6Z,9Z,12Z)/18)	C43H80NO8P	M-H	768.5549	-2.2
HMDB0114071	PE-NMe2(18:2(9Z,12Z)/18:1(11Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0114072	PE-NMe2(18:2(9Z,12Z)/18:1(9Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0114044	PE-NMe2(18:1(9Z)/18:2(9Z,12Z))	C43H80NO8P	M-H	768.5549	-2.2
HMDB0114017	PE-NMe2(18:1(11Z)/18:2(9Z,12Z))	C43H80NO8P	M-H	768.5549	-2.2

	HMDB0113991	PE-NMe2(18/18:3(6Z,9Z,12Z))	C43H80NO8P	M-H	768.5549	-2.2
	HMDB0113992	PE-NMe2(18/18:3(9Z,12Z,15Z))	C43H80NO8P	M-H	768.5549	-2.2
	HMDB0113950	PE-NMe2(16/:3(8Z,11Z,14Z))	C43H80NO8P	M-H	768.5549	-2.2
	HMDB0113949	PE-NMe2(16/:3(5Z,8Z,11Z))	C43H80NO8P	M-H	768.5549	-2.2
	HMDB0113911	PE-NMe2(14:1(9Z)/22:2(13Z,16Z))	C43H80NO8P	M-H	768.5549	-2.2
769.5041	HMDB0116606	PG(:4(5Z,8Z,11Z,14Z)/16)	C42H75O10P	M-H	769.5025	2.1
	HMDB0010650	PG(18:2(9Z,12Z)/18:2(9Z,12Z))	C42H75O10P	M-H	769.5025	2.1
	HMDB0010663	PG(18:3(6Z,9Z,12Z)/18:1(11Z))	C42H75O10P	M-H	769.5025	2.1
	HMDB0010637	PG(18:1(9Z)/18:3(9Z,12Z,15Z))	C42H75O10P	M-H	769.5025	2.1
	HMDB0010636	PG(18:1(9Z)/18:3(6Z,9Z,12Z))	C42H75O10P	M-H	769.5025	2.1
	HMDB0010622	PG(18:1(11Z)/18:3(9Z,12Z,15Z))	C42H75O10P	M-H	769.5025	2.1
	HMDB0010621	PG(18:1(11Z)/18:3(6Z,9Z,12Z))	C42H75O10P	M-H	769.5025	2.1
	HMDB0010580	PG(16/:4(5Z,8Z,11Z,14Z))	C42H75O10P	M-H	769.5025	2.1
	HMDB0010593	PG(16:1(9Z)/:3(5Z,8Z,11Z))	C42H75O10P	M-H	769.5025	2.1
	HMDB0010594	PG(16:1(9Z)/:3(8Z,11Z,14Z))	C42H75O10P	M-H	769.5025	2.1
	HMDB0010664	PG(18:3(6Z,9Z,12Z)/18:1(9Z))	C42H75O10P	M-H	769.5025	2.1
	HMDB0010678	PG(18:3(9Z,12Z,15Z)/18:1(11Z))	C42H75O10P	M-H	769.5025	2.1
	HMDB0010679	PG(18:3(9Z,12Z,15Z)/18:1(9Z))	C42H75O10P	M-H	769.5025	2.1
	HMDB0115326	PA(22:4(7Z,Z,13Z,16Z)/16)	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0115493	PA(:2(11Z,14Z)/18:2(9Z,12Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0115517	PA(18:1(11Z)/:3(8Z,11Z,14Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0115519	PA(18:1(9Z)/:3(8Z,11Z,14Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0115520	PA(18:2(9Z,12Z)/:2(11Z,14Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0115568	PA(:3(8Z,11Z,14Z)/18:1(9Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0115567	PA(:3(8Z,11Z,14Z)/18:1(11Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0115125	PA(:3(5Z,8Z,11Z)/18:1(9Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0115176	PA(:4(8Z,11Z,14Z,17Z)/18)	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0115149	PA(:4(5Z,8Z,11Z,14Z)/18)	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0114884	PA(18/:4(5Z,8Z,11Z,14Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0114885	PA(18/:4(8Z,11Z,14Z,17Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0114908	PA(18:1(11Z)/:3(5Z,8Z,11Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0114933	PA(18:1(9Z)/:3(5Z,8Z,11Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0114986	PA(18:3(6Z,9Z,12Z)/:1(11Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0115013	PA(18:3(9Z,12Z,15Z)/:1(11Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0115039	PA(18:4(6Z,9Z,12Z,15Z)/)	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0115073	PA(/18:4(6Z,9Z,12Z,15Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0115100	PA(:1(11Z)/18:3(6Z,9Z,12Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0115101	PA(:1(11Z)/18:3(9Z,12Z,15Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0115124	PA(:3(5Z,8Z,11Z)/18:1(11Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0114846	PA(16/22:4(7Z,Z,13Z,16Z))	C41H73O8P	M+FA-H	769.5025	2.1
	HMDB0113867	PE-NMe2(16:1(9Z)/:1(11Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0113868	PE-NMe2(18:1(9Z)/18:1(11Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0113870	PE-NMe2(18:1(11Z)/18:1(11Z))	C43H82NO8P	M-H	770.5705	0.6

770.5710	HMDB0113869	PE-NMe2(18:1(11Z)/18:1(9Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0114438	PE-NMe2(22:1(13Z)/14:1(9Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0114466	PE-NMe2(22:2(13Z,16Z)/14)	C43H82NO8P	M-H	770.5705	0.6
	HMDB0113948	PE-NMe2(16/:2(11Z,14Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0114242	PE-NMe2(:2(11Z,14Z)/16)	C43H82NO8P	M-H	770.5705	0.6
	HMDB0114214	PE-NMe2(:1(11Z)/16:1(9Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0114070	PE-NMe2(18:2(9Z,12Z)/18)	C43H82NO8P	M-H	770.5705	0.6
	HMDB0113910	PE-NMe2(14:1(9Z)/22:1(13Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0113033	PE-NMe(15/22:2(13Z,16Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0113565	PE-NMe(22:2(13Z,16Z)/15)	C43H82NO8P	M-H	770.5705	0.6
	HMDB0113892	PE-NMe2(14/22:2(13Z,16Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0113990	PE-NMe2(18/18:2(9Z,12Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0009225	PE(/18:2(9Z,12Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0009256	PE(:1(11Z)/18:1(11Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0009257	PE(:1(11Z)/18:1(9Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0009288	PE(:2(11Z,14Z)/18)	C43H82NO8P	M-H	770.5705	0.6
	HMDB0009518	PE(22:1(13Z)/16:1(9Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0009550	PE(22:2(13Z,16Z)/16)	C43H82NO8P	M-H	770.5705	0.6
	HMDB0009097	PE(18:2(9Z,12Z)/)	C43H82NO8P	M-H	770.5705	0.6
	HMDB0009065	PE(18:1(9Z)/:1(11Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0009032	PE(18:1(11Z)/:1(11Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0009000	PE(18/:2(11Z,14Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0008974	PE(16:1(9Z)/22:1(13Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0008942	PE(16/22:2(13Z,16Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0008882	PE(14:1(9Z)/24:1(15Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0008330	PC(:2(11Z,14Z)/15)	C43H82NO8P	M-H	770.5705	0.6
	HMDB0007946	PC(15/:2(11Z,14Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0009746	PE(24:1(15Z)/14:1(9Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0010564	PE-NMe2(18:1(9Z)/18:1(9Z))	C43H82NO8P	M-H	770.5705	0.6
	HMDB0010648	PG(18:2(9Z,12Z)/18:1(11Z))	C42H77O10P	M-H	771.5182	0.3
	HMDB0010578	PG(16/:3(5Z,8Z,11Z))	C42H77O10P	M-H	771.5182	0.3
	HMDB0010579	PG(16/:3(8Z,11Z,14Z))	C42H77O10P	M-H	771.5182	0.3

771.5184	HMDB0010606	PG(18/18:3(6Z,9Z,12Z))	C42H77O10P	M-H	771.5182	0.3
	HMDB0010607	PG(18/18:3(9Z,12Z,15Z))	C42H77O10P	M-H	771.5182	0.3
	HMDB0010620	PG(18:1(11Z)/18:2(9Z,12Z))	C42H77O10P	M-H	771.5182	0.3
	HMDB0010635	PG(18:1(9Z)/18:2(9Z,12Z))	C42H77O10P	M-H	771.5182	0.3
	HMDB0010649	PG(18:2(9Z,12Z)/18:1(9Z))	C42H77O10P	M-H	771.5182	0.3
	HMDB0010662	PG(18:3(6Z,9Z,12Z)/18)	C42H77O10P	M-H	771.5182	0.3
	HMDB0010677	PG(18:3(9Z,12Z,15Z)/18)	C42H77O10P	M-H	771.5182	0.3
	HMDB0115300	PA(22:2(13Z,16Z)/16:1(9Z))	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0115516	PA(18:1(11Z)/:2(11Z,14Z))	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0115515	PA(18/:3(8Z,11Z,14Z))	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0115518	PA(18:1(9Z)/:2(11Z,14Z))	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0115538	PA(:2(11Z,14Z)/18:1(11Z))	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0115539	PA(:2(11Z,14Z)/18:1(9Z))	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0115566	PA(:3(8Z,11Z,14Z)/18)	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0115123	PA(:3(5Z,8Z,11Z)/18)	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0115099	PA(:1(11Z)/18:2(9Z,12Z))	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0115071	PA(/18:3(6Z,9Z,12Z))	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0115072	PA(/18:3(9Z,12Z,15Z))	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0115012	PA(18:3(9Z,12Z,15Z)/)	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0114985	PA(18:3(6Z,9Z,12Z)/)	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0114959	PA(18:2(9Z,12Z)/:1(11Z))	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0114883	PA(18/:3(5Z,8Z,11Z))	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0114866	PA(16:1(9Z)/22:2(13Z,16Z))	C41H75O8P	M+FA-H	771.5182	0.3
	HMDB0009711	PE(22:6(4Z,7Z,Z,13Z,16Z,19Z)/P-18:1(9Z))	C45H76NO7P	M-H	772.5287	1.0
	HMDB0009710	PE(22:6(4Z,7Z,Z,13Z,16Z,19Z)/P-18:1(11Z))	C45H76NO7P	M-H	772.5287	1.0
	HMDB0011427	PE(P-18:1(11Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C45H76NO7P	M-H	772.5287	1.0
	HMDB0011460	PE(P-18:1(9Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C45H76NO7P	M-H	772.5287	1.0
	HMDB0113959	PE-NMe2(16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C45H78NO8P	M-H20-H	772.5281	1.7
	HMDB0113981	PE-NMe2(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C45H78NO8P	M-H20-H	772.5281	1.7
	HMDB0114388	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C45H78NO8P	M-H20-H	772.5281	1.7
	HMDB0114526	PE-NMe2(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C45H78NO8P	M-H20-H	772.5281	1.7
	HMDB0114553	PE-NMe2(22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C45H78NO8P	M-H20-H	772.5281	1.7
	HMDB0114579	PE-NMe2(22:6(4Z,7Z,Z,13Z,16Z,19Z)/16)	C45H78NO8P	M-H20-H	772.5281	1.7
	HMDB0114166	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/:2(11Z,14Z))	C45H78NO8P	M-H20-H	772.5281	1.7
	HMDB0114250	PE-NMe2(:2(11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C45H78NO8P	M-H20-H	772.5281	1.7
	HMDB0114387	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C45H78NO8P	M-H20-H	772.5281	1.7
	HMDB0114360	PE-NMe2(:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C45H78NO8P	M-H20-H	772.5281	1.7
	HMDB0114028	PE-NMe2(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C45H78NO8P	M-H20-H	772.5281	1.7
	HMDB0114055	PE-NMe2(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C45H78NO8P	M-H20-H	772.5281	1.7
	HMDB0114083	PE-NMe2(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C45H78NO8P	M-H20-H	772.5281	1.7

772.5294

HMDB0114082	PE-NMe2(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0114109	PE-NMe2(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0114110	PE-NMe2(18:3(6Z,9Z,12Z)/:3(8Z,11Z,14Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0114138	PE-NMe2(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0114139	PE-NMe2(18:3(9Z,12Z,15Z)/:3(8Z,11Z,14Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0114277	PE-NMe2(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0114278	PE-NMe2(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0114305	PE-NMe2(:3(8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0114306	PE-NMe2(:3(8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0114332	PE-NMe2(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0113980	PE-NMe2(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0007958	PC(15/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009396	PE(:4(5Z,8Z,11Z,14Z)/:2(11Z,14Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009429	PE(:4(8Z,11Z,14Z,17Z)/:2(11Z,14Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009461	PE(:5(5Z,8Z,11Z,14Z,17Z)/:1(11Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009558	PE(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009588	PE(22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009620	PE(22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009619	PE(22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009652	PE(22:5(7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009653	PE(22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009684	PE(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18)	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009365	PE(:3(8Z,11Z,14Z)/:3(8Z,11Z,14Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009364	PE(:3(8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0008724	PC(22:6(4Z,7Z,Z,13Z,16Z,19Z)/15)	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009012	PE(18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009044	PE(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009043	PE(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009076	PE(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009077	PE(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009108	PE(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C45H78NO8P	M-H20-H	772.5281	1.7
HMDB0009206	PE(18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C45H78NO8P	M-H20-H	772.5281	1.7

	HMDB0009269	PE(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C45H78NO8P	M-H2O-H	772.5281	1.7
	HMDB0009300	PE(:2(11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C45H78NO8P	M-H2O-H	772.5281	1.7
	HMDB0009301	PE(:2(11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C45H78NO8P	M-H2O-H	772.5281	1.7
	HMDB0009331	PE(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z))	C45H78NO8P	M-H2O-H	772.5281	1.7
	HMDB0009332	PE(:3(5Z,8Z,11Z)/:3(8Z,11Z,14Z))	C45H78NO8P	M-H2O-H	772.5281	1.7
773.5333	HMDB0114811	PA(14:1(9Z)/24:1(15Z))	C41H77O8P	M+FA-H	773.5338	-0.7
	HMDB0114845	PA(16/22:2(13Z,16Z))	C41H77O8P	M+FA-H	773.5338	-0.7
	HMDB0114865	PA(16:1(9Z)/22:1(13Z))	C41H77O8P	M+FA-H	773.5338	-0.7
	HMDB0114907	PA(18:1(11Z)/:1(11Z))	C41H77O8P	M+FA-H	773.5338	-0.7
	HMDB0114932	PA(18:1(9Z)/:1(11Z))	C41H77O8P	M+FA-H	773.5338	-0.7
	HMDB0114958	PA(18:2(9Z,12Z)/)	C41H77O8P	M+FA-H	773.5338	-0.7
	HMDB0115070	PA(/18:2(9Z,12Z))	C41H77O8P	M+FA-H	773.5338	-0.7
	HMDB0115097	PA(:1(11Z)/18:1(11Z))	C41H77O8P	M+FA-H	773.5338	-0.7
	HMDB0115098	PA(:1(11Z)/18:1(9Z))	C41H77O8P	M+FA-H	773.5338	-0.7
	HMDB0115274	PA(22:1(13Z)/16:1(9Z))	C41H77O8P	M+FA-H	773.5338	-0.7
	HMDB0115299	PA(22:2(13Z,16Z)/16)	C41H77O8P	M+FA-H	773.5338	-0.7
	HMDB0115514	PA(18/:2(11Z,14Z))	C41H77O8P	M+FA-H	773.5338	-0.7
	HMDB0115456	PA(24:1(15Z)/14:1(9Z))	C41H77O8P	M+FA-H	773.5338	-0.7
	HMDB0115537	PA(:2(11Z,14Z)/18)	C41H77O8P	M+FA-H	773.5338	-0.7
	HMDB0010605	PG(18/18:2(9Z,12Z))	C42H79O10P	M-H	773.5338	-0.7
	HMDB0010647	PG(18:2(9Z,12Z)/18)	C42H79O10P	M-H	773.5338	-0.7
	HMDB0010633	PG(18:1(9Z)/18:1(11Z))	C42H79O10P	M-H	773.5338	-0.7
	HMDB0010619	PG(18:1(11Z)/18:1(9Z))	C42H79O10P	M-H	773.5338	-0.7
	HMDB0010634	PG(18:1(9Z)/18:1(9Z))	C42H79O10P	M-H	773.5338	-0.7
	HMDB0010618	PG(18:1(11Z)/18:1(11Z))	C42H79O10P	M-H	773.5338	-0.7
775.5508	HMDB0010604	PG(18/18:1(9Z))	C42H81O10P	M-H	775.5495	1.7
	HMDB0010617	PG(18:1(11Z)/18)	C42H81O10P	M-H	775.5495	1.7
	HMDB0010632	PG(18:1(9Z)/18)	C42H81O10P	M-H	775.5495	1.7
	HMDB0010603	PG(18/18:1(11Z))	C42H81O10P	M-H	775.5495	1.7
	HMDB0115244	PA(22/16:1(9Z))	C41H79O8P	M+FA-H	775.5495	1.7
	HMDB0115273	PA(22:1(13Z)/16)	C41H79O8P	M+FA-H	775.5495	1.7
	HMDB0115429	PA(24/14:1(9Z))	C41H79O8P	M+FA-H	775.5495	1.7
	HMDB0115455	PA(24:1(15Z)/14)	C41H79O8P	M+FA-H	775.5495	1.7
	HMDB0115096	PA(:1(11Z)/18)	C41H79O8P	M+FA-H	775.5495	1.7
	HMDB0115068	PA(/18:1(11Z))	C41H79O8P	M+FA-H	775.5495	1.7
	HMDB0114931	PA(18:1(9Z)/)	C41H79O8P	M+FA-H	775.5495	1.7
	HMDB0114906	PA(18:1(11Z)/)	C41H79O8P	M+FA-H	775.5495	1.7
	HMDB0114882	PA(18/:1(11Z))	C41H79O8P	M+FA-H	775.5495	1.7
	HMDB0114864	PA(16:1(9Z)/22)	C41H79O8P	M+FA-H	775.5495	1.7
	HMDB0114844	PA(16/22:1(13Z))	C41H79O8P	M+FA-H	775.5495	1.7
	HMDB0114810	PA(14:1(9Z)/24)	C41H79O8P	M+FA-H	775.5495	1.7
	HMDB0114794	PA(14/24:1(15Z))	C41H79O8P	M+FA-H	775.5495	1.7
	HMDB0115069	PA(/18:1(9Z))	C41H79O8P	M+FA-H	775.5495	1.7
	HMDB0009585	PE(22:4(7Z,Z,13Z,16Z)/18)	C45H82NO8P	M-H2O-H	776.5594	-1.2
	HMDB0009265	PE(:1(11Z)/:3(5Z,8Z,11Z))	C45H82NO8P	M-H2O-H	776.5594	-1.2
	HMDB0009172	PE(18:3(9Z,12Z,15Z)/22:1(13Z))	C45H82NO8P	M-H2O-H	776.5594	-1.2

776.5585

HMDB0009204	PE(18:4(6Z,9Z,12Z,15Z)/22)	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0009394	PE(:4(5Z,8Z,11Z,14Z)/)	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0009362	PE(:3(8Z,11Z,14Z)/:1(11Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0009329	PE(:3(5Z,8Z,11Z)/:1(11Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0009235	PE(/:4(8Z,11Z,14Z,17Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0009297	PE(:2(11Z,14Z)/:2(11Z,14Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0009234	PE(/:4(5Z,8Z,11Z,14Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0009266	PE(:1(11Z)/:3(8Z,11Z,14Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0009427	PE(:4(8Z,11Z,14Z,17Z)/)	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0009139	PE(18:3(6Z,9Z,12Z)/22:1(13Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0009555	PE(22:2(13Z,16Z)/18:2(9Z,12Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0007955	PC(15/22:4(7Z,Z,13Z,16Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0008625	PC(22:4(7Z,Z,13Z,16Z)/15)	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0009009	PE(18/22:4(7Z,Z,13Z,16Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0009523	PE(22:1(13Z)/18:3(6Z,9Z,12Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0009524	PE(22:1(13Z)/18:3(9Z,12Z,15Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0009107	PE(18:2(9Z,12Z)/22:2(13Z,16Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0009492	PE(22/18:4(6Z,9Z,12Z,15Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0114000	PE-NMe2(18/:4(8Z,11Z,14Z,17Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0113956	PE-NMe2(16/22:4(7Z,Z,13Z,16Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0113999	PE-NMe2(18/:4(5Z,8Z,11Z,14Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0114025	PE-NMe2(18:1(11Z)/:3(8Z,11Z,14Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0114302	PE-NMe2(:3(8Z,11Z,14Z)/18:1(11Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0114329	PE-NMe2(:4(5Z,8Z,11Z,14Z)/18)	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0114357	PE-NMe2(:4(8Z,11Z,14Z,17Z)/18)	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0114498	PE-NMe2(22:4(7Z,Z,13Z,16Z)/16)	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0114079	PE-NMe2(18:2(9Z,12Z)/:2(11Z,14Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0114247	PE-NMe2(:2(11Z,14Z)/18:2(9Z,12Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0114274	PE-NMe2(:3(5Z,8Z,11Z)/18:1(11Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0114275	PE-NMe2(:3(5Z,8Z,11Z)/18:1(9Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0114303	PE-NMe2(:3(8Z,11Z,14Z)/18:1(9Z))	C45H82NO8P	M-H20-H	776.5594	-1.2
HMDB0114024	PE-NMe2(18:1(11Z)/:3(5Z,8Z,11Z))	C45H82NO8P	M-H20-H	776.5594	-1.2

HMDB0114052	PE-NMe2(18:1(9Z)/:3(8Z,11Z,14Z))	C45H82NO8P	M-H2O-H	776.5594	-1.2
HMDB0114051	PE-NMe2(18:1(9Z)/:3(5Z,8Z,11Z))	C45H82NO8P	M-H2O-H	776.5594	-1.2
HMDB0114107	PE-NMe2(18:3(6Z,9Z,12Z)/:1(11Z))	C45H82NO8P	M-H2O-H	776.5594	-1.2
HMDB0114136	PE-NMe2(18:3(9Z,12Z,15Z)/:1(11Z))	C45H82NO8P	M-H2O-H	776.5594	-1.2
HMDB0114164	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/)	C45H82NO8P	M-H2O-H	776.5594	-1.2
HMDB0114192	PE-NMe2(/18:4(6Z,9Z,12Z,15Z))	C45H82NO8P	M-H2O-H	776.5594	-1.2
HMDB0114220	PE-NMe2(:1(11Z)/18:3(9Z,12Z,15Z))	C45H82NO8P	M-H2O-H	776.5594	-1.2
HMDB0114219	PE-NMe2(:1(11Z)/18:3(6Z,9Z,12Z))	C45H82NO8P	M-H2O-H	776.5594	-1.2
HMDB0011447	PE(P-18:1(9Z)/:1(11Z))	C43H82NO7P	M+Na-2H	776.5576	1.2
HMDB0011414	PE(P-18:1(11Z)/:1(11Z))	C43H82NO7P	M+Na-2H	776.5576	1.2
HMDB0011382	PE(P-18/:2(11Z,14Z))	C43H82NO7P	M+Na-2H	776.5576	1.2
HMDB0011357	PE(P-16/22:2(13Z,16Z))	C43H82NO7P	M+Na-2H	776.5576	1.2
HMDB0009313	PE(:2(11Z,14Z)/P-18)	C43H82NO7P	M+Na-2H	776.5576	1.2
HMDB0009282	PE(:1(11Z)/P-18:1(9Z))	C43H82NO7P	M+Na-2H	776.5576	1.2
HMDB0009281	PE(:1(11Z)/P-18:1(11Z))	C43H82NO7P	M+Na-2H	776.5576	1.2
HMDB0009576	PE(22:2(13Z,16Z)/P-16)	C43H82NO7P	M+Na-2H	776.5576	1.2
HMDB0011393	PE(P-18/22:5(7Z,Z,13Z,16Z,19Z))	C45H80NO7P	M-H	776.5600	-1.9
HMDB0011392	PE(P-18/22:5(4Z,7Z,Z,13Z,16Z))	C45H80NO7P	M-H	776.5600	-1.9
HMDB0009676	PE(22:5(7Z,Z,13Z,16Z,19Z)/P-18)	C45H80NO7P	M-H	776.5600	-1.9
HMDB0009643	PE(22:5(4Z,7Z,Z,13Z,16Z)/P-18)	C45H80NO7P	M-H	776.5600	-1.9
HMDB0009612	PE(22:4(7Z,Z,13Z,16Z)/P-18:1(9Z))	C45H80NO7P	M-H	776.5600	-1.9
HMDB0009611	PE(22:4(7Z,Z,13Z,16Z)/P-18:1(11Z))	C45H80NO7P	M-H	776.5600	-1.9
HMDB0011424	PE(P-18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C45H80NO7P	M-H	776.5600	-1.9
HMDB0011457	PE(P-18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C45H80NO7P	M-H	776.5600	-1.9
HMDB0116379	(2S)-1-{[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate	C47H80O7	M+Na-2H	777.5651	-1.4
HMDB0116373	(2S)-1-{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C47H80O7	M+Na-2H	777.5651	-1.4
HMDB0116401	(2S)-1-hydroxy-3-{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C47H80O7	M+Na-2H	777.5651	-1.4
HMDB0116405	(2S)-2-{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C47H80O7	M+Na-2H	777.5651	-1.4
HMDB0116412	(2S)-2-{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-hydroxypropyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C47H80O7	M+Na-2H	777.5651	-1.4

777.5640

HMDB0116435	(2S)-1-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-3-hydroxypropan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate	C47H80O7	M+Na-2H	777.5651	-1.4
HMDB0116417	(2S)-3-hydroxy-2-{{11-(3-methyl-5-pentylfuran-2-yl)undecanoyl}oxy}propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate	C47H80O7	M+Na-2H	777.5651	-1.4
HMDB0115730	PA(a-21/a-17)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115721	PA(a-21/17)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115702	PA(a-13/a-25)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115940	PA(i-24/i-14)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115672	PA(22/i-16)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115738	PA(a-21/i-17)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115747	PA(a-25/13)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115923	PA(i-24/14)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115912	PA(i-22/i-16)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115895	PA(i-22/16)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115883	PA(i-21/i-17)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115866	PA(i-21/17)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115854	PA(i-/i-18)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115837	PA(i-/18)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115825	PA(i-19/i-19)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115798	PA(i-13/a-25)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115764	PA(a-25/i-13)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115758	PA(a-25/a-13)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115656	PA(21/i-17)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115648	PA(21/a-17)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115640	PA(i-/18)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0114793	PA(14/24)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0114843	PA(16/22)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0114881	PA(18/)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115054	PA(19/19)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115067	PA(/18)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115230	PA(21/17)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115243	PA(22/16)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115428	PA(24/14)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0115875	PA(i-21/a-17)	C41H81O8P	M+FA-H	777.5651	-1.4
HMDB0010602	PG(18/18)	C42H83O10P	M-H	777.5651	-1.4
HMDB0116671	PG(i-12/i-24)	C42H83O10P	M-H	777.5651	-1.4
HMDB0011391	PE(P-18/22:4(7Z,Z,13Z,16Z))	C45H82NO7P	M-H	778.5756	0.1
HMDB0009610	PE(22:4(7Z,Z,13Z,16Z)/P-18)	C45H82NO7P	M-H	778.5756	0.1
HMDB0113978	PE-NMe2(16:1(9Z)/22:2(13Z,16Z))	C45H84NO8P	M-H2O-H	778.5751	0.8
HMDB0113997	PE-NMe2(18:/3(5Z,8Z,11Z))	C45H84NO8P	M-H2O-H	778.5751	0.8
HMDB0113998	PE-NMe2(18:/3(8Z,11Z,14Z))	C45H84NO8P	M-H2O-H	778.5751	0.8
HMDB0114246	PE-NMe2(:2(11Z,14Z)/18:1(9Z))	C45H84NO8P	M-H2O-H	778.5751	0.8
HMDB0114245	PE-NMe2(:2(11Z,14Z)/18:1(11Z))	C45H84NO8P	M-H2O-H	778.5751	0.8
HMDB0114023	PE-NMe2(18:1(11Z)/:2(11Z,14Z))	C45H84NO8P	M-H2O-H	778.5751	0.8
HMDB0114050	PE-NMe2(18:1(9Z)/:2(11Z,14Z))	C45H84NO8P	M-H2O-H	778.5751	0.8
HMDB0114301	PE-NMe2(:3(8Z,11Z,14Z)/18)	C45H84NO8P	M-H2O-H	778.5751	0.8
HMDB0114273	PE-NMe2(:3(5Z,8Z,11Z)/18)	C45H84NO8P	M-H2O-H	778.5751	0.8
HMDB0114218	PE-NMe2(:1(11Z)/18:2(9Z,12Z))	C45H84NO8P	M-H2O-H	778.5751	0.8

778.5757

HMDB0114190	PE-NMe2(/18:3(6Z,9Z,12Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0114191	PE-NMe2(/18:3(9Z,12Z,15Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0114135	PE-NMe2(18:3(9Z,12Z,15Z)/)	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0114106	PE-NMe2(18:3(6Z,9Z,12Z)/)	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0114078	PE-NMe2(18:2(9Z,12Z)/:1(11Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0114470	PE-NMe2(22:2(13Z,16Z)/16:1(9Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009361	PE(:3(8Z,11Z,14Z)/)	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009490	PE(22/18:3(6Z,9Z,12Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009491	PE(22/18:3(9Z,12Z,15Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009522	PE(22:1(13Z)/18:2(9Z,12Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009553	PE(22:2(13Z,16Z)/18:1(11Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009328	PE(:3(5Z,8Z,11Z)/)	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009296	PE(:2(11Z,14Z)/:1(11Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009264	PE(:1(11Z)/:2(11Z,14Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009233	PE(/:3(8Z,11Z,14Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009232	PE(/:3(5Z,8Z,11Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009171	PE(18:3(9Z,12Z,15Z)/22)	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009138	PE(18:3(6Z,9Z,12Z)/22)	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009106	PE(18:2(9Z,12Z)/22:1(13Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009074	PE(18:1(9Z)/22:2(13Z,16Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009554	PE(22:2(13Z,16Z)/18:1(9Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0009041	PE(18:1(11Z)/22:2(13Z,16Z))	C45H84NO8P	M-H20-H	778.5751	0.8
HMDB0112410	PS(18:1(9Z)/18:3(6Z,9Z,12Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0112391	PS(18:1(11Z)/18:3(9Z,12Z,15Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0112390	PS(18:1(11Z)/18:3(6Z,9Z,12Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0112374	PS(18/18:4(6Z,9Z,12Z,15Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0112361	PS(16:1(9Z)/:3(5Z,8Z,11Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0112450	PS(18:3(6Z,9Z,12Z)/18:1(9Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0116750	PS(16/:4(8Z,11Z,14Z,17Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0112449	PS(18:3(6Z,9Z,12Z)/18:1(11Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0112468	PS(18:3(9Z,12Z,15Z)/18:1(11Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0112303	PS(14/22:4(7Z,Z,13Z,16Z))	C42H74NO10P	M-H	782.4978	0.4

782.4981

HMDB0112788	PS(22:4(7Z,Z,13Z,16Z)/14)	C42H74NO10P	M-H	782.4978	0.4
HMDB0112657	PS(:4(8Z,11Z,14Z,17Z)/16)	C42H74NO10P	M-H	782.4978	0.4
HMDB0112597	PS(:3(5Z,8Z,11Z)/16:1(9Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0112490	PS(18:4(6Z,9Z,12Z,15Z)/18)	C42H74NO10P	M-H	782.4978	0.4
HMDB0012412	PS(18:3(9Z,12Z,15Z)/18:1(9Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0012402	PS(18:2(9Z,12Z)/18:2(9Z,12Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0012361	PS(16/:4(5Z,8Z,11Z,14Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0012371	PS(16:1(9Z)/:3(8Z,11Z,14Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0012392	PS(18:1(9Z)/18:3(9Z,12Z,15Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0012421	PS(:3(8Z,11Z,14Z)/16:1(9Z))	C42H74NO10P	M-H	782.4978	0.4
HMDB0012431	PS(:4(5Z,8Z,11Z,14Z)/16)	C42H74NO10P	M-H	782.4978	0.4
HMDB0113030	PE-NMe(15/:5(5Z,8Z,11Z,14Z,17Z))	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0113908	PE-NMe2(14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0114381	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/14)	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0114353	PE-NMe2(:4(8Z,11Z,14Z,17Z)/14:1(9Z))	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0114325	PE-NMe2(:4(5Z,8Z,11Z,14Z)/14:1(9Z))	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0114156	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/16:1(9Z))	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0113969	PE-NMe2(16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0113907	PE-NMe2(14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0113889	PE-NMe2(14/:5(5Z,8Z,11Z,14Z,17Z))	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0113481	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/15)	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0008846	PE(14/22:5(7Z,Z,13Z,16Z,19Z))	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0009190	PE(18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0009386	PE(:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0009419	PE(:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0009451	PE(:5(5Z,8Z,11Z,14Z,17Z)/16)	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0009581	PE(22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0009613	PE(22:5(4Z,7Z,Z,13Z,16Z)/14)	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0009646	PE(22:5(7Z,Z,13Z,16Z,19Z)/14)	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0009191	PE(18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0009159	PE(18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C41H72NO8P	M+FA-H	782.4978	0.4
HMDB0008845	PE(14/22:5(4Z,7Z,Z,13Z,16Z))	C41H72NO8P	M+FA-H	782.4978	0.4

	HMDB0008877	PE(14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C41H72NO8P	M+FA-H	782.4978	0.4
	HMDB0008939	PE(16/:5(5Z,8Z,11Z,14Z,17Z))	C41H72NO8P	M+FA-H	782.4978	0.4
	HMDB0008970	PE(16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C41H72NO8P	M+FA-H	782.4978	0.4
	HMDB0008971	PE(16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C41H72NO8P	M+FA-H	782.4978	0.4
	HMDB0009030	PE(18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO8P	M+FA-H	782.4978	0.4
	HMDB0009063	PE(18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C41H72NO8P	M+FA-H	782.4978	0.4
	HMDB0009095	PE(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C41H72NO8P	M+FA-H	782.4978	0.4
	HMDB0009094	PE(18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C41H72NO8P	M+FA-H	782.4978	0.4
	HMDB0009126	PE(18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C41H72NO8P	M+FA-H	782.4978	0.4
782.5330	HMDB0112763	PS(22:2(13Z,16Z)/15)	C43H80NO10P	M-H20-H	782.5336	-0.8
	HMDB0116749	PS(15/22:2(13Z,16Z))	C43H80NO10P	M-H20-H	782.5336	-0.8
	HMDB0011214	PC(P-16/18:4(6Z,9Z,12Z,15Z))	C42H76NO7P	M+FA-H	782.5341	-1.5
	HMDB0008258	PC(18:4(6Z,9Z,12Z,15Z)/P-16)	C42H76NO7P	M+FA-H	782.5341	-1.5
	HMDB0113028	PE-NMe(15/:4(5Z,8Z,11Z,14Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0113029	PE-NMe(15/:4(8Z,11Z,14Z,17Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0113424	PE-NMe(:4(5Z,8Z,11Z,14Z)/15)	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0114352	PE-NMe2(:4(8Z,11Z,14Z,17Z)/14)	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0114324	PE-NMe2(:4(5Z,8Z,11Z,14Z)/14)	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0114297	PE-NMe2(:3(8Z,11Z,14Z)/14:1(9Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0114269	PE-NMe2(:3(5Z,8Z,11Z)/14:1(9Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0113452	PE-NMe(:4(8Z,11Z,14Z,17Z)/15)	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0113887	PE-NMe2(14/:4(5Z,8Z,11Z,14Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0113888	PE-NMe2(14/:4(8Z,11Z,14Z,17Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0113905	PE-NMe2(14:1(9Z)/:3(5Z,8Z,11Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0113906	PE-NMe2(14:1(9Z)/:3(8Z,11Z,14Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0113946	PE-NMe2(16/18:4(6Z,9Z,12Z,15Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0113967	PE-NMe2(16:1(9Z)/18:3(6Z,9Z,12Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0113968	PE-NMe2(16:1(9Z)/18:3(9Z,12Z,15Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0114098	PE-NMe2(18:3(6Z,9Z,12Z)/16:1(9Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0114127	PE-NMe2(18:3(9Z,12Z,15Z)/16:1(9Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0114155	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/16)	C41H74NO8P	M+FA-H	784.5134	-1.2
	HMDB0009580	PE(22:4(7Z,Z,13Z,16Z)/14)	C41H74NO8P	M+FA-H	784.5134	-1.2

784.5125

HMDB0009029	PE(18:1(11Z)/18:3(9Z,12Z,15Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0009061	PE(18:1(9Z)/18:3(6Z,9Z,12Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0009062	PE(18:1(9Z)/18:3(9Z,12Z,15Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0009320	PE(:3(5Z,8Z,11Z)/16:1(9Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0009093	PE(18:2(9Z,12Z)/18:2(9Z,12Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0009418	PE(:4(8Z,11Z,14Z,17Z)/16)	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0009385	PE(:4(5Z,8Z,11Z,14Z)/16)	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0009353	PE(:3(8Z,11Z,14Z)/16:1(9Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0009189	PE(18:4(6Z,9Z,12Z,15Z)/18)	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0009157	PE(18:3(9Z,12Z,15Z)/18:1(11Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0009158	PE(18:3(9Z,12Z,15Z)/18:1(9Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0009125	PE(18:3(6Z,9Z,12Z)/18:1(9Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0009124	PE(18:3(6Z,9Z,12Z)/18:1(11Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0009028	PE(18:1(11Z)/18:3(6Z,9Z,12Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0008997	PE(18/18:4(6Z,9Z,12Z,15Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0008938	PE(16/:4(8Z,11Z,14Z,17Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0008937	PE(16/:4(5Z,8Z,11Z,14Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0008844	PE(14/22:4(7Z,Z,13Z,16Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0008231	PC(18:4(6Z,9Z,12Z,15Z)/15)	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0007943	PC(15/18:4(6Z,9Z,12Z,15Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0008968	PE(16:1(9Z)/:3(5Z,8Z,11Z))	C41H74NO8P	M+FA-H	784.5134	-1.2
HMDB0012360	PS(16/:3(8Z,11Z,14Z))	C42H76NO10P	M-H	784.5134	-1.2
HMDB0012420	PS(:3(8Z,11Z,14Z)/16)	C42H76NO10P	M-H	784.5134	-1.2
HMDB0012401	PS(18:2(9Z,12Z)/18:1(9Z))	C42H76NO10P	M-H	784.5134	-1.2
HMDB0012381	PS(18/18:3(9Z,12Z,15Z))	C42H76NO10P	M-H	784.5134	-1.2
HMDB0012391	PS(18:1(9Z)/18:2(9Z,12Z))	C42H76NO10P	M-H	784.5134	-1.2
HMDB0012411	PS(18:3(9Z,12Z,15Z)/18)	C42H76NO10P	M-H	784.5134	-1.2
HMDB0112596	PS(:3(5Z,8Z,11Z)/16)	C42H76NO10P	M-H	784.5134	-1.2
HMDB0112762	PS(22:2(13Z,16Z)/14:1(9Z))	C42H76NO10P	M-H	784.5134	-1.2
HMDB0112360	PS(16:1(9Z)/:2(11Z,14Z))	C42H76NO10P	M-H	784.5134	-1.2
HMDB0112571	PS(:2(11Z,14Z)/16:1(9Z))	C42H76NO10P	M-H	784.5134	-1.2
HMDB0112426	PS(18:2(9Z,12Z)/18:1(11Z))	C42H76NO10P	M-H	784.5134	-1.2

HMDB0112448	PS(18:3(6Z,9Z,12Z)/18)	C42H76NO10P	M-H	784.5134	-1.2
HMDB0112347	PS(16/:3(5Z,8Z,11Z))	C42H76NO10P	M-H	784.5134	-1.2
HMDB0112389	PS(18:1(11Z)/18:2(9Z,12Z))	C42H76NO10P	M-H	784.5134	-1.2
HMDB0112315	PS(14:1(9Z)/22:2(13Z,16Z))	C42H76NO10P	M-H	784.5134	-1.2
HMDB0112373	PS(18/18:3(6Z,9Z,12Z))	C42H76NO10P	M-H	784.5134	-1.2
HMDB0112511	PS(/14)	C40H78NO10P	M+Na-2H	784.5110	1.9
HMDB0012376	PS(18/16)	C40H78NO10P	M+Na-2H	784.5110	1.9
HMDB0112295	PS(14/)	C40H78NO10P	M+Na-2H	784.5110	1.9
HMDB0012356	PS(16/18)	C40H78NO10P	M+Na-2H	784.5110	1.9
HMDB0113026	PE-NMe(15/:3(5Z,8Z,11Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0113027	PE-NMe(15/:3(8Z,11Z,14Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0114268	PE-NMe2(:3(5Z,8Z,11Z)/14)	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0114296	PE-NMe2(:3(8Z,11Z,14Z)/14)	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0113904	PE-NMe2(14:1(9Z)/:2(11Z,14Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0114240	PE-NMe2(:2(11Z,14Z)/14:1(9Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0114126	PE-NMe2(18:3(9Z,12Z,15Z)/16)	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0114097	PE-NMe2(18:3(6Z,9Z,12Z)/16)	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0113368	PE-NMe(:3(5Z,8Z,11Z)/15)	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0113396	PE-NMe(:3(8Z,11Z,14Z)/15)	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0113886	PE-NMe2(14/:3(8Z,11Z,14Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0113885	PE-NMe2(14/:3(5Z,8Z,11Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0113944	PE-NMe2(16/18:3(6Z,9Z,12Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0113945	PE-NMe2(16/18:3(9Z,12Z,15Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0113966	PE-NMe2(16:1(9Z)/18:2(9Z,12Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0114069	PE-NMe2(18:2(9Z,12Z)/16:1(9Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0007942	PC(15/18:3(9Z,12Z,15Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0009092	PE(18:2(9Z,12Z)/18:1(9Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0009123	PE(18:3(6Z,9Z,12Z)/18)	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0009156	PE(18:3(9Z,12Z,15Z)/18)	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0009287	PE(:2(11Z,14Z)/16:1(9Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0009319	PE(:3(5Z,8Z,11Z)/16)	C41H76NO8P	M+FA-H	786.5291	-1.9
HMDB0009352	PE(:3(8Z,11Z,14Z)/16)	C41H76NO8P	M+FA-H	786.5291	-1.9

786.5276	HMDB0009548	PE(22:2(13Z,16Z)/14:1(9Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
	HMDB0009091	PE(18:2(9Z,12Z)/18:1(11Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
	HMDB0009060	PE(18:1(9Z)/18:2(9Z,12Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
	HMDB0007941	PC(15/18:3(6Z,9Z,12Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
	HMDB0008165	PC(18:3(6Z,9Z,12Z)/15)	C41H76NO8P	M+FA-H	786.5291	-1.9
	HMDB0008198	PC(18:3(9Z,12Z,15Z)/15)	C41H76NO8P	M+FA-H	786.5291	-1.9
	HMDB0008876	PE(14:1(9Z)/22:2(13Z,16Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
	HMDB0008936	PE(16/:3(8Z,11Z,14Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
	HMDB0008935	PE(16/:3(5Z,8Z,11Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
	HMDB0008967	PE(16:1(9Z)/:2(11Z,14Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
	HMDB0008996	PE(18/18:3(9Z,12Z,15Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
	HMDB0008995	PE(18/18:3(6Z,9Z,12Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
	HMDB0009027	PE(18:1(11Z)/18:2(9Z,12Z))	C41H76NO8P	M+FA-H	786.5291	-1.9
	HMDB0012400	PS(18:2(9Z,12Z)/18)	C42H78NO10P	M-H	786.5291	-1.9
	HMDB0012380	PS(18/18:2(9Z,12Z))	C42H78NO10P	M-H	786.5291	-1.9
	HMDB0112737	PS(22:1(13Z)/14:1(9Z))	C42H78NO10P	M-H	786.5291	-1.9
	HMDB0112761	PS(22:2(13Z,16Z)/14)	C42H78NO10P	M-H	786.5291	-1.9
	HMDB0112346	PS(16/:2(11Z,14Z))	C42H78NO10P	M-H	786.5291	-1.9
	HMDB0112570	PS(:2(11Z,14Z)/16)	C42H78NO10P	M-H	786.5291	-1.9
	HMDB0112272	PS(18:1(11Z)/18:1(11Z))	C42H78NO10P	M-H	786.5291	-1.9
	HMDB0112544	PS(:1(11Z)/16:1(9Z))	C42H78NO10P	M-H	786.5291	-1.9
	HMDB0112314	PS(14:1(9Z)/22:1(13Z))	C42H78NO10P	M-H	786.5291	-1.9
	HMDB0012390	PS(18:1(9Z)/18:1(9Z))	C42H78NO10P	M-H	786.5291	-1.9
	HMDB0112290	PS(18:1(11Z)/18:1(9Z))	C42H78NO10P	M-H	786.5291	-1.9
	HMDB0112291	PS(18:1(9Z)/18:1(11Z))	C42H78NO10P	M-H	786.5291	-1.9
	HMDB0112288	PS(16:1(9Z)/:1(11Z))	C42H78NO10P	M-H	786.5291	-1.9
	HMDB0112302	PS(14/22:2(13Z,16Z))	C42H78NO10P	M-H	786.5291	-1.9
	HMDB0112603	PS(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C44H74NO10P	M-H20-H	788.4866	0.3
	HMDB0112474	PS(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C44H74NO10P	M-H20-H	788.4866	0.3
	HMDB0112456	PS(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C44H74NO10P	M-H20-H	788.4866	0.3
	HMDB0112457	PS(18:3(6Z,9Z,12Z)/:3(8Z,11Z,14Z))	C44H74NO10P	M-H20-H	788.4866	0.3
	HMDB0112433	PS(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C44H74NO10P	M-H20-H	788.4866	0.3

788.4869	HMDB0112416	PS(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0112399	PS(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0112369	PS(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0112602	PS(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0112623	PS(:3(8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0112662	PS(:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0112577	PS(:2(11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0112843	PS(22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0112818	PS(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0112685	PS(:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0112686	PS(:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0112368	PS(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0112498	PS(18:4(6Z,9Z,12Z,15Z)/:2(11Z,14Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0012442	PS(22:6(4Z,7Z,Z,13Z,16Z,19Z)/16)	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0012435	PS(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0012425	PS(:3(8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0012415	PS(18:3(9Z,12Z,15Z)/:3(8Z,11Z,14Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0012405	PS(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0012362	PS(16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C44H74NO10P	M-H2O-H	788.4866	0.3
	HMDB0113857	PE-NMe2(16:1(9Z)/18:1(9Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0113856	PE-NMe2(14:1(9Z)/:1(11Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0113858	PE-NMe2(16:1(9Z)/18:1(11Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0114068	PE-NMe2(18:2(9Z,12Z)/16)	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0114211	PE-NMe2(:1(11Z)/14:1(9Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0113025	PE-NMe(15/:2(11Z,14Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0113339	PE-NMe(:2(11Z,14Z)/15)	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0113884	PE-NMe2(14/:2(11Z,14Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0114239	PE-NMe2(:2(11Z,14Z)/14)	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0114042	PE-NMe2(18:1(9Z)/16:1(9Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0114015	PE-NMe2(18:1(11Z)/16:1(9Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0113943	PE-NMe2(16/18:2(9Z,12Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0007940	PC(15/18:2(9Z,12Z))	C41H78NO8P	M+FA-H	788.5447	-1.7

788.5434	HMDB0009547	PE(22:2(13Z,16Z)/14)	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0009515	PE(22:1(13Z)/14:1(9Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0009286	PE(:2(11Z,14Z)/16)	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0008132	PC(18:2(9Z,12Z)/15)	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0008843	PE(14/22:2(13Z,16Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0008875	PE(14:1(9Z)/22:1(13Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0008934	PE(16/:2(11Z,14Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0008966	PE(16:1(9Z)/:1(11Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0008994	PE(18/18:2(9Z,12Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0009025	PE(18:1(11Z)/18:1(11Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0009026	PE(18:1(11Z)/18:1(9Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0009058	PE(18:1(9Z)/18:1(11Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0009059	PE(18:1(9Z)/18:1(9Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0009090	PE(18:2(9Z,12Z)/18)	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0009254	PE(:1(11Z)/16:1(9Z))	C41H78NO8P	M+FA-H	788.5447	-1.7
	HMDB0112301	PS(14/22:1(13Z))	C42H80NO10P	M-H	788.5447	-1.7
	HMDB0112388	PS(18:1(11Z)/18)	C42H80NO10P	M-H	788.5447	-1.7
	HMDB0112515	PS(/16:1(9Z))	C42H80NO10P	M-H	788.5447	-1.7
	HMDB0112543	PS(:1(11Z)/16)	C42H80NO10P	M-H	788.5447	-1.7
	HMDB0112708	PS(22/14:1(9Z))	C42H80NO10P	M-H	788.5447	-1.7
	HMDB0112736	PS(22:1(13Z)/14)	C42H80NO10P	M-H	788.5447	-1.7
	HMDB0112289	PS(18/18:1(11Z))	C42H80NO10P	M-H	788.5447	-1.7
	HMDB0112287	PS(16:1(9Z)/)	C42H80NO10P	M-H	788.5447	-1.7
	HMDB0112286	PS(16/:1(11Z))	C42H80NO10P	M-H	788.5447	-1.7
	HMDB0112279	PS(14:1(9Z)/22)	C42H80NO10P	M-H	788.5447	-1.7
	HMDB0012389	PS(18:1(9Z)/18)	C42H80NO10P	M-H	788.5447	-1.7
	HMDB0010163	PS(18/18:1(9Z))	C42H80NO10P	M-H	788.5447	-1.7
790.4874	HMDB0112425	PS(18:2(9Z,12Z)/15)	C39H72NO10P	M+FA-H	790.4876	-0.2
	HMDB0112323	PS(15/18:2(9Z,12Z))	C39H72NO10P	M+FA-H	790.4876	-0.2
	HMDB0009408	PE(:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C47H74NO8P	M-H20-H	792.4968	1.4
	HMDB0114178	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C47H74NO8P	M-H20-H	792.4968	1.4

792.4979	HMDB0114400	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/:5(5Z,8Z,11Z,14Z,17Z))	C47H74NO8P	M-H20-H	792.4968	1.4
	HMDB0114587	PE-NMe2(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z))	C47H74NO8P	M-H20-H	792.4968	1.4
	HMDB0009441	PE(:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C47H74NO8P	M-H20-H	792.4968	1.4
	HMDB0009472	PE(:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C47H74NO8P	M-H20-H	792.4968	1.4
	HMDB0009473	PE(:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C47H74NO8P	M-H20-H	792.4968	1.4
	HMDB0009632	PE(22:5(4Z,7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C47H74NO8P	M-H20-H	792.4968	1.4
	HMDB0009665	PE(22:5(7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C47H74NO8P	M-H20-H	792.4968	1.4
	HMDB0009696	PE(22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C47H74NO8P	M-H20-H	792.4968	1.4
	HMDB0009697	PE(22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C47H74NO8P	M-H20-H	792.4968	1.4
	HMDB0113957	PE-NMe2(16/22:5(4Z,7Z,Z,13Z,16Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114359	PE-NMe2(:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114386	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/18)	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114499	PE-NMe2(22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0116717	PE-NMe2(22:5(4Z,7Z,Z,13Z,16Z)/16)	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114552	PE-NMe2(22:5(7Z,Z,13Z,16Z,19Z)/16)	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114108	PE-NMe2(18:3(6Z,9Z,12Z)/:2(11Z,14Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114137	PE-NMe2(18:3(9Z,12Z,15Z)/:2(11Z,14Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114249	PE-NMe2(:2(11Z,14Z)/18:3(9Z,12Z,15Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114248	PE-NMe2(:2(11Z,14Z)/18:3(6Z,9Z,12Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114358	PE-NMe2(:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114331	PE-NMe2(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114304	PE-NMe2(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0113958	PE-NMe2(16/22:5(7Z,Z,13Z,16Z,19Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0113979	PE-NMe2(16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114001	PE-NMe2(18/:5(5Z,8Z,11Z,14Z,17Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114026	PE-NMe2(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114027	PE-NMe2(18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114053	PE-NMe2(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114054	PE-NMe2(18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114080	PE-NMe2(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C45H80NO8P	M-H	792.5549	0.7
	HMDB0114081	PE-NMe2(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C45H80NO8P	M-H	792.5549	0.7

792.5554

HMDB0114165	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0114221	PE-NMe2(:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0114276	PE-NMe2(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0114330	PE-NMe2(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009299	PE(:2(11Z,14Z)/:3(8Z,11Z,14Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009330	PE(:3(5Z,8Z,11Z)/:2(11Z,14Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009363	PE(:3(8Z,11Z,14Z)/:2(11Z,14Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009395	PE(:4(5Z,8Z,11Z,14Z)/:1(11Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009428	PE(:4(8Z,11Z,14Z,17Z)/:1(11Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009460	PE(:5(5Z,8Z,11Z,14Z,17Z)/)	C45H80NO8P	M-H	792.5549	0.7
HMDB0009525	PE(22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009556	PE(22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009557	PE(22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009586	PE(22:4(7Z,Z,13Z,16Z)/18:1(11Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009587	PE(22:4(7Z,Z,13Z,16Z)/18:1(9Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009618	PE(22:5(4Z,7Z,Z,13Z,16Z)/18)	C45H80NO8P	M-H	792.5549	0.7
HMDB0009298	PE(:2(11Z,14Z)/:3(5Z,8Z,11Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009267	PE(:1(11Z)/:4(5Z,8Z,11Z,14Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0007956	PC(15/22:5(4Z,7Z,Z,13Z,16Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0007957	PC(15/22:5(7Z,Z,13Z,16Z,19Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0008658	PC(22:5(4Z,7Z,Z,13Z,16Z)/15)	C45H80NO8P	M-H	792.5549	0.7
HMDB0008691	PC(22:5(7Z,Z,13Z,16Z,19Z)/15)	C45H80NO8P	M-H	792.5549	0.7
HMDB0009011	PE(18/22:5(7Z,Z,13Z,16Z,19Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009010	PE(18/22:5(4Z,7Z,Z,13Z,16Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009042	PE(18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009075	PE(18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009140	PE(18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009173	PE(18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009205	PE(18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009236	PE(/:5(5Z,8Z,11Z,14Z,17Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009268	PE(:1(11Z)/:4(8Z,11Z,14Z,17Z))	C45H80NO8P	M-H	792.5549	0.7
HMDB0009651	PE(22:5(7Z,Z,13Z,16Z,19Z)/18)	C45H80NO8P	M-H	792.5549	0.7

793.5031	HMDB0116575	PG(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C44H75O10P	M-H	793.5025	0.7
	HMDB0116584	PG(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C44H75O10P	M-H	793.5025	0.7
	HMDB0116591	PG(:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C44H75O10P	M-H	793.5025	0.7
	HMDB0116615	PG(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C44H75O10P	M-H	793.5025	0.7
	HMDB0116629	PG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/16)	C44H75O10P	M-H	793.5025	0.7
	HMDB0116623	PG(22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C44H75O10P	M-H	793.5025	0.7
	HMDB0010684	PG(18:3(9Z,12Z,15Z)/:3(8Z,11Z,14Z))	C44H75O10P	M-H	793.5025	0.7
	HMDB0010683	PG(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C44H75O10P	M-H	793.5025	0.7
	HMDB0010669	PG(18:3(6Z,9Z,12Z)/:3(8Z,11Z,14Z))	C44H75O10P	M-H	793.5025	0.7
	HMDB0010668	PG(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C44H75O10P	M-H	793.5025	0.7
	HMDB0010655	PG(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C44H75O10P	M-H	793.5025	0.7
	HMDB0010598	PG(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C44H75O10P	M-H	793.5025	0.7
	HMDB0010597	PG(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C44H75O10P	M-H	793.5025	0.7
	HMDB0010584	PG(16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C44H75O10P	M-H	793.5025	0.7
	HMDB0115498	PA(:4(5Z,8Z,11Z,14Z)/:2(11Z,14Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115500	PA(:4(8Z,11Z,14Z,17Z)/:2(11Z,14Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115549	PA(:2(11Z,14Z)/:4(8Z,11Z,14Z,17Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115047	PA(18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115494	PA(:3(5Z,8Z,11Z)/:3(8Z,11Z,14Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115497	PA(:3(8Z,11Z,14Z)/:3(8Z,11Z,14Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115496	PA(:3(8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0114893	PA(18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0114917	PA(18:1(11Z)/22:5(7Z,Z,13Z,16Z,19Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0114916	PA(18:1(11Z)/22:5(4Z,7Z,Z,13Z,16Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0114942	PA(18:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0114941	PA(18:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0114967	PA(18:2(9Z,12Z)/22:4(7Z,Z,13Z,16Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115108	PA(:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115132	PA(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115210	PA(:5(5Z,8Z,11Z,14Z,17Z)/:1(11Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115307	PA(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115331	PA(22:4(7Z,Z,13Z,16Z)/18:2(9Z,12Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115355	PA(22:5(4Z,7Z,Z,13Z,16Z)/18:1(11Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115356	PA(22:5(4Z,7Z,Z,13Z,16Z)/18:1(9Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115381	PA(22:5(7Z,Z,13Z,16Z,19Z)/18:1(11Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115382	PA(22:5(7Z,Z,13Z,16Z,19Z)/18:1(9Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115406	PA(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18)	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0115548	PA(:2(11Z,14Z)/:4(5Z,8Z,11Z,14Z))	C43H73O8P	M+FA-H	793.5025	0.7
	HMDB0114891	PA(18/22:5(4Z,7Z,Z,13Z,16Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115380	PA(22:5(7Z,Z,13Z,16Z,19Z)/18)	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115354	PA(22:5(4Z,7Z,Z,13Z,16Z)/18)	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115330	PA(22:4(7Z,Z,13Z,16Z)/18:1(9Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115306	PA(22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115305	PA(22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115281	PA(22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115209	PA(:5(5Z,8Z,11Z,14Z,17Z)/)	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0114892	PA(18/22:5(7Z,Z,13Z,16Z,19Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115184	PA(:4(8Z,11Z,14Z,17Z)/:1(11Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115157	PA(:4(5Z,8Z,11Z,14Z)/:1(11Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115106	PA(:1(11Z)/:4(5Z,8Z,11Z,14Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115107	PA(:1(11Z)/:4(8Z,11Z,14Z,17Z))	C43H75O8P	M+FA-H	795.5182	-0.1

795.5181	HMDB0115080	PA(/:5(5Z,8Z,11Z,14Z,17Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115046	PA(18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0114993	PA(18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0114940	PA(18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0114915	PA(18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115329	PA(22:4(7Z,Z,13Z,16Z)/18:1(11Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115020	PA(18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115560	PA(:3(5Z,8Z,11Z)/:2(11Z,14Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115546	PA(:2(11Z,14Z)/:3(5Z,8Z,11Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115574	PA(:3(8Z,11Z,14Z)/:2(11Z,14Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0115547	PA(:2(11Z,14Z)/:3(8Z,11Z,14Z))	C43H75O8P	M+FA-H	795.5182	-0.1
	HMDB0010625	PG(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C44H77O10P	M-H	795.5182	-0.1
	HMDB0010640	PG(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C44H77O10P	M-H	795.5182	-0.1
	HMDB0010583	PG(16/22:5(7Z,Z,13Z,16Z,19Z))	C44H77O10P	M-H	795.5182	-0.1
	HMDB0010653	PG(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C44H77O10P	M-H	795.5182	-0.1
	HMDB0010596	PG(16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C44H77O10P	M-H	795.5182	-0.1
	HMDB0010582	PG(16/22:5(4Z,7Z,Z,13Z,16Z))	C44H77O10P	M-H	795.5182	-0.1
	HMDB0010654	PG(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C44H77O10P	M-H	795.5182	-0.1
	HMDB0116743	PG(22:5(4Z,7Z,Z,13Z,16Z)/16)	C44H77O10P	M-H	795.5182	-0.1
	HMDB0116578	PG(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C44H77O10P	M-H	795.5182	-0.1
	HMDB0116609	PG(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C44H77O10P	M-H	795.5182	-0.1
	HMDB0116610	PG(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C44H77O10P	M-H	795.5182	-0.1
	HMDB0116621	PG(22:5(7Z,Z,13Z,16Z,19Z)/16)	C44H77O10P	M-H	795.5182	-0.1
	HMDB0116581	PG(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C44H77O10P	M-H	795.5182	-0.1
	HMDB0010634	PG(18:1(9Z)/18:1(9Z))	C42H79O10P	M+Na-2H	795.5158	3.0
	HMDB0010618	PG(18:1(11Z)/18:1(11Z))	C42H79O10P	M+Na-2H	795.5158	3.0
	HMDB0010605	PG(18/18:2(9Z,12Z))	C42H79O10P	M+Na-2H	795.5158	3.0
	HMDB0010619	PG(18:1(11Z)/18:1(9Z))	C42H79O10P	M+Na-2H	795.5158	3.0
	HMDB0010633	PG(18:1(9Z)/18:1(11Z))	C42H79O10P	M+Na-2H	795.5158	3.0
	HMDB0010647	PG(18:2(9Z,12Z)/18)	C42H79O10P	M+Na-2H	795.5158	3.0
	HMDB0112336	PS(15/22:4(7Z,Z,13Z,16Z))	C43H76NO10P	M-H	796.5134	0.2
	HMDB0112790	PS(22:4(7Z,Z,13Z,16Z)/15)	C43H76NO10P	M-H	796.5134	0.2
	HMDB0113173	PE-NMe(18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113174	PE-NMe(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113146	PE-NMe(18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113119	PE-NMe(18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113073	PE-NMe(16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113072	PE-NMe(16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C42H74NO8P	M+FA-H	796.5134	0.2

796.5136	HMDB0113051	PE-NMe(16:5(5Z,8Z,11Z,14Z,17Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113012	PE-NMe(14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0112994	PE-NMe(14/22:5(4Z,7Z,Z,13Z,16Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0112995	PE-NMe(14/22:5(7Z,Z,13Z,16Z,19Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0116726	PE-NMe(18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113229	PE-NMe(18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0114383	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/15)	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113930	PE-NMe2(15/:5(5Z,8Z,11Z,14Z,17Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113646	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/14)	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113620	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/14)	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113593	PE-NMe(22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113482	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/16)	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113454	PE-NMe(:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113426	PE-NMe(:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113257	PE-NMe(18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0113256	PE-NMe(18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0009648	PE(22:5(7Z,Z,13Z,16Z,19Z)/15)	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0009615	PE(22:5(4Z,7Z,Z,13Z,16Z)/15)	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0008912	PE(15/22:5(7Z,Z,13Z,16Z,19Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0008911	PE(15/22:5(4Z,7Z,Z,13Z,16Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0008492	PC(:5(5Z,8Z,11Z,14Z,17Z)/14)	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0008460	PC(:4(8Z,11Z,14Z,17Z)/14:1(9Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0008427	PC(:4(5Z,8Z,11Z,14Z)/14:1(9Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0008233	PC(18:4(6Z,9Z,12Z,15Z)/16:1(9Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0008009	PC(16:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0007917	PC(14:1(9Z)/:4(8Z,11Z,14Z,17Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0007916	PC(14:1(9Z)/:4(5Z,8Z,11Z,14Z))	C42H74NO8P	M+FA-H	796.5134	0.2
	HMDB0007885	PC(14/:5(5Z,8Z,11Z,14Z,17Z))	C42H74NO8P	M+FA-H	796.5134	0.2
797.5314	HMDB0010604	PG(18/18:1(9Z))	C42H81O10P	M+Na-2H	797.5314	0.0
	HMDB0010632	PG(18:1(9Z)/18)	C42H81O10P	M+Na-2H	797.5314	0.0
	HMDB0010617	PG(18:1(11Z)/18)	C42H81O10P	M+Na-2H	797.5314	0.0
	HMDB0010603	PG(18/18:1(11Z))	C42H81O10P	M+Na-2H	797.5314	0.0

798.5301	HMDB0113092	PE-NMe(18:18:4(6Z,9Z,12Z,15Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113118	PE-NMe(18:1(11Z)/18:3(9Z,12Z,15Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113117	PE-NMe(18:1(11Z)/18:3(6Z,9Z,12Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113145	PE-NMe(18:1(9Z)/18:3(9Z,12Z,15Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113144	PE-NMe(18:1(9Z)/18:3(6Z,9Z,12Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113070	PE-NMe(16:1(9Z)/:3(5Z,8Z,11Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0112993	PE-NMe(14/22:4(7Z,Z,13Z,16Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113050	PE-NMe(16:/4(5Z,8Z,11Z,14Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0116725	PE-NMe(16:/4(8Z,11Z,14Z,17Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113071	PE-NMe(16:1(9Z)/:3(8Z,11Z,14Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113172	PE-NMe(18:2(9Z,12Z)/18:2(9Z,12Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113199	PE-NMe(18:3(6Z,9Z,12Z)/18:1(11Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113200	PE-NMe(18:3(6Z,9Z,12Z)/18:1(9Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113370	PE-NMe(:3(5Z,8Z,11Z)/16:1(9Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0114354	PE-NMe2(:4(8Z,11Z,14Z,17Z)/15)	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0114326	PE-NMe2(:4(5Z,8Z,11Z,14Z)/15)	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113928	PE-NMe2(15:/4(5Z,8Z,11Z,14Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113929	PE-NMe2(15:/4(8Z,11Z,14Z,17Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113592	PE-NMe(22:4(7Z,Z,13Z,16Z)/14)	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113453	PE-NMe(:4(8Z,11Z,14Z,17Z)/16)	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113425	PE-NMe(:4(5Z,8Z,11Z,14Z)/16)	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113398	PE-NMe(:3(8Z,11Z,14Z)/16:1(9Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113255	PE-NMe(18:4(6Z,9Z,12Z,15Z)/18)	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113228	PE-NMe(18:3(9Z,12Z,15Z)/18:1(9Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0113227	PE-NMe(18:3(9Z,12Z,15Z)/18:1(11Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0007883	PC(14:/4(5Z,8Z,11Z,14Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0008426	PC(:4(5Z,8Z,11Z,14Z)/14)	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0008459	PC(:4(8Z,11Z,14Z,17Z)/14)	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0008910	PE(15/22:4(7Z,Z,13Z,16Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0009582	PE(22:4(7Z,Z,13Z,16Z)/15)	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0008395	PC(:3(8Z,11Z,14Z)/14:1(9Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0008362	PC(:3(5Z,8Z,11Z)/14:1(9Z))	C42H76NO8P	M+FA-H	798.5291	1.3

	HMDB0008232	PC(18:4(6Z,9Z,12Z,15Z)/16)	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0007884	PC(14:4(8Z,11Z,14Z,17Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0007914	PC(14:1(9Z)/:3(5Z,8Z,11Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0007915	PC(14:1(9Z)/:3(8Z,11Z,14Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0007976	PC(16/18:4(6Z,9Z,12Z,15Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0008007	PC(16:1(9Z)/18:3(6Z,9Z,12Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0008008	PC(16:1(9Z)/18:3(9Z,12Z,15Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0008167	PC(18:3(6Z,9Z,12Z)/16:1(9Z))	C42H76NO8P	M+FA-H	798.5291	1.3
	HMDB0008200	PC(18:3(9Z,12Z,15Z)/16:1(9Z))	C42H76NO8P	M+FA-H	798.5291	1.3
800.5436	HMDB0113198	PE-NMe(18:3(6Z,9Z,12Z)/18)	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113170	PE-NMe(18:2(9Z,12Z)/18:1(11Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113171	PE-NMe(18:2(9Z,12Z)/18:1(9Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113143	PE-NMe(18:1(9Z)/18:2(9Z,12Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113090	PE-NMe(18/18:3(6Z,9Z,12Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113091	PE-NMe(18/18:3(9Z,12Z,15Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113049	PE-NMe(16/:3(8Z,11Z,14Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113048	PE-NMe(16/:3(5Z,8Z,11Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113011	PE-NMe(14:1(9Z)/22:2(13Z,16Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113226	PE-NMe(18:3(9Z,12Z,15Z)/18)	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113369	PE-NMe(:3(5Z,8Z,11Z)/16)	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113341	PE-NMe(:2(11Z,14Z)/16:1(9Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113069	PE-NMe(16:1(9Z)/:2(11Z,14Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0114298	PE-NMe2(:3(8Z,11Z,14Z)/15)	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0114270	PE-NMe2(:3(5Z,8Z,11Z)/15)	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113927	PE-NMe2(15/:3(8Z,11Z,14Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113926	PE-NMe2(15/:3(5Z,8Z,11Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113564	PE-NMe(22:2(13Z,16Z)/14:1(9Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113397	PE-NMe(:3(8Z,11Z,14Z)/16)	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0008394	PC(:3(8Z,11Z,14Z)/14)	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0008361	PC(:3(5Z,8Z,11Z)/14)	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0008329	PC(:2(11Z,14Z)/14:1(9Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0008199	PC(18:3(9Z,12Z,15Z)/16)	C42H78NO8P	M+FA-H	800.5447	-1.4

	HMDB0008166	PC(18:3(6Z,9Z,12Z)/16)	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0008134	PC(18:2(9Z,12Z)/16:1(9Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0008006	PC(16:1(9Z)/18:2(9Z,12Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0007974	PC(16/18:3(6Z,9Z,12Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0007975	PC(16/18:3(9Z,12Z,15Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0007913	PC(14:1(9Z):2(11Z,14Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0007881	PC(14/:3(5Z,8Z,11Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0007882	PC(14/:3(8Z,11Z,14Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0113116	PE-NMe(18:1(11Z)/18:2(9Z,12Z))	C42H78NO8P	M+FA-H	800.5447	-1.4
	HMDB0112763	PS(22:2(13Z,16Z)/15)	C43H80NO10P	M-H	800.5447	-1.4
	HMDB0116749	PS(15/22:2(13Z,16Z))	C43H80NO10P	M-H	800.5447	-1.4
801.5407	HMDB0114999	PA(18:3(6Z,9Z,12Z)/24:1(15Z))	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115593	PA(22:1(13Z):3(8Z,11Z,14Z))	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115579	PA(:3(8Z,11Z,14Z)/22:1(13Z))	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115553	PA(:2(11Z,14Z)/22:2(13Z,16Z))	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115464	PA(24:1(15Z)/18:3(6Z,9Z,12Z))	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115465	PA(24:1(15Z)/18:3(9Z,12Z,15Z))	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115439	PA(24/18:4(6Z,9Z,12Z,15Z))	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115334	PA(22:4(7Z,Z,13Z,16Z)/)	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115283	PA(22:1(13Z):3(5Z,8Z,11Z))	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115257	PA(22/:4(8Z,11Z,14Z,17Z))	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115256	PA(22/:4(5Z,8Z,11Z,14Z))	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115189	PA(:4(8Z,11Z,14Z,17Z)/22)	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115162	PA(:4(5Z,8Z,11Z,14Z)/22)	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115137	PA(:3(5Z,8Z,11Z)/22:1(13Z))	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115085	PA(/22:4(7Z,Z,13Z,16Z))	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115052	PA(18:4(6Z,9Z,12Z,15Z)/24)	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115026	PA(18:3(9Z,12Z,15Z)/24:1(15Z))	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0115594	PA(22:2(13Z,16Z):2(11Z,14Z))	C45H81O8P	M+Na-2H	801.5416	-1.1
	HMDB0010565	PE-NMe(18:1(9Z)/18:1(9Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0009549	PE(22:2(13Z,16Z)/15)	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0007880	PC(14/:2(11Z,14Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0007912	PC(14:1(9Z):1(11Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0007973	PC(16/18:2(9Z,12Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0008005	PC(16:1(9Z)/18:1(9Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0008004	PC(16:1(9Z)/18:1(11Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0008068	PC(18:1(11Z)/16:1(9Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0008101	PC(18:1(9Z)/16:1(9Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0008133	PC(18:2(9Z,12Z)/16)	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0008296	PC(:1(11Z)/14:1(9Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0008328	PC(:2(11Z,14Z)/14)	C42H80NO8P	M+FA-H	802.5604	-2.9

802.5580	HMDB0008909	PE(15/22:2(13Z,16Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0112967	PE-NMe(18:1(9Z)/18:1(11Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0112968	PE-NMe(18:1(11Z)/18:1(9Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0112969	PE-NMe(18:1(11Z)/18:1(11Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0112992	PE-NMe(14/22:2(13Z,16Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0113010	PE-NMe(14:1(9Z)/22:1(13Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0114241	PE-NMe2(2(11Z,14Z)/15)	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0113925	PE-NMe2(15/:2(11Z,14Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0113340	PE-NMe(2(11Z,14Z)/16)	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0113047	PE-NMe(16/:2(11Z,14Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0113563	PE-NMe(22:2(13Z,16Z)/14)	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0113536	PE-NMe(22:1(13Z)/14:1(9Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0113312	PE-NMe(1(11Z)/16:1(9Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0113169	PE-NMe(18:2(9Z,12Z)/18)	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0113089	PE-NMe(18/18:2(9Z,12Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0112966	PE-NMe(16:1(9Z)/:1(11Z))	C42H80NO8P	M+FA-H	802.5604	-2.9
	HMDB0112738	PS(22:1(13Z)/15)	C43H82NO10P	M-H	802.5604	-2.9
	HMDB0112335	PS(15/22:1(13Z))	C43H82NO10P	M-H	802.5604	-2.9
803.5616	HMDB0115472	PA(24:1(15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C47H81O8P	M-H	803.5596	2.5
	HMDB0115419	PA(22:6(4Z,7Z,Z,13Z,16Z,19Z)/22)	C47H81O8P	M-H	803.5596	2.5
	HMDB0115393	PA(22:5(7Z,Z,13Z,16Z,19Z)/22:1(13Z))	C47H81O8P	M-H	803.5596	2.5
	HMDB0115368	PA(22:5(4Z,7Z,Z,13Z,16Z)/22:1(13Z))	C47H81O8P	M-H	803.5596	2.5
	HMDB0115342	PA(22:4(7Z,Z,13Z,16Z)/22:2(13Z,16Z))	C47H81O8P	M-H	803.5596	2.5
	HMDB0115317	PA(22:2(13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C47H81O8P	M-H	803.5596	2.5
	HMDB0115291	PA(22:1(13Z)/22:5(4Z,7Z,Z,13Z,16Z))	C47H81O8P	M-H	803.5596	2.5
	HMDB0115292	PA(22:1(13Z)/22:5(7Z,Z,13Z,16Z,19Z))	C47H81O8P	M-H	803.5596	2.5
	HMDB0115266	PA(22/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C47H81O8P	M-H	803.5596	2.5
	HMDB0115223	PA(:5(5Z,8Z,11Z,14Z,17Z)/24:1(15Z))	C47H81O8P	M-H	803.5596	2.5
807.5021	HMDB0009779	PI(16/16:1(9Z))	C41H77O13P	M-H	807.5029	-1.0
	HMDB0009797	PI(16:1(9Z)/16)	C41H77O13P	M-H	807.5029	-1.0
	HMDB0113036	PE-NMe(15/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
	HMDB0114576	PE-NMe2(22:6(4Z,7Z,Z,13Z,16Z,19Z)/14)	C43H74NO8P	M+FA-H	808.5134	-0.7
	HMDB0114550	PE-NMe2(22:5(7Z,Z,13Z,16Z,19Z)/14:1(9Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
	HMDB0114524	PE-NMe2(22:5(4Z,7Z,Z,13Z,16Z)/14:1(9Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
	HMDB0114385	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/16:1(9Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
	HMDB0113675	PE-NMe(22:6(4Z,7Z,Z,13Z,16Z,19Z)/15)	C43H74NO8P	M+FA-H	808.5134	-0.7
	HMDB0113896	PE-NMe2(14/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H74NO8P	M+FA-H	808.5134	-0.7

HMDB0113914	PE-NMe2(14:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0113913	PE-NMe2(14:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0113975	PE-NMe2(16:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0114076	PE-NMe2(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0114104	PE-NMe2(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0114103	PE-NMe2(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0114132	PE-NMe2(18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0114133	PE-NMe2(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0114160	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009166	PE(18:3(9Z,12Z,15Z)/:3(5Z,8Z,11Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009133	PE(18:3(6Z,9Z,12Z)/:3(5Z,8Z,11Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009134	PE(18:3(6Z,9Z,12Z)/:3(8Z,11Z,14Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009102	PE(18:2(9Z,12Z)/:4(5Z,8Z,11Z,14Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009198	PE(18:4(6Z,9Z,12Z,15Z)/:2(11Z,14Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009167	PE(18:3(9Z,12Z,15Z)/:3(8Z,11Z,14Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009326	PE(:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009682	PE(22:6(4Z,7Z,Z,13Z,16Z,19Z)/16)	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009103	PE(18:2(9Z,12Z)/:4(8Z,11Z,14Z,17Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009390	PE(:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009359	PE(:3(8Z,11Z,14Z)/18:3(9Z,12Z,15Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0008977	PE(16:1(9Z)/22:5(4Z,7Z,Z,13Z,16Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0008946	PE(16/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009358	PE(:3(8Z,11Z,14Z)/18:3(6Z,9Z,12Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009325	PE(:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009294	PE(:2(11Z,14Z)/18:4(6Z,9Z,12Z,15Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009423	PE(:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009071	PE(18:1(9Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009038	PE(18:1(11Z)/:5(5Z,8Z,11Z,14Z,17Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0008978	PE(16:1(9Z)/22:5(7Z,Z,13Z,16Z,19Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009650	PE(22:5(7Z,Z,13Z,16Z,19Z)/16:1(9Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009617	PE(22:5(4Z,7Z,Z,13Z,16Z)/16:1(9Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0009455	PE(:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	C43H74NO8P	M+FA-H	808.5134	-0.7

808.5128

HMDB0009454	PE(:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))	C43H74NO8P	M+FA-H	808.5134	-0.7
HMDB0012404	PS(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0061528	(2-aminoethoxy)[(2R)-2-{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0012394	PS(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0012424	PS(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0061476	(2-aminoethoxy)[(2R)-3-{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-2-{[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0061547	(2-aminoethoxy)[(2R)-2-{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0061479	(2-aminoethoxy)[(2R)-3-{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-2-{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0061512	(2-aminoethoxy)[(2R)-3-{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-2-{[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0061543	(2-aminoethoxy)[(2R)-2-{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-3-{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0061520	(2-aminoethoxy)[(2R)-2-{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-{[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0061515	(2-aminoethoxy)[(2R)-3-{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-2-{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0061504	(2-aminoethoxy)[(2R)-3-{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-2-{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0012434	PS(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0061516	(2-aminoethoxy)[(2R)-2-{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-3-{[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112817	PS(22:5(4Z,7Z,Z,13Z,16Z)/16)	C44H76NO10P	M-H	808.5134	-0.8
HMDB0116758	PS(18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0116761	PS(:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112601	PS(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112637	PS(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112660	PS(:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112661	PS(:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C44H76NO10P	M-H	808.5134	-0.8

HMDB0112684	PS(:5(5Z,8Z,11Z,14Z,17Z)/18)	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112792	PS(22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112473	PS(18:3(9Z,12Z,15Z)/:2(11Z,14Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112842	PS(22:5(7Z,Z,13Z,16Z,19Z)/16)	C44H76NO10P	M-H	808.5134	-0.8
HMDB0114722	[(2R)-3-{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-2-{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0114716	[(2R)-3-{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-2-{[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0113836	[(2R)-2,3-bis({[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy})propoxy][2-(methylamino)ethoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0113830	[(2R)-3-{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}-2-{[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0113825	[(2R)-3-{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-2-{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0113817	[(2R)-2-{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0113810	[(2R)-3-{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-2-{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0113782	[(2R)-2-{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-{[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0113776	[(2R)-2,3-bis({[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy})propoxy][2-(methylamino)ethoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0113762	[(2R)-2-{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112576	PS(:2(11Z,14Z)/18:3(9Z,12Z,15Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0116763	PS(:2(11Z,14Z)/18:3(6Z,9Z,12Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0116754	PS(18:3(6Z,9Z,12Z)/:2(11Z,14Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0114684	[(2R)-2-{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-{[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0114737	[(2R)-2-{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3-{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112432	PS(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112415	PS(18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C44H76NO10P	M-H	808.5134	-0.8

HMDB0112354	PS(16/22:5(7Z,Z,13Z,16Z,19Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112353	PS(16/22:5(4Z,7Z,Z,13Z,16Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112367	PS(16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112378	PS(18/:5(5Z,8Z,11Z,14Z,17Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112397	PS(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0112398	PS(18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C44H76NO10P	M-H	808.5134	-0.8
HMDB0061420	[2,3-bis({[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy})propoxy][2-(trimethylazaniumyl)ethoxy]phosphinic acid	C44H77NO10P	M-H	808.5140	-1.4
HMDB0112290	PS(18:1(11Z)/18:1(9Z))	C42H78NO10P	M+Na-2H	808.5110	2.2
HMDB0112272	PS(18:1(11Z)/18:1(11Z))	C42H78NO10P	M+Na-2H	808.5110	2.2
HMDB0112544	PS(:1(11Z)/16:1(9Z))	C42H78NO10P	M+Na-2H	808.5110	2.2
HMDB0112737	PS(22:1(13Z)/14:1(9Z))	C42H78NO10P	M+Na-2H	808.5110	2.2
HMDB0112761	PS(22:2(13Z,16Z)/14)	C42H78NO10P	M+Na-2H	808.5110	2.2
HMDB0112314	PS(14:1(9Z)/22:1(13Z))	C42H78NO10P	M+Na-2H	808.5110	2.2
HMDB0112302	PS(14/22:2(13Z,16Z))	C42H78NO10P	M+Na-2H	808.5110	2.2
HMDB0112346	PS(16/:2(11Z,14Z))	C42H78NO10P	M+Na-2H	808.5110	2.2
HMDB0012390	PS(18:1(9Z)/18:1(9Z))	C42H78NO10P	M+Na-2H	808.5110	2.2
HMDB0112570	PS(:2(11Z,14Z)/16)	C42H78NO10P	M+Na-2H	808.5110	2.2
HMDB0112291	PS(18:1(9Z)/18:1(11Z))	C42H78NO10P	M+Na-2H	808.5110	2.2
HMDB0112288	PS(16:1(9Z)/:1(11Z))	C42H78NO10P	M+Na-2H	808.5110	2.2
HMDB0012400	PS(18:2(9Z,12Z)/18)	C42H78NO10P	M+Na-2H	808.5110	2.2
HMDB0012380	PS(18/18:2(9Z,12Z))	C42H78NO10P	M+Na-2H	808.5110	2.2
HMDB0113974	PE-NMe2(16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0114020	PE-NMe2(18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0114047	PE-NMe2(18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0114074	PE-NMe2(18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0114075	PE-NMe2(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0114102	PE-NMe2(18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0114131	PE-NMe2(18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0114159	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0114158	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0114328	PE-NMe2(:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0114356	PE-NMe2(:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C43H76NO8P	M+FA-H	810.5291	-1.2

HMDB0114384	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/16)	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0114496	PE-NMe2(22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0114523	PE-NMe2(22:5(4Z,7Z,Z,13Z,16Z)/14)	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0113952	PE-NMe2(16/:5(5Z,8Z,11Z,14Z,17Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0113912	PE-NMe2(14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0113895	PE-NMe2(14/22:5(7Z,Z,13Z,16Z,19Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0113973	PE-NMe2(16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0112978	PE-NMe(15/22:5(7Z,Z,13Z,16Z,19Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0113035	PE-NMe(15/22:5(4Z,7Z,Z,13Z,16Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0113622	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/15)	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0113648	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/15)	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0113894	PE-NMe2(14/22:5(4Z,7Z,Z,13Z,16Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0114549	PE-NMe2(22:5(7Z,Z,13Z,16Z,19Z)/14)	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0007951	PC(15/:5(5Z,8Z,11Z,14Z,17Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009324	PE(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009357	PE(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009388	PE(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009389	PE(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009421	PE(:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009422	PE(:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009453	PE(:5(5Z,8Z,11Z,14Z,17Z)/18)	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009584	PE(22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009616	PE(22:5(4Z,7Z,Z,13Z,16Z)/16)	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009649	PE(22:5(7Z,Z,13Z,16Z,19Z)/16)	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009037	PE(18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009293	PE(:2(11Z,14Z)/18:3(9Z,12Z,15Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009292	PE(:2(11Z,14Z)/18:3(6Z,9Z,12Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009261	PE(:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0008494	PC(:5(5Z,8Z,11Z,14Z,17Z)/15)	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0008944	PE(16/22:5(4Z,7Z,Z,13Z,16Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0008945	PE(16/22:5(7Z,Z,13Z,16Z,19Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0008976	PE(16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C43H76NO8P	M+FA-H	810.5291	-1.2

HMDB0009005	PE(18/:5(5Z,8Z,11Z,14Z,17Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009036	PE(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009070	PE(18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009069	PE(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009100	PE(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009101	PE(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009132	PE(18:3(6Z,9Z,12Z)/:2(11Z,14Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009165	PE(18:3(9Z,12Z,15Z)/:2(11Z,14Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0009197	PE(18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C43H76NO8P	M+FA-H	810.5291	-1.2
HMDB0012383	PS(18/:4(5Z,8Z,11Z,14Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0012433	PS(:4(5Z,8Z,11Z,14Z)/18)	C44H78NO10P	M-H	810.5291	-1.2
HMDB0012423	PS(:3(8Z,11Z,14Z)/18:1(9Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0012393	PS(18:1(9Z)/:3(8Z,11Z,14Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0010165	PS(18/:4(8Z,11Z,14Z,17Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112414	PS(18:1(9Z)/:3(5Z,8Z,11Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112455	PS(18:3(6Z,9Z,12Z)/:1(11Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112497	PS(18:4(6Z,9Z,12Z,15Z)/)	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112522	PS(/18:4(6Z,9Z,12Z,15Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112549	PS(:1(11Z)/18:3(6Z,9Z,12Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112431	PS(18:2(9Z,12Z)/:2(11Z,14Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112550	PS(:1(11Z)/18:3(9Z,12Z,15Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112472	PS(18:3(9Z,12Z,15Z)/:1(11Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112575	PS(:2(11Z,14Z)/18:2(9Z,12Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112791	PS(22:4(7Z,Z,13Z,16Z)/16)	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112659	PS(:4(8Z,11Z,14Z,17Z)/18)	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112622	PS(:3(8Z,11Z,14Z)/18:1(11Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112599	PS(:3(5Z,8Z,11Z)/18:1(11Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112395	PS(18:1(11Z)/:3(5Z,8Z,11Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112396	PS(18:1(11Z)/:3(8Z,11Z,14Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112600	PS(:3(5Z,8Z,11Z)/18:1(9Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112352	PS(16/22:4(7Z,Z,13Z,16Z))	C44H78NO10P	M-H	810.5291	-1.2
HMDB0112388	PS(18:1(11Z)/18)	C42H80NO10P	M+Na-2H	810.5267	1.8

HMDB0012389	PS(18:1(9Z)/18)	C42H80NO10P	M+Na-2H	810.5267	1.8
HMDB0010163	PS(18/18:1(9Z))	C42H80NO10P	M+Na-2H	810.5267	1.8
HMDB0112736	PS(22:1(13Z)/14)	C42H80NO10P	M+Na-2H	810.5267	1.8
HMDB0112301	PS(14/22:1(13Z))	C42H80NO10P	M+Na-2H	810.5267	1.8
HMDB0112289	PS(18/18:1(11Z))	C42H80NO10P	M+Na-2H	810.5267	1.8
HMDB0112287	PS(16:1(9Z)/)	C42H80NO10P	M+Na-2H	810.5267	1.8
HMDB0112515	PS(/16:1(9Z))	C42H80NO10P	M+Na-2H	810.5267	1.8
HMDB0112543	PS(:1(11Z)/16)	C42H80NO10P	M+Na-2H	810.5267	1.8
HMDB0112286	PS(16/:1(11Z))	C42H80NO10P	M+Na-2H	810.5267	1.8
HMDB0112708	PS(22/14:1(9Z))	C42H80NO10P	M+Na-2H	810.5267	1.8
HMDB0112279	PS(14:1(9Z)/22)	C42H80NO10P	M+Na-2H	810.5267	1.8
HMDB0112707	PS(22/14)	C42H82NO10P	M+Na-2H	812.5423	1.1
HMDB0012378	PS(18/18)	C42H82NO10P	M+Na-2H	812.5423	1.1
HMDB0112300	PS(14/22)	C42H82NO10P	M+Na-2H	812.5423	1.1
HMDB0112345	PS(16/)	C42H82NO10P	M+Na-2H	812.5423	1.1
HMDB0112514	PS(/16)	C42H82NO10P	M+Na-2H	812.5423	1.1
HMDB0113034	PE-NMe(15/22:4(7Z,Z,13Z,16Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0113594	PE-NMe(22:4(7Z,Z,13Z,16Z)/15)	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0113893	PE-NMe2(14/22:4(7Z,Z,13Z,16Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0113951	PE-NMe2(16/:4(5Z,8Z,11Z,14Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0116711	PE-NMe2(16/:4(8Z,11Z,14Z,17Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0113972	PE-NMe2(16:1(9Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0113971	PE-NMe2(16:1(9Z)/:3(5Z,8Z,11Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0114495	PE-NMe2(22:4(7Z,Z,13Z,16Z)/14)	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0114355	PE-NMe2(:4(8Z,11Z,14Z,17Z)/16)	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0113993	PE-NMe2(18/18:4(6Z,9Z,12Z,15Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0114019	PE-NMe2(18:1(11Z)/18:3(9Z,12Z,15Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0114018	PE-NMe2(18:1(11Z)/18:3(6Z,9Z,12Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0114045	PE-NMe2(18:1(9Z)/18:3(6Z,9Z,12Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0114046	PE-NMe2(18:1(9Z)/18:3(9Z,12Z,15Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0114073	PE-NMe2(18:2(9Z,12Z)/18:2(9Z,12Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0114100	PE-NMe2(18:3(6Z,9Z,12Z)/18:1(11Z))	C43H78NO8P	M+FA-H	812.5447	-1.9

812.5432

HMDB0114101	PE-NMe ₂ (18:3(6Z,9Z,12Z)/18:1(9Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0114129	PE-NMe ₂ (18:3(9Z,12Z,15Z)/18:1(11Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0114130	PE-NMe ₂ (18:3(9Z,12Z,15Z)/18:1(9Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0114157	PE-NMe ₂ (18:4(6Z,9Z,12Z,15Z)/18)	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0114272	PE-NMe ₂ (:3(5Z,8Z,11Z)/16:1(9Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0114300	PE-NMe ₂ (:3(8Z,11Z,14Z)/16:1(9Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0114327	PE-NMe ₂ (:4(5Z,8Z,11Z,14Z)/16)	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0007950	PC(15/:4(8Z,11Z,14Z,17Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009259	PE(:1(11Z)/18:3(6Z,9Z,12Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009260	PE(:1(11Z)/18:3(9Z,12Z,15Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009291	PE(:2(11Z,14Z)/18:2(9Z,12Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009323	PE(:3(5Z,8Z,11Z)/18:1(9Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009322	PE(:3(5Z,8Z,11Z)/18:1(11Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009356	PE(:3(8Z,11Z,14Z)/18:1(9Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009355	PE(:3(8Z,11Z,14Z)/18:1(11Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009387	PE(:4(5Z,8Z,11Z,14Z)/18)	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009420	PE(:4(8Z,11Z,14Z,17Z)/18)	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009583	PE(22:4(7Z,Z,13Z,16Z)/16)	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009228	PE(/18:4(6Z,9Z,12Z,15Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009034	PE(18:1(11Z)/:3(5Z,8Z,11Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0007949	PC(15/:4(5Z,8Z,11Z,14Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0008428	PC(:4(5Z,8Z,11Z,14Z)/15)	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0008461	PC(:4(8Z,11Z,14Z,17Z)/15)	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0008943	PE(16/22:4(7Z,Z,13Z,16Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0008969	PE(16:1(9Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009004	PE(18/:4(8Z,11Z,14Z,17Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009003	PE(18/:4(5Z,8Z,11Z,14Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009035	PE(18:1(11Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009067	PE(18:1(9Z)/:3(5Z,8Z,11Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009068	PE(18:1(9Z)/:3(8Z,11Z,14Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009099	PE(18:2(9Z,12Z)/:2(11Z,14Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009131	PE(18:3(6Z,9Z,12Z)/:1(11Z))	C43H78NO8P	M+FA-H	812.5447	-1.9

HMDB0009164	PE(18:3(9Z,12Z,15Z)/:1(11Z))	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0009196	PE(18:4(6Z,9Z,12Z,15Z)/)	C43H78NO8P	M+FA-H	812.5447	-1.9
HMDB0012382	PS(18/:3(8Z,11Z,14Z))	C44H80NO10P	M-H	812.5447	-1.9
HMDB0012422	PS(:3(8Z,11Z,14Z)/18)	C44H80NO10P	M-H	812.5447	-1.9
HMDB0112765	PS(22:2(13Z,16Z)/16:1(9Z))	C44H80NO10P	M-H	812.5447	-1.9
HMDB0112366	PS(16:1(9Z)/22:2(13Z,16Z))	C44H80NO10P	M-H	812.5447	-1.9
HMDB0112548	PS(:1(11Z)/18:2(9Z,12Z))	C44H80NO10P	M-H	812.5447	-1.9
HMDB0112377	PS(18/:3(5Z,8Z,11Z))	C44H80NO10P	M-H	812.5447	-1.9
HMDB0112394	PS(18:1(11Z)/:2(11Z,14Z))	C44H80NO10P	M-H	812.5447	-1.9
HMDB0112598	PS(:3(5Z,8Z,11Z)/18)	C44H80NO10P	M-H	812.5447	-1.9
HMDB0112574	PS(:2(11Z,14Z)/18:1(9Z))	C44H80NO10P	M-H	812.5447	-1.9
HMDB0112573	PS(:2(11Z,14Z)/18:1(11Z))	C44H80NO10P	M-H	812.5447	-1.9
HMDB0112521	PS(/18:3(9Z,12Z,15Z))	C44H80NO10P	M-H	812.5447	-1.9
HMDB0112520	PS(/18:3(6Z,9Z,12Z))	C44H80NO10P	M-H	812.5447	-1.9
HMDB0112471	PS(18:3(9Z,12Z,15Z)/)	C44H80NO10P	M-H	812.5447	-1.9
HMDB0112454	PS(18:3(6Z,9Z,12Z)/)	C44H80NO10P	M-H	812.5447	-1.9
HMDB0112430	PS(18:2(9Z,12Z)/:1(11Z))	C44H80NO10P	M-H	812.5447	-1.9
HMDB0112413	PS(18:1(9Z)/:2(11Z,14Z))	C44H80NO10P	M-H	812.5447	-1.9
HMDB0009551	PE(22:2(13Z,16Z)/16:1(9Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0009033	PE(18:1(11Z)/:2(11Z,14Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0009002	PE(18/:3(8Z,11Z,14Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0009001	PE(18/:3(5Z,8Z,11Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0008975	PE(16:1(9Z)/22:2(13Z,16Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0008396	PC(:3(8Z,11Z,14Z)/15)	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0008363	PC(:3(5Z,8Z,11Z)/15)	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0007948	PC(15/:3(8Z,11Z,14Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0007947	PC(15/:3(5Z,8Z,11Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0009066	PE(18:1(9Z)/:2(11Z,14Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0009098	PE(18:2(9Z,12Z)/:1(11Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0009130	PE(18:3(6Z,9Z,12Z)/)	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0009354	PE(:3(8Z,11Z,14Z)/18)	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0009321	PE(:3(5Z,8Z,11Z)/18)	C43H80NO8P	M+FA-H	814.5604	-1.7

814.5590

HMDB0009289	PE(:2(11Z,14Z)/18:1(11Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0009290	PE(:2(11Z,14Z)/18:1(9Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0009258	PE(:1(11Z)/18:2(9Z,12Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0009226	PE(/18:3(6Z,9Z,12Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0009227	PE(/18:3(9Z,12Z,15Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0009163	PE(18:3(9Z,12Z,15Z)/)	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0114271	PE-NMe2(:3(5Z,8Z,11Z)/16)	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0114299	PE-NMe2(:3(8Z,11Z,14Z)/16)	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0114467	PE-NMe2(22:2(13Z,16Z)/14:1(9Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0113970	PE-NMe2(16:1(9Z)/:2(11Z,14Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0114128	PE-NMe2(18:3(9Z,12Z,15Z)/18)	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0114099	PE-NMe2(18:3(6Z,9Z,12Z)/18)	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0114071	PE-NMe2(18:2(9Z,12Z)/18:1(11Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0114072	PE-NMe2(18:2(9Z,12Z)/18:1(9Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0114044	PE-NMe2(18:1(9Z)/18:2(9Z,12Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0114017	PE-NMe2(18:1(11Z)/18:2(9Z,12Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0113991	PE-NMe2(18/18:3(6Z,9Z,12Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0113992	PE-NMe2(18/18:3(9Z,12Z,15Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0114243	PE-NMe2(:2(11Z,14Z)/16:1(9Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0113950	PE-NMe2(16/:3(8Z,11Z,14Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0113911	PE-NMe2(14:1(9Z)/22:2(13Z,16Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0113949	PE-NMe2(16/:3(5Z,8Z,11Z))	C43H80NO8P	M+FA-H	814.5604	-1.7
HMDB0112519	PS(/18:2(9Z,12Z))	C44H82NO10P	M-H	814.5604	-1.7
HMDB0112412	PS(18:1(9Z)/:1(11Z))	C44H82NO10P	M-H	814.5604	-1.7
HMDB0112429	PS(18:2(9Z,12Z)/)	C44H82NO10P	M-H	814.5604	-1.7
HMDB0112393	PS(18:1(11Z)/:1(11Z))	C44H82NO10P	M-H	814.5604	-1.7
HMDB0112365	PS(16:1(9Z)/22:1(13Z))	C44H82NO10P	M-H	814.5604	-1.7
HMDB0112546	PS(:1(11Z)/18:1(11Z))	C44H82NO10P	M-H	814.5604	-1.7
HMDB0112740	PS(22:1(13Z)/16:1(9Z))	C44H82NO10P	M-H	814.5604	-1.7
HMDB0112764	PS(22:2(13Z,16Z)/16)	C44H82NO10P	M-H	814.5604	-1.7
HMDB0112911	PS(24:1(15Z)/14:1(9Z))	C44H82NO10P	M-H	814.5604	-1.7
HMDB0112351	PS(16/22:2(13Z,16Z))	C44H82NO10P	M-H	814.5604	-1.7

	HMDB0112292	PS(14:1(9Z)/24:1(15Z))	C44H82NO10P	M-H	814.5604	-1.7
	HMDB0112376	PS(18/:2(11Z,14Z))	C44H82NO10P	M-H	814.5604	-1.7
	HMDB0112572	PS(:2(11Z,14Z)/18)	C44H82NO10P	M-H	814.5604	-1.7
	HMDB0112547	PS(:1(11Z)/18:1(9Z))	C44H82NO10P	M-H	814.5604	-1.7
816.5747	HMDB0010564	PE-NMe2(18:1(9Z)/18:1(9Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0007946	PC(15/:2(11Z,14Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0008330	PC(:2(11Z,14Z)/15)	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0008882	PE(14:1(9Z)/24:1(15Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0008942	PE(16/22:2(13Z,16Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0008974	PE(16:1(9Z)/22:1(13Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0009000	PE(18/:2(11Z,14Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0009032	PE(18:1(11Z)/:1(11Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0009065	PE(18:1(9Z)/:1(11Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0009097	PE(18:2(9Z,12Z)/)	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0009746	PE(24:1(15Z)/14:1(9Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0009550	PE(22:2(13Z,16Z)/16)	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0009518	PE(22:1(13Z)/16:1(9Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0009288	PE(:2(11Z,14Z)/18)	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0009257	PE(:1(11Z)/18:1(9Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0009256	PE(:1(11Z)/18:1(11Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0009225	PE(/18:2(9Z,12Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0113033	PE-NMe(15/22:2(13Z,16Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0113869	PE-NMe2(18:1(11Z)/18:1(9Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0113870	PE-NMe2(18:1(11Z)/18:1(11Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0113868	PE-NMe2(18:1(9Z)/18:1(11Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0113565	PE-NMe(22:2(13Z,16Z)/15)	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0113892	PE-NMe2(14/22:2(13Z,16Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0113910	PE-NMe2(14:1(9Z)/22:1(13Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0114242	PE-NMe2(:2(11Z,14Z)/16)	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0113948	PE-NMe2(16/:2(11Z,14Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0114466	PE-NMe2(22:2(13Z,16Z)/14)	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0114438	PE-NMe2(22:1(13Z)/14:1(9Z))	C43H82NO8P	M+FA-H	816.5760	-1.6

	HMDB0114214	PE-NMe2(:1(11Z)/16:1(9Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0114070	PE-NMe2(18:2(9Z,12Z)/18)	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0113990	PE-NMe2(18/18:2(9Z,12Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0113867	PE-NMe2(16:1(9Z)/:1(11Z))	C43H82NO8P	M+FA-H	816.5760	-1.6
	HMDB0112910	PS(24:1(15Z)/14)	C44H84NO10P	M-H	816.5760	-1.6
	HMDB0112882	PS(24/14:1(9Z))	C44H84NO10P	M-H	816.5760	-1.6
	HMDB0112739	PS(22:1(13Z)/16)	C44H84NO10P	M-H	816.5760	-1.6
	HMDB0112711	PS(22/16:1(9Z))	C44H84NO10P	M-H	816.5760	-1.6
	HMDB0112319	PS(14:1(9Z)/24)	C44H84NO10P	M-H	816.5760	-1.6
	HMDB0112350	PS(16/22:1(13Z))	C44H84NO10P	M-H	816.5760	-1.6
	HMDB0112364	PS(16:1(9Z)/22)	C44H84NO10P	M-H	816.5760	-1.6
	HMDB0112375	PS(18/:1(11Z))	C44H84NO10P	M-H	816.5760	-1.6
	HMDB0112392	PS(18:1(11Z)/)	C44H84NO10P	M-H	816.5760	-1.6
	HMDB0112411	PS(18:1(9Z)/)	C44H84NO10P	M-H	816.5760	-1.6
	HMDB0112517	PS(/18:1(11Z))	C44H84NO10P	M-H	816.5760	-1.6
	HMDB0112518	PS(/18:1(9Z))	C44H84NO10P	M-H	816.5760	-1.6
	HMDB0112545	PS(:1(11Z)/18)	C44H84NO10P	M-H	816.5760	-1.6
	HMDB0112307	PS(14/24:1(15Z))	C44H84NO10P	M-H	816.5760	-1.6
817.5070	HMDB0014916	Roxithromycin	C41H76N2O15	M-H20-H	817.5062	1.0
818.5167	HMDB0112328	PS(15/:2(11Z,14Z))	C41H76NO10P	M+FA-H	818.5189	-2.7
	HMDB0112569	PS(:2(11Z,14Z)/15)	C41H76NO10P	M+FA-H	818.5189	-2.7
820.5284	HMDB0009605	PE(22:4(7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C49H78NO8P	M-H20-H	820.5281	0.3
	HMDB0114349	PE-NMe2(:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C49H78NO8P	M-H20-H	820.5281	0.3
	HMDB0114378	PE-NMe2(:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C49H78NO8P	M-H20-H	820.5281	0.3
	HMDB0114405	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/22:5(4Z,7Z,Z,13Z,16Z))	C49H78NO8P	M-H20-H	820.5281	0.3
	HMDB0114406	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,Z,13Z,16Z,19Z))	C49H78NO8P	M-H20-H	820.5281	0.3
	HMDB0114540	PE-NMe2(22:5(4Z,7Z,Z,13Z,16Z)/:5(5Z,8Z,11Z,14Z,17Z))	C49H78NO8P	M-H20-H	820.5281	0.3
	HMDB0114567	PE-NMe2(22:5(7Z,Z,13Z,16Z,19Z)/:5(5Z,8Z,11Z,14Z,17Z))	C49H78NO8P	M-H20-H	820.5281	0.3
	HMDB0114593	PE-NMe2(22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(8Z,11Z,14Z,17Z))	C49H78NO8P	M-H20-H	820.5281	0.3

HMDB0116722	PE-NMe ₂ (22:6(4Z,7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C49H78NO8P	M-H20-H	820.5281	0.3
HMDB0009638	PE(22:5(4Z,7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C49H78NO8P	M-H20-H	820.5281	0.3
HMDB0009637	PE(22:5(4Z,7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C49H78NO8P	M-H20-H	820.5281	0.3
HMDB0009670	PE(22:5(7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C49H78NO8P	M-H20-H	820.5281	0.3
HMDB0009671	PE(22:5(7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C49H78NO8P	M-H20-H	820.5281	0.3
HMDB0009702	PE(22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C49H78NO8P	M-H20-H	820.5281	0.3
HMDB0112335	PS(15/22:1(13Z))	C43H82NO10P	M+Na-2H	824.5423	0.8
HMDB0112738	PS(22:1(13Z)/15)	C43H82NO10P	M+Na-2H	824.5423	0.8
HMDB0113263	PE-NMe(18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113402	PE-NMe(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113152	PE-NMe(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113153	PE-NMe(18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113179	PE-NMe(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113374	PE-NMe(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113319	PE-NMe(:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113180	PE-NMe(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113057	PE-NMe(16/22:5(7Z,Z,13Z,16Z,19Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113056	PE-NMe(16/22:5(4Z,7Z,Z,13Z,16Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113078	PE-NMe(16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113100	PE-NMe(18/:5(5Z,8Z,11Z,14Z,17Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113126	PE-NMe(18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113125	PE-NMe(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113428	PE-NMe(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113429	PE-NMe(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113456	PE-NMe(:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113206	PE-NMe(18:3(6Z,9Z,12Z)/:2(11Z,14Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113235	PE-NMe(18:3(9Z,12Z,15Z)/:2(11Z,14Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113347	PE-NMe(:2(11Z,14Z)/18:3(9Z,12Z,15Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113346	PE-NMe(:2(11Z,14Z)/18:3(6Z,9Z,12Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0008235	PC(18:4(6Z,9Z,12Z,15Z)/18:1(11Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0114551	PE-NMe ₂ (22:5(7Z,Z,13Z,16Z,19Z)/15)	C44H78NO8P	M+FA-H	824.5447	-2.1
HMDB0113457	PE-NMe(:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C44H78NO8P	M+FA-H	824.5447	-2.1

824.5430	HMDB0113596	PE-NMe(22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0116733	PE-NMe(22:5(4Z,7Z,Z,13Z,16Z)/16)	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0113649	PE-NMe(22:5(7Z,Z,13Z,16Z,19Z)/16)	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0113936	PE-NMe2(15/22:5(7Z,Z,13Z,16Z,19Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0113935	PE-NMe2(15/22:5(4Z,7Z,Z,13Z,16Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0114525	PE-NMe2(22:5(4Z,7Z,Z,13Z,16Z)/15)	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0113484	PE-NMe(:5(5Z,8Z,11Z,14Z,17Z)/18)	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0007890	PC(14/22:5(4Z,7Z,Z,13Z,16Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0008463	PC(:4(8Z,11Z,14Z,17Z)/16:1(9Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0008495	PC(:5(5Z,8Z,11Z,14Z,17Z)/16)	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0008624	PC(22:4(7Z,Z,13Z,16Z)/14:1(9Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0008656	PC(22:5(4Z,7Z,Z,13Z,16Z)/14)	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0008689	PC(22:5(7Z,Z,13Z,16Z,19Z)/14)	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0008430	PC(:4(5Z,8Z,11Z,14Z)/16:1(9Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0008236	PC(18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0007891	PC(14/22:5(7Z,Z,13Z,16Z,19Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0007922	PC(14:1(9Z)/22:4(7Z,Z,13Z,16Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0007984	PC(16/:5(5Z,8Z,11Z,14Z,17Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0008015	PC(16:1(9Z)/:4(5Z,8Z,11Z,14Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0008016	PC(16:1(9Z)/:4(8Z,11Z,14Z,17Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0008075	PC(18:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0008108	PC(18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0008140	PC(18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0008141	PC(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0008171	PC(18:3(6Z,9Z,12Z)/18:2(9Z,12Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
	HMDB0008204	PC(18:3(9Z,12Z,15Z)/18:2(9Z,12Z))	C44H78NO8P	M+FA-H	824.5447	-2.1
825.3505	HMDB0034949	Rebaudioside B	C38H60O18	M+Na-2H	825.3526	-2.6
	HMDB0182204	SCHEMBL142651	C38H60O18	M+Na-2H	825.3526	-2.6
	HMDB0034945	stevioside	C38H60O18	M+Na-2H	825.3526	-2.6
826.5574	HMDB0112334	PS(15/22)	C43H84NO10P	M+Na-2H	826.5580	-0.7
	HMDB0112709	PS(22/15)	C43H84NO10P	M+Na-2H	826.5580	-0.7
	HMDB0009846	PI(18:2(9Z,12Z)/16)	C43H79O13P	M-H	833.5186	-1.5
	HMDB0009800	PI(16:1(9Z)/18:1(11Z))	C43H79O13P	M-H	833.5186	-1.5
	HMDB0009801	PI(16:1(9Z)/18:1(9Z))	C43H79O13P	M-H	833.5186	-1.5

833.5173	HMDB0009803	PI(16:2(9Z,12Z)/18)	C43H79O13P	M-H	833.5186	-1.5
	HMDB0009807	PI(18/16:2(9Z,12Z))	C43H79O13P	M-H	833.5186	-1.5
	HMDB0009823	PI(18:1(11Z)/16:1(9Z))	C43H79O13P	M-H	833.5186	-1.5
	HMDB0009835	PI(18:1(9Z)/16:1(9Z))	C43H79O13P	M-H	833.5186	-1.5
	HMDB0062653	Phosphatidylinositol(34:2)	C43H79O13P	M-H	833.5186	-1.5
	HMDB0009784	PI(16/18:2(9Z,12Z))	C43H79O13P	M-H	833.5186	-1.5
834.5253	HMDB0012382	PS(18/3(8Z,11Z,14Z))	C44H80NO10P	M+Na-2H	834.5267	-1.6
	HMDB0012422	PS(:3(8Z,11Z,14Z)/18)	C44H80NO10P	M+Na-2H	834.5267	-1.6
	HMDB0112548	PS(:1(11Z)/18:2(9Z,12Z))	C44H80NO10P	M+Na-2H	834.5267	-1.6
	HMDB0112598	PS(:3(5Z,8Z,11Z)/18)	C44H80NO10P	M+Na-2H	834.5267	-1.6
	HMDB0112765	PS(22:2(13Z,16Z)/16:1(9Z))	C44H80NO10P	M+Na-2H	834.5267	-1.6
	HMDB0112394	PS(18:1(11Z)/:2(11Z,14Z))	C44H80NO10P	M+Na-2H	834.5267	-1.6
	HMDB0112413	PS(18:1(9Z)/:2(11Z,14Z))	C44H80NO10P	M+Na-2H	834.5267	-1.6
	HMDB0112574	PS(:2(11Z,14Z)/18:1(9Z))	C44H80NO10P	M+Na-2H	834.5267	-1.6
	HMDB0112573	PS(:2(11Z,14Z)/18:1(11Z))	C44H80NO10P	M+Na-2H	834.5267	-1.6
	HMDB0112521	PS(/18:3(9Z,12Z,15Z))	C44H80NO10P	M+Na-2H	834.5267	-1.6
	HMDB0112520	PS(/18:3(6Z,9Z,12Z))	C44H80NO10P	M+Na-2H	834.5267	-1.6
	HMDB0112471	PS(18:3(9Z,12Z,15Z)/)	C44H80NO10P	M+Na-2H	834.5267	-1.6
	HMDB0112454	PS(18:3(6Z,9Z,12Z)/)	C44H80NO10P	M+Na-2H	834.5267	-1.6
	HMDB0112430	PS(18:2(9Z,12Z)/:1(11Z))	C44H80NO10P	M+Na-2H	834.5267	-1.6
	HMDB0112377	PS(18/:3(5Z,8Z,11Z))	C44H80NO10P	M+Na-2H	834.5267	-1.6
	HMDB0112366	PS(16:1(9Z)/22:2(13Z,16Z))	C44H80NO10P	M+Na-2H	834.5267	-1.6
835.5326	HMDB0009783	PI(16/18:1(9Z))	C43H81O13P	M-H	835.5342	-1.9
	HMDB0009834	PI(18:1(9Z)/16)	C43H81O13P	M-H	835.5342	-1.9
	HMDB0009822	PI(18:1(11Z)/16)	C43H81O13P	M-H	835.5342	-1.9
	HMDB0009806	PI(18/16:1(9Z))	C43H81O13P	M-H	835.5342	-1.9
	HMDB0009799	PI(16:1(9Z)/18)	C43H81O13P	M-H	835.5342	-1.9
	HMDB0009782	PI(16/18:1(11Z))	C43H81O13P	M-H	835.5342	-1.9
	HMDB0112740	PS(22:1(13Z)/16:1(9Z))	C44H82NO10P	M+Na-2H	836.5423	-1.3
	HMDB0112764	PS(22:2(13Z,16Z)/16)	C44H82NO10P	M+Na-2H	836.5423	-1.3
	HMDB0112911	PS(24:1(15Z)/14:1(9Z))	C44H82NO10P	M+Na-2H	836.5423	-1.3
	HMDB0112376	PS(18/:2(11Z,14Z))	C44H82NO10P	M+Na-2H	836.5423	-1.3

836.5412

HMDB0112572	PS(:2(11Z,14Z)/18)	C44H82NO10P	M+Na-2H	836.5423	-1.3
HMDB0112547	PS(:1(11Z)/18:1(9Z))	C44H82NO10P	M+Na-2H	836.5423	-1.3
HMDB0112546	PS(:1(11Z)/18:1(11Z))	C44H82NO10P	M+Na-2H	836.5423	-1.3
HMDB0112519	PS(/18:2(9Z,12Z))	C44H82NO10P	M+Na-2H	836.5423	-1.3
HMDB0112429	PS(18:2(9Z,12Z)/)	C44H82NO10P	M+Na-2H	836.5423	-1.3
HMDB0112412	PS(18:1(9Z)/:1(11Z))	C44H82NO10P	M+Na-2H	836.5423	-1.3
HMDB0112393	PS(18:1(11Z)/:1(11Z))	C44H82NO10P	M+Na-2H	836.5423	-1.3
HMDB0112365	PS(16:1(9Z)/22:1(13Z))	C44H82NO10P	M+Na-2H	836.5423	-1.3
HMDB0112351	PS(16/22:2(13Z,16Z))	C44H82NO10P	M+Na-2H	836.5423	-1.3
HMDB0112292	PS(14:1(9Z)/24:1(15Z))	C44H82NO10P	M+Na-2H	836.5423	-1.3
HMDB0112606	PS(:3(5Z,8Z,11Z)/:1(11Z))	C46H82NO10P	M-H	838.5604	0.9
HMDB0112665	PS(:4(8Z,11Z,14Z,17Z)/)	C46H82NO10P	M-H	838.5604	0.9
HMDB0112626	PS(:3(8Z,11Z,14Z)/:1(11Z))	C46H82NO10P	M-H	838.5604	0.9
HMDB0112504	PS(18:4(6Z,9Z,12Z,15Z)/22)	C46H82NO10P	M-H	838.5604	0.9
HMDB0112554	PS(:1(11Z)/:3(5Z,8Z,11Z))	C46H82NO10P	M-H	838.5604	0.9
HMDB0112555	PS(:1(11Z)/:3(8Z,11Z,14Z))	C46H82NO10P	M-H	838.5604	0.9
HMDB0112529	PS(/:4(8Z,11Z,14Z,17Z))	C46H82NO10P	M-H	838.5604	0.9
HMDB0112528	PS(/:4(5Z,8Z,11Z,14Z))	C46H82NO10P	M-H	838.5604	0.9
HMDB0112478	PS(18:3(9Z,12Z,15Z)/22:1(13Z))	C46H82NO10P	M-H	838.5604	0.9
HMDB0112461	PS(18:3(6Z,9Z,12Z)/22:1(13Z))	C46H82NO10P	M-H	838.5604	0.9
HMDB0112437	PS(18:2(9Z,12Z)/22:2(13Z,16Z))	C46H82NO10P	M-H	838.5604	0.9
HMDB0112382	PS(18/22:4(7Z,Z,13Z,16Z))	C46H82NO10P	M-H	838.5604	0.9
HMDB0112718	PS(22/18:4(6Z,9Z,12Z,15Z))	C46H82NO10P	M-H	838.5604	0.9
HMDB0112746	PS(22:1(13Z)/18:3(9Z,12Z,15Z))	C46H82NO10P	M-H	838.5604	0.9
HMDB0112580	PS(:2(11Z,14Z)/:2(11Z,14Z))	C46H82NO10P	M-H	838.5604	0.9
HMDB0112640	PS(:4(5Z,8Z,11Z,14Z)/)	C46H82NO10P	M-H	838.5604	0.9
HMDB0112769	PS(22:2(13Z,16Z)/18:2(9Z,12Z))	C46H82NO10P	M-H	838.5604	0.9
HMDB0112793	PS(22:4(7Z,Z,13Z,16Z)/18)	C46H82NO10P	M-H	838.5604	0.9
HMDB0112745	PS(22:1(13Z)/18:3(6Z,9Z,12Z))	C46H82NO10P	M-H	838.5604	0.9
HMDB0114026	PE-NMe2(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114001	PE-NMe2(18/:5(5Z,8Z,11Z,14Z,17Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0113979	PE-NMe2(16:1(9Z)/22:4(7Z,Z,13Z,16Z))	C45H80NO8P	M+FA-H	838.5604	0.9

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HMDB0113958	PE-NMe2(16/22:5(7Z,Z,13Z,16Z,19Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0113957	PE-NMe2(16/22:5(4Z,7Z,Z,13Z,16Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114027	PE-NMe2(18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114499	PE-NMe2(22:4(7Z,Z,13Z,16Z)/16:1(9Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0116717	PE-NMe2(22:5(4Z,7Z,Z,13Z,16Z)/16)	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114552	PE-NMe2(22:5(7Z,Z,13Z,16Z,19Z)/16)	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114108	PE-NMe2(18:3(6Z,9Z,12Z)/:2(11Z,14Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114137	PE-NMe2(18:3(9Z,12Z,15Z)/:2(11Z,14Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114249	PE-NMe2(:2(11Z,14Z)/18:3(9Z,12Z,15Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114248	PE-NMe2(:2(11Z,14Z)/18:3(6Z,9Z,12Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114386	PE-NMe2(:5(5Z,8Z,11Z,14Z,17Z)/18)	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114358	PE-NMe2(:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114053	PE-NMe2(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114054	PE-NMe2(18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114080	PE-NMe2(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114081	PE-NMe2(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114165	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/:1(11Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114221	PE-NMe2(:1(11Z)/18:4(6Z,9Z,12Z,15Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114276	PE-NMe2(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114304	PE-NMe2(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114331	PE-NMe2(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114330	PE-NMe2(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0114359	PE-NMe2(:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009395	PE(:4(5Z,8Z,11Z,14Z)/:1(11Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009330	PE(:3(5Z,8Z,11Z)/:2(11Z,14Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009299	PE(:2(11Z,14Z)/:3(8Z,11Z,14Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009363	PE(:3(8Z,11Z,14Z)/:2(11Z,14Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009428	PE(:4(8Z,11Z,14Z,17Z)/:1(11Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009460	PE(:5(5Z,8Z,11Z,14Z,17Z)/)	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009525	PE(22:1(13Z)/18:4(6Z,9Z,12Z,15Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009556	PE(22:2(13Z,16Z)/18:3(6Z,9Z,12Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009557	PE(22:2(13Z,16Z)/18:3(9Z,12Z,15Z))	C45H80NO8P	M+FA-H	838.5604	0.9

HMDB0009586	PE(22:4(7Z,Z,13Z,16Z)/18:1(11Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009587	PE(22:4(7Z,Z,13Z,16Z)/18:1(9Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009298	PE(:2(11Z,14Z)/:3(5Z,8Z,11Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009267	PE(:1(11Z)/:4(5Z,8Z,11Z,14Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009268	PE(:1(11Z)/:4(8Z,11Z,14Z,17Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0007956	PC(15/22:5(4Z,7Z,Z,13Z,16Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0007957	PC(15/22:5(7Z,Z,13Z,16Z,19Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0008658	PC(22:5(4Z,7Z,Z,13Z,16Z)/15)	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0008691	PC(22:5(7Z,Z,13Z,16Z,19Z)/15)	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009011	PE(18/22:5(7Z,Z,13Z,16Z,19Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009010	PE(18/22:5(4Z,7Z,Z,13Z,16Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009042	PE(18:1(11Z)/22:4(7Z,Z,13Z,16Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009075	PE(18:1(9Z)/22:4(7Z,Z,13Z,16Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009140	PE(18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009173	PE(18:3(9Z,12Z,15Z)/22:2(13Z,16Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009205	PE(18:4(6Z,9Z,12Z,15Z)/22:1(13Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009236	PE(/:5(5Z,8Z,11Z,14Z,17Z))	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009618	PE(22:5(4Z,7Z,Z,13Z,16Z)/18)	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0009651	PE(22:5(7Z,Z,13Z,16Z,19Z)/18)	C45H80NO8P	M+FA-H	838.5604	0.9
HMDB0169206	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{[(19Z)-16-hydroxy-(5-methyl-2-oxooxolan-3-yl)triacont-19-en-15-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C45H81N3O9S	M-H	838.5621	-1.2
HMDB0169205	2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-{[16-hydroxy-1-(5-methyl-2-oxooxolan-3-yl)triacont-11-en-15-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid	C45H81N3O9S	M-H	838.5621	-1.2
HMDB0112306	PS(14/24)	C44H86NO10P	M+Na-2H	840.5736	1.4
HMDB0010164	PS(18/)	C44H86NO10P	M+Na-2H	840.5736	1.4
HMDB0112881	PS(24/14)	C44H86NO10P	M+Na-2H	840.5736	1.4
HMDB0112710	PS(22/16)	C44H86NO10P	M+Na-2H	840.5736	1.4
HMDB0112516	PS(/18)	C44H86NO10P	M+Na-2H	840.5736	1.4
HMDB0112349	PS(16/22)	C44H86NO10P	M+Na-2H	840.5736	1.4
HMDB0007955	PC(15/22:4(7Z,Z,13Z,16Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009265	PE(:1(11Z)/:3(5Z,8Z,11Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009266	PE(:1(11Z)/:3(8Z,11Z,14Z))	C45H82NO8P	M+FA-H	840.5760	-1.4

840.5748

HMDB0009234	PE(/:4(5Z,8Z,11Z,14Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009235	PE(/:4(8Z,11Z,14Z,17Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009204	PE(18:4(6Z,9Z,12Z,15Z)/22)	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009172	PE(18:3(9Z,12Z,15Z)/22:1(13Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009139	PE(18:3(6Z,9Z,12Z)/22:1(13Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009107	PE(18:2(9Z,12Z)/22:2(13Z,16Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009009	PE(18/22:4(7Z,Z,13Z,16Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0008625	PC(22:4(7Z,Z,13Z,16Z)/15)	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009297	PE(:2(11Z,14Z)/:2(11Z,14Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009329	PE(:3(5Z,8Z,11Z)/:1(11Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009362	PE(:3(8Z,11Z,14Z)/:1(11Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009585	PE(22:4(7Z,Z,13Z,16Z)/18)	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009555	PE(22:2(13Z,16Z)/18:2(9Z,12Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009394	PE(:4(5Z,8Z,11Z,14Z)/)	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009427	PE(:4(8Z,11Z,14Z,17Z)/)	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009492	PE(22/18:4(6Z,9Z,12Z,15Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009524	PE(22:1(13Z)/18:3(9Z,12Z,15Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0009523	PE(22:1(13Z)/18:3(6Z,9Z,12Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0114303	PE-NMe2(:3(8Z,11Z,14Z)/18:1(9Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0114302	PE-NMe2(:3(8Z,11Z,14Z)/18:1(11Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0114274	PE-NMe2(:3(5Z,8Z,11Z)/18:1(11Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0114275	PE-NMe2(:3(5Z,8Z,11Z)/18:1(9Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0114219	PE-NMe2(:1(11Z)/18:3(6Z,9Z,12Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0114220	PE-NMe2(:1(11Z)/18:3(9Z,12Z,15Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0114192	PE-NMe2(/18:4(6Z,9Z,12Z,15Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0114164	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/)	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0114329	PE-NMe2(:4(5Z,8Z,11Z,14Z)/18)	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0114357	PE-NMe2(:4(8Z,11Z,14Z,17Z)/18)	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0114498	PE-NMe2(22:4(7Z,Z,13Z,16Z)/16)	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0114247	PE-NMe2(:2(11Z,14Z)/18:2(9Z,12Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0114079	PE-NMe2(18:2(9Z,12Z)/:2(11Z,14Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
HMDB0114136	PE-NMe2(18:3(9Z,12Z,15Z)/:1(11Z))	C45H82NO8P	M+FA-H	840.5760	-1.4

	HMDB0114107	PE-NMe2(18:3(6Z,9Z,12Z)/:1(11Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
	HMDB0113956	PE-NMe2(16/22:4(7Z,Z,13Z,16Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
	HMDB0113999	PE-NMe2(18/:4(5Z,8Z,11Z,14Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
	HMDB0114000	PE-NMe2(18/:4(8Z,11Z,14Z,17Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
	HMDB0114025	PE-NMe2(18:1(11Z)/:3(8Z,11Z,14Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
	HMDB0114024	PE-NMe2(18:1(11Z)/:3(5Z,8Z,11Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
	HMDB0114052	PE-NMe2(18:1(9Z)/:3(8Z,11Z,14Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
	HMDB0114051	PE-NMe2(18:1(9Z)/:3(5Z,8Z,11Z))	C45H82NO8P	M+FA-H	840.5760	-1.4
	HMDB0112553	PS(:1(11Z)/:2(11Z,14Z))	C46H84NO10P	M-H	840.5760	-1.4
	HMDB0112579	PS(:2(11Z,14Z)/:1(11Z))	C46H84NO10P	M-H	840.5760	-1.4
	HMDB0112526	PS(/:3(5Z,8Z,11Z))	C46H84NO10P	M-H	840.5760	-1.4
	HMDB0112768	PS(22:2(13Z,16Z)/18:1(9Z))	C46H84NO10P	M-H	840.5760	-1.4
	HMDB0112419	PS(18:1(9Z)/22:2(13Z,16Z))	C46H84NO10P	M-H	840.5760	-1.4
	HMDB0112436	PS(18:2(9Z,12Z)/22:1(13Z))	C46H84NO10P	M-H	840.5760	-1.4
	HMDB0112460	PS(18:3(6Z,9Z,12Z)/22)	C46H84NO10P	M-H	840.5760	-1.4
	HMDB0112477	PS(18:3(9Z,12Z,15Z)/22)	C46H84NO10P	M-H	840.5760	-1.4
	HMDB0112527	PS(/:3(8Z,11Z,14Z))	C46H84NO10P	M-H	840.5760	-1.4
	HMDB0112605	PS(:3(5Z,8Z,11Z)/)	C46H84NO10P	M-H	840.5760	-1.4
	HMDB0112625	PS(:3(8Z,11Z,14Z)/)	C46H84NO10P	M-H	840.5760	-1.4
	HMDB0112716	PS(22/18:3(6Z,9Z,12Z))	C46H84NO10P	M-H	840.5760	-1.4
	HMDB0112717	PS(22/18:3(9Z,12Z,15Z))	C46H84NO10P	M-H	840.5760	-1.4
	HMDB0112744	PS(22:1(13Z)/18:2(9Z,12Z))	C46H84NO10P	M-H	840.5760	-1.4
	HMDB0112767	PS(22:2(13Z,16Z)/18:1(11Z))	C46H84NO10P	M-H	840.5760	-1.4
	HMDB0112402	PS(18:1(11Z)/22:2(13Z,16Z))	C46H84NO10P	M-H	840.5760	-1.4
842.5195	HMDB0112336	PS(15/22:4(7Z,Z,13Z,16Z))	C43H76NO10P	M+FA-H	842.5189	0.7
	HMDB0112790	PS(22:4(7Z,Z,13Z,16Z)/15)	C43H76NO10P	M+FA-H	842.5189	0.7
	HMDB0009554	PE(22:2(13Z,16Z)/18:1(9Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
	HMDB0009041	PE(18:1(11Z)/22:2(13Z,16Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
	HMDB0009074	PE(18:1(9Z)/22:2(13Z,16Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
	HMDB0009106	PE(18:2(9Z,12Z)/22:1(13Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
	HMDB0009138	PE(18:3(6Z,9Z,12Z)/22)	C45H84NO8P	M+FA-H	842.5917	-1.8
	HMDB0009171	PE(18:3(9Z,12Z,15Z)/22)	C45H84NO8P	M+FA-H	842.5917	-1.8

842.5901

HMDB0009232	PE(/:3(5Z,8Z,11Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0009233	PE(/:3(8Z,11Z,14Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0009264	PE(:1(11Z)/:2(11Z,14Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0009296	PE(:2(11Z,14Z)/:1(11Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0009553	PE(22:2(13Z,16Z)/18:1(11Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0009522	PE(22:1(13Z)/18:2(9Z,12Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0009491	PE(22/18:3(9Z,12Z,15Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0009490	PE(22/18:3(6Z,9Z,12Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0009361	PE(:3(8Z,11Z,14Z)/)	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0009328	PE(:3(5Z,8Z,11Z)/)	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0114301	PE-NMe2(:3(8Z,11Z,14Z)/18)	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0114273	PE-NMe2(:3(5Z,8Z,11Z)/18)	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0114218	PE-NMe2(:1(11Z)/18:2(9Z,12Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0114190	PE-NMe2(/18:3(6Z,9Z,12Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0114191	PE-NMe2(/18:3(9Z,12Z,15Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0114135	PE-NMe2(18:3(9Z,12Z,15Z)/)	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0114106	PE-NMe2(18:3(6Z,9Z,12Z)/)	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0114078	PE-NMe2(18:2(9Z,12Z)/:1(11Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0114470	PE-NMe2(22:2(13Z,16Z)/16:1(9Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0114246	PE-NMe2(:2(11Z,14Z)/18:1(9Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0114245	PE-NMe2(:2(11Z,14Z)/18:1(11Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0114023	PE-NMe2(18:1(11Z)/:2(11Z,14Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0114050	PE-NMe2(18:1(9Z)/:2(11Z,14Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0113998	PE-NMe2(18/:3(8Z,11Z,14Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0113997	PE-NMe2(18/:3(5Z,8Z,11Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0113978	PE-NMe2(16:1(9Z)/22:2(13Z,16Z))	C45H84NO8P	M+FA-H	842.5917	-1.8
HMDB0112578	PS(:2(11Z,14Z)/)	C46H86NO10P	M-H	842.5917	-1.9
HMDB0112525	PS(/:2(11Z,14Z))	C46H86NO10P	M-H	842.5917	-1.9
HMDB0112914	PS(24:1(15Z)/16:1(9Z))	C46H86NO10P	M-H	842.5917	-1.9
HMDB0112371	PS(16:1(9Z)/24:1(15Z))	C46H86NO10P	M-H	842.5917	-1.9
HMDB0112381	PS(18/22:2(13Z,16Z))	C46H86NO10P	M-H	842.5917	-1.9
HMDB0112401	PS(18:1(11Z)/22:1(13Z))	C46H86NO10P	M-H	842.5917	-1.9

	HMDB0112435	PS(18:2(9Z,12Z)/22)	C46H86NO10P	M-H	842.5917	-1.9
	HMDB0112552	PS(:1(11Z):1(11Z))	C46H86NO10P	M-H	842.5917	-1.9
	HMDB0112715	PS(22/18:2(9Z,12Z))	C46H86NO10P	M-H	842.5917	-1.9
	HMDB0112743	PS(22:1(13Z)/18:1(9Z))	C46H86NO10P	M-H	842.5917	-1.9
	HMDB0112742	PS(22:1(13Z)/18:1(11Z))	C46H86NO10P	M-H	842.5917	-1.9
	HMDB0112766	PS(22:2(13Z,16Z)/18)	C46H86NO10P	M-H	842.5917	-1.9
	HMDB0112418	PS(18:1(9Z)/22:1(13Z))	C46H86NO10P	M-H	842.5917	-1.9
843.5199	HMDB0116626	PG(22:5(7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C48H77O10P	M-H	843.5182	2.1
	HMDB0116744	PG(22:5(4Z,7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C48H77O10P	M-H	843.5182	2.1
	HMDB0116612	PG(:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C48H77O10P	M-H	843.5182	2.1
	HMDB0116611	PG(:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C48H77O10P	M-H	843.5182	2.1
	HMDB0116602	PG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3(5Z,8Z,11Z))	C48H77O10P	M-H	843.5182	2.1
	HMDB0116603	PG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3(8Z,11Z,14Z))	C48H77O10P	M-H	843.5182	2.1
	HMDB0115395	PA(22:5(7Z,Z,13Z,16Z,19Z)/22:4(7Z,Z,13Z,16Z))	C47H75O8P	M+FA-H	843.5182	2.1
	HMDB0115370	PA(22:5(4Z,7Z,Z,13Z,16Z)/22:4(7Z,Z,13Z,16Z))	C47H75O8P	M+FA-H	843.5182	2.1
	HMDB0115345	PA(22:4(7Z,Z,13Z,16Z)/22:5(7Z,Z,13Z,16Z,19Z))	C47H75O8P	M+FA-H	843.5182	2.1
	HMDB0115344	PA(22:4(7Z,Z,13Z,16Z)/22:5(4Z,7Z,Z,13Z,16Z))	C47H75O8P	M+FA-H	843.5182	2.1
	HMDB0009749	PE(24:1(15Z)/16:1(9Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0007954	PC(15/22:2(13Z,16Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0008592	PC(22:2(13Z,16Z)/15)	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0008981	PE(16:1(9Z)/24:1(15Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0009008	PE(18/22:2(13Z,16Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0009040	PE(18:1(11Z)/22:1(13Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0009073	PE(18:1(9Z)/22:1(13Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0009105	PE(18:2(9Z,12Z)/22)	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0009231	PE(/:2(11Z,14Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0009552	PE(22:2(13Z,16Z)/18)	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0009521	PE(22:1(13Z)/18:1(9Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0009520	PE(22:1(13Z)/18:1(11Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0009489	PE(22/18:2(9Z,12Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0009295	PE(:2(11Z,14Z)/)	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0009263	PE(:1(11Z):1(11Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0114216	PE-NMe2(:1(11Z)/18:1(11Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
	HMDB0114217	PE-NMe2(:1(11Z)/18:1(9Z))	C45H86NO8P	M+FA-H	844.6073	-1.9

844.6057

HMDB0114189	PE-NMe2(18:2(9Z,12Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
HMDB0114077	PE-NMe2(18:2(9Z,12Z)/)	C45H86NO8P	M+FA-H	844.6073	-1.9
HMDB0114049	PE-NMe2(18:1(9Z)/:1(11Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
HMDB0114022	PE-NMe2(18:1(11Z)/:1(11Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
HMDB0113977	PE-NMe2(16:1(9Z)/22:1(13Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
HMDB0114441	PE-NMe2(22:1(13Z)/16:1(9Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
HMDB0114469	PE-NMe2(22:2(13Z,16Z)/16)	C45H86NO8P	M+FA-H	844.6073	-1.9
HMDB0114632	PE-NMe2(24:1(15Z)/14:1(9Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
HMDB0113996	PE-NMe2(18/:2(11Z,14Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
HMDB0114244	PE-NMe2(:2(11Z,14Z)/18)	C45H86NO8P	M+FA-H	844.6073	-1.9
HMDB0113955	PE-NMe2(16/22:2(13Z,16Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
HMDB0113878	PE-NMe2(14:1(9Z)/24:1(15Z))	C45H86NO8P	M+FA-H	844.6073	-1.9
HMDB0112913	PS(24:1(15Z)/16)	C46H88NO10P	M-H	844.6073	-1.9
HMDB0112356	PS(16/24:1(15Z))	C46H88NO10P	M-H	844.6073	-1.9
HMDB0112885	PS(24/16:1(9Z))	C46H88NO10P	M-H	844.6073	-1.9
HMDB0112741	PS(22:1(13Z)/18)	C46H88NO10P	M-H	844.6073	-1.9
HMDB0112713	PS(22/18:1(11Z))	C46H88NO10P	M-H	844.6073	-1.9
HMDB0112714	PS(22/18:1(9Z))	C46H88NO10P	M-H	844.6073	-1.9
HMDB0112551	PS(:1(11Z)/)	C46H88NO10P	M-H	844.6073	-1.9
HMDB0112524	PS(/:1(11Z))	C46H88NO10P	M-H	844.6073	-1.9
HMDB0112417	PS(18:1(9Z)/22)	C46H88NO10P	M-H	844.6073	-1.9
HMDB0112400	PS(18:1(11Z)/22)	C46H88NO10P	M-H	844.6073	-1.9
HMDB0112380	PS(18/22:1(13Z))	C46H88NO10P	M-H	844.6073	-1.9
HMDB0112370	PS(16:1(9Z)/24)	C46H88NO10P	M-H	844.6073	-1.9
HMDB0009782	PI(16/18:1(11Z))	C43H81O13P	M+Na-2H	857.5161	1.0
HMDB0009799	PI(16:1(9Z)/18)	C43H81O13P	M+Na-2H	857.5161	1.0
HMDB0009806	PI(18/16:1(9Z))	C43H81O13P	M+Na-2H	857.5161	1.0
HMDB0009822	PI(18:1(11Z)/16)	C43H81O13P	M+Na-2H	857.5161	1.0
HMDB0009834	PI(18:1(9Z)/16)	C43H81O13P	M+Na-2H	857.5161	1.0
HMDB0009783	PI(16/18:1(9Z))	C43H81O13P	M+Na-2H	857.5161	1.0
HMDB0009860	PI(18:3(6Z,9Z,12Z)/18:1(9Z))	C45H79O13P	M-H	857.5186	-1.8
HMDB0009899	PI(:4(8Z,11Z,14Z,17Z)/16)	C45H79O13P	M-H	857.5186	-1.8

857.5170	HMDB0009893	PI(:4(5Z,8Z,11Z,14Z)/16)	C45H79O13P	M-H	857.5186	-1.8
	HMDB0009863	PI(18:3(9Z,12Z,15Z)/18:1(11Z))	C45H79O13P	M-H	857.5186	-1.8
	HMDB0009864	PI(18:3(9Z,12Z,15Z)/18:1(9Z))	C45H79O13P	M-H	857.5186	-1.8
	HMDB0009859	PI(18:3(6Z,9Z,12Z)/18:1(11Z))	C45H79O13P	M-H	857.5186	-1.8
	HMDB0009840	PI(18:1(9Z)/18:3(9Z,12Z,15Z))	C45H79O13P	M-H	857.5186	-1.8
	HMDB0009839	PI(18:1(9Z)/18:3(6Z,9Z,12Z))	C45H79O13P	M-H	857.5186	-1.8
	HMDB0009827	PI(18:1(11Z)/18:3(6Z,9Z,12Z))	C45H79O13P	M-H	857.5186	-1.8
	HMDB0009828	PI(18:1(11Z)/18:3(9Z,12Z,15Z))	C45H79O13P	M-H	857.5186	-1.8
	HMDB0009790	PI(16/:4(8Z,11Z,14Z,17Z))	C45H79O13P	M-H	857.5186	-1.8
	HMDB0009850	PI(18:2(9Z,12Z)/18:2(9Z,12Z))	C45H79O13P	M-H	857.5186	-1.8
	HMDB0009789	PI(16/:4(5Z,8Z,11Z,14Z))	C45H79O13P	M-H	857.5186	-1.8
	HMDB0062771	1,2-dilinooleoyl-sn-glycero-3-phospho-1D-myo-inositol	C45H79O13P	M-H	857.5186	-1.8
859.5327	HMDB0062582	Phosphatidylinositol(34)	C43H83O13P	M+Na-2H	859.5318	1.1
	HMDB0009781	PI(16/18)	C43H83O13P	M+Na-2H	859.5318	1.1
	HMDB0009805	PI(18/16)	C43H83O13P	M+Na-2H	859.5318	1.1
	HMDB0009787	PI(16/:3(5Z,8Z,11Z))	C45H81O13P	M-H	859.5342	-1.7
	HMDB0009788	PI(16/:3(8Z,11Z,14Z))	C45H81O13P	M-H	859.5342	-1.7
	HMDB0009810	PI(18/18:3(6Z,9Z,12Z))	C45H81O13P	M-H	859.5342	-1.7
	HMDB0009811	PI(18/18:3(9Z,12Z,15Z))	C45H81O13P	M-H	859.5342	-1.7
	HMDB0009826	PI(18:1(11Z)/18:2(9Z,12Z))	C45H81O13P	M-H	859.5342	-1.7
	HMDB0009838	PI(18:1(9Z)/18:2(9Z,12Z))	C45H81O13P	M-H	859.5342	-1.7
	HMDB0009848	PI(18:2(9Z,12Z)/18:1(11Z))	C45H81O13P	M-H	859.5342	-1.7
	HMDB0009849	PI(18:2(9Z,12Z)/18:1(9Z))	C45H81O13P	M-H	859.5342	-1.7
	HMDB0009858	PI(18:3(6Z,9Z,12Z)/18)	C45H81O13P	M-H	859.5342	-1.7
	HMDB0009886	PI(:3(8Z,11Z,14Z)/16)	C45H81O13P	M-H	859.5342	-1.7
	HMDB0009862	PI(18:3(9Z,12Z,15Z)/18)	C45H81O13P	M-H	859.5342	-1.7
	HMDB0009879	PI(:3(5Z,8Z,11Z)/16)	C45H81O13P	M-H	859.5342	-1.7
861.5487	HMDB0009786	PI(16/:2(11Z,14Z))	C45H83O13P	M-H	861.5499	-1.3
	HMDB0009875	PI(:2(11Z,14Z)/16)	C45H83O13P	M-H	861.5499	-1.3
	HMDB0009809	PI(18/18:2(9Z,12Z))	C45H83O13P	M-H	861.5499	-1.3
	HMDB0009824	PI(18:1(11Z)/18:1(11Z))	C45H83O13P	M-H	861.5499	-1.3
	HMDB0009825	PI(18:1(11Z)/18:1(9Z))	C45H83O13P	M-H	861.5499	-1.3

	HMDB0009836	PI(18:1(9Z)/18:1(11Z))	C45H83O13P	M-H	861.5499	-1.3
	HMDB0009837	PI(18:1(9Z)/18:1(9Z))	C45H83O13P	M-H	861.5499	-1.3
	HMDB0009847	PI(18:2(9Z,12Z)/18)	C45H83O13P	M-H	861.5499	-1.3
865.5014	HMDB0116605	PG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C50H75O10P	M-H	865.5025	-1.3
	HMDB0116603	PG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3(8Z,11Z,14Z))	C48H77O10P	M+Na-2H	865.5001	1.5
	HMDB0116602	PG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/:3(5Z,8Z,11Z))	C48H77O10P	M+Na-2H	865.5001	1.5
	HMDB0116611	PG(:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,Z,13Z,16Z))	C48H77O10P	M+Na-2H	865.5001	1.5
	HMDB0116612	PG(:4(5Z,8Z,11Z,14Z)/22:5(7Z,Z,13Z,16Z,19Z))	C48H77O10P	M+Na-2H	865.5001	1.5
	HMDB0116744	PG(22:5(4Z,7Z,Z,13Z,16Z)/:4(5Z,8Z,11Z,14Z))	C48H77O10P	M+Na-2H	865.5001	1.5
	HMDB0116626	PG(22:5(7Z,Z,13Z,16Z,19Z)/:4(5Z,8Z,11Z,14Z))	C48H77O10P	M+Na-2H	865.5001	1.5
867.5187	HMDB0116620	PG(22:5(4Z,7Z,Z,13Z,16Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C50H77O10P	M-H	867.5182	0.6
	HMDB0116745	PG(22:5(7Z,Z,13Z,16Z,19Z)/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C50H77O10P	M-H	867.5182	0.6
	HMDB0116634	PG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(4Z,7Z,Z,13Z,16Z))	C50H77O10P	M-H	867.5182	0.6
	HMDB0116635	PG(22:6(4Z,7Z,Z,13Z,16Z,19Z)/22:5(7Z,Z,13Z,16Z,19Z))	C50H77O10P	M-H	867.5182	0.6
	HMDB0112355	PS(16/24)	C46H90NO10P	M+Na-2H	868.6049	0.5
	HMDB0112379	PS(18/22)	C46H90NO10P	M+Na-2H	868.6049	0.5
	HMDB0112523	PS(/)	C46H90NO10P	M+Na-2H	868.6049	0.5
	HMDB0112712	PS(22/18)	C46H90NO10P	M+Na-2H	868.6049	0.5
	HMDB0112884	PS(24/16)	C46H90NO10P	M+Na-2H	868.6049	0.5
	HMDB0009435	PE(:4(8Z,11Z,14Z,17Z)/22)	C47H86NO8P	M+FA-H	868.6073	-2.3
	HMDB0009402	PE(:4(5Z,8Z,11Z,14Z)/22)	C47H86NO8P	M+FA-H	868.6073	-2.3
	HMDB0009370	PE(:3(8Z,11Z,14Z)/22:1(13Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
	HMDB0009337	PE(:3(5Z,8Z,11Z)/22:1(13Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
	HMDB0009305	PE(:2(11Z,14Z)/22:2(13Z,16Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
	HMDB0009240	PE(/22:4(7Z,Z,13Z,16Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
	HMDB0009211	PE(18:4(6Z,9Z,12Z,15Z)/24)	C47H86NO8P	M+FA-H	868.6073	-2.3
	HMDB0009179	PE(18:3(9Z,12Z,15Z)/24:1(15Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
	HMDB0009146	PE(18:3(6Z,9Z,12Z)/24:1(15Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
	HMDB0009499	PE(22/:4(8Z,11Z,14Z,17Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
	HMDB0009498	PE(22/:4(5Z,8Z,11Z,14Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
	HMDB0009754	PE(24:1(15Z)/18:3(6Z,9Z,12Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
	HMDB0009755	PE(24:1(15Z)/18:3(9Z,12Z,15Z))	C47H86NO8P	M+FA-H	868.6073	-2.3

868.6053

HMDB0009723	PE(24/18:4(6Z,9Z,12Z,15Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0009592	PE(22:4(7Z,Z,13Z,16Z)/)	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0009561	PE(22:2(13Z,16Z)/:2(11Z,14Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0009530	PE(22:1(13Z)/:3(8Z,11Z,14Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0009529	PE(22:1(13Z)/:3(5Z,8Z,11Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114336	PE-NMe2(:4(5Z,8Z,11Z,14Z)/)	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114281	PE-NMe2(:3(5Z,8Z,11Z)/:1(11Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114309	PE-NMe2(:3(8Z,11Z,14Z)/:1(11Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114226	PE-NMe2(:1(11Z)/:3(8Z,11Z,14Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114225	PE-NMe2(:1(11Z)/:3(5Z,8Z,11Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114198	PE-NMe2(/:4(5Z,8Z,11Z,14Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114199	PE-NMe2(/:4(8Z,11Z,14Z,17Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114364	PE-NMe2(:4(8Z,11Z,14Z,17Z)/)	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114421	PE-NMe2(22/18:4(6Z,9Z,12Z,15Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114446	PE-NMe2(22:1(13Z)/18:3(6Z,9Z,12Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114447	PE-NMe2(22:1(13Z)/18:3(9Z,12Z,15Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114474	PE-NMe2(22:2(13Z,16Z)/18:2(9Z,12Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114500	PE-NMe2(22:4(7Z,Z,13Z,16Z)/18)	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114253	PE-NMe2(:2(11Z,14Z)/:2(11Z,14Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114172	PE-NMe2(18:4(6Z,9Z,12Z,15Z)/22)	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114144	PE-NMe2(18:3(9Z,12Z,15Z)/22:1(13Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114115	PE-NMe2(18:3(6Z,9Z,12Z)/22:1(13Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114087	PE-NMe2(18:2(9Z,12Z)/22:2(13Z,16Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0114005	PE-NMe2(18/22:4(7Z,Z,13Z,16Z))	C47H86NO8P	M+FA-H	868.6073	-2.3
HMDB0112890	PS(24/18:3(6Z,9Z,12Z))	C48H88NO10P	M-H	868.6073	-2.3
HMDB0112891	PS(24/18:3(9Z,12Z,15Z))	C48H88NO10P	M-H	868.6073	-2.3
HMDB0112749	PS(22:1(13Z)/:2(11Z,14Z))	C48H88NO10P	M-H	868.6073	-2.3
HMDB0112918	PS(24:1(15Z)/18:2(9Z,12Z))	C48H88NO10P	M-H	868.6073	-2.3
HMDB0112586	PS(:2(11Z,14Z)/22:1(13Z))	C48H88NO10P	M-H	868.6073	-2.3
HMDB0112774	PS(22:2(13Z,16Z)/:1(11Z))	C48H88NO10P	M-H	868.6073	-2.3
HMDB0112723	PS(22/:3(8Z,11Z,14Z))	C48H88NO10P	M-H	868.6073	-2.3
HMDB0112630	PS(:3(8Z,11Z,14Z)/22)	C48H88NO10P	M-H	868.6073	-2.3

	HMDB0112613	PS(:3(5Z,8Z,11Z)/22)	C48H88NO10 P	M-H	868.6073	-2.3
	HMDB0112560	PS(:1(11Z)/22:2(13Z,16Z))	C48H88NO10 P	M-H	868.6073	-2.3
	HMDB0112483	PS(18:3(9Z,12Z,15Z)/24)	C48H88NO10 P	M-H	868.6073	-2.3
	HMDB0112466	PS(18:3(6Z,9Z,12Z)/24)	C48H88NO10 P	M-H	868.6073	-2.3
	HMDB0112442	PS(18:2(9Z,12Z)/24:1(15Z))	C48H88NO10 P	M-H	868.6073	-2.3
	HMDB0112722	PS(22/:3(5Z,8Z,11Z))	C48H88NO10 P	M-H	868.6073	-2.3
870.6216	HMDB0009753	PE(24:1(15Z)/18:2(9Z,12Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0009113	PE(18:2(9Z,12Z)/24:1(15Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0009145	PE(18:3(6Z,9Z,12Z)/24)	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0009178	PE(18:3(9Z,12Z,15Z)/24)	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0009272	PE(:1(11Z)/22:2(13Z,16Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0009304	PE(:2(11Z,14Z)/22:1(13Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0009336	PE(:3(5Z,8Z,11Z)/22)	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0009369	PE(:3(8Z,11Z,14Z)/22)	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0009496	PE(22/:3(5Z,8Z,11Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0009497	PE(22/:3(8Z,11Z,14Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0009528	PE(22:1(13Z)/:2(11Z,14Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0009560	PE(22:2(13Z,16Z)/:1(11Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0009721	PE(24/18:3(6Z,9Z,12Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0009722	PE(24/18:3(9Z,12Z,15Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0114197	PE-NMe2(/:3(8Z,11Z,14Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0114196	PE-NMe2(/:3(5Z,8Z,11Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0114143	PE-NMe2(18:3(9Z,12Z,15Z)/22)	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0114114	PE-NMe2(18:3(6Z,9Z,12Z)/22)	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0114086	PE-NMe2(18:2(9Z,12Z)/22:1(13Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0114058	PE-NMe2(18:1(9Z)/22:2(13Z,16Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0114280	PE-NMe2(:3(5Z,8Z,11Z)/)	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0114308	PE-NMe2(:3(8Z,11Z,14Z)/)	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0114419	PE-NMe2(22/18:3(6Z,9Z,12Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0114420	PE-NMe2(22/18:3(9Z,12Z,15Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0114445	PE-NMe2(22:1(13Z)/18:2(9Z,12Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0114472	PE-NMe2(22:2(13Z,16Z)/18:1(11Z))	C47H88NO8P	M+FA-H	870.6230	-1.6

	HMDB0114473	PE-NMe2(22:2(13Z,16Z)/18:1(9Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0114224	PE-NMe2(:1(11Z)/:2(11Z,14Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0114252	PE-NMe2(:2(11Z,14Z)/:1(11Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0114031	PE-NMe2(18:1(11Z)/22:2(13Z,16Z))	C47H88NO8P	M+FA-H	870.6230	-1.6
	HMDB0112917	PS(24:1(15Z)/18:1(9Z))	C48H90NO10P	M-H	870.6230	-1.6
	HMDB0112916	PS(24:1(15Z)/18:1(11Z))	C48H90NO10P	M-H	870.6230	-1.6
	HMDB0112585	PS(:2(11Z,14Z)/22)	C48H90NO10P	M-H	870.6230	-1.6
	HMDB0112721	PS(22/:2(11Z,14Z))	C48H90NO10P	M-H	870.6230	-1.6
	HMDB0112889	PS(24/18:2(9Z,12Z))	C48H90NO10P	M-H	870.6230	-1.6
	HMDB0112773	PS(22:2(13Z,16Z)/)	C48H90NO10P	M-H	870.6230	-1.6
	HMDB0112748	PS(22:1(13Z)/:1(11Z))	C48H90NO10P	M-H	870.6230	-1.6
	HMDB0112559	PS(:1(11Z)/22:1(13Z))	C48H90NO10P	M-H	870.6230	-1.6
	HMDB0112533	PS(/22:2(13Z,16Z))	C48H90NO10P	M-H	870.6230	-1.6
	HMDB0112441	PS(18:2(9Z,12Z)/24)	C48H90NO10P	M-H	870.6230	-1.6
	HMDB0112424	PS(18:1(9Z)/24:1(15Z))	C48H90NO10P	M-H	870.6230	-1.6
	HMDB0112408	PS(18:1(11Z)/24:1(15Z))	C48H90NO10P	M-H	870.6230	-1.6
871.5378	HMDB0034248	Styrene	C53H70N4O4	M+FA-H	871.5379	-0.1
	HMDB0009047	PE(18:1(11Z)/24:1(15Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0009751	PE(24:1(15Z)/18:1(11Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0009080	PE(18:1(9Z)/24:1(15Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0009112	PE(18:2(9Z,12Z)/24)	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0009239	PE(/22:2(13Z,16Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0009271	PE(:1(11Z)/22:1(13Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0009303	PE(:2(11Z,14Z)/22)	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0009495	PE(22/:2(11Z,14Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0009527	PE(22:1(13Z)/:1(11Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0009559	PE(22:2(13Z,16Z)/)	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0009720	PE(24/18:2(9Z,12Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0009752	PE(24:1(15Z)/18:1(9Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0114443	PE-NMe2(22:1(13Z)/18:1(11Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0114444	PE-NMe2(22:1(13Z)/18:1(9Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0114418	PE-NMe2(22/18:2(9Z,12Z))	C47H90NO8P	M+FA-H	872.6386	-1.8

872.6370	HMDB0114223	PE-NMe2(:1(11Z):1(11Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0114085	PE-NMe2(18:2(9Z,12Z)/22)	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0114057	PE-NMe2(18:1(9Z)/22:1(13Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0114471	PE-NMe2(22:2(13Z,16Z)/18)	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0114635	PE-NMe2(24:1(15Z)/16:1(9Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0114195	PE-NMe2(/:2(11Z,14Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0114251	PE-NMe2(:2(11Z,14Z)/)	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0114030	PE-NMe2(18:1(11Z)/22:1(13Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0114004	PE-NMe2(18/22:2(13Z,16Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0113984	PE-NMe2(16:1(9Z)/24:1(15Z))	C47H90NO8P	M+FA-H	872.6386	-1.8
	HMDB0112915	PS(24:1(15Z)/18)	C48H92NO10P	M-H	872.6386	-1.8
	HMDB0112888	PS(24/18:1(9Z))	C48H92NO10P	M-H	872.6386	-1.8
	HMDB0112887	PS(24/18:1(11Z))	C48H92NO10P	M-H	872.6386	-1.8
	HMDB0112747	PS(22:1(13Z)/)	C48H92NO10P	M-H	872.6386	-1.8
	HMDB0112720	PS(22/:1(11Z))	C48H92NO10P	M-H	872.6386	-1.8
	HMDB0112558	PS(:1(11Z)/22)	C48H92NO10P	M-H	872.6386	-1.8
	HMDB0112532	PS(/22:1(13Z))	C48H92NO10P	M-H	872.6386	-1.8
	HMDB0112423	PS(18:1(9Z)/24)	C48H92NO10P	M-H	872.6386	-1.8
	HMDB0112385	PS(18/24:1(15Z))	C48H92NO10P	M-H	872.6386	-1.8
	HMDB0112407	PS(18:1(11Z)/24)	C48H92NO10P	M-H	872.6386	-1.8
873.6413	HMDB0055513	TG(18:4(6Z,9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	C59H88O6	M-H20-H	873.6397	1.8
	HMDB0055503	TG(18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z)/:5(5Z,8Z,11Z,14Z,17Z))	C59H88O6	M-H20-H	873.6397	1.8
881.5179	HMDB0009862	PI(18:3(9Z,12Z,15Z)/18)	C45H81O13P	M+Na-2H	881.5161	2.0
	HMDB0009858	PI(18:3(6Z,9Z,12Z)/18)	C45H81O13P	M+Na-2H	881.5161	2.0
	HMDB0009849	PI(18:2(9Z,12Z)/18:1(9Z))	C45H81O13P	M+Na-2H	881.5161	2.0
	HMDB0009848	PI(18:2(9Z,12Z)/18:1(11Z))	C45H81O13P	M+Na-2H	881.5161	2.0
	HMDB0009838	PI(18:1(9Z)/18:2(9Z,12Z))	C45H81O13P	M+Na-2H	881.5161	2.0
	HMDB0009826	PI(18:1(11Z)/18:2(9Z,12Z))	C45H81O13P	M+Na-2H	881.5161	2.0
	HMDB0009811	PI(18/18:3(9Z,12Z,15Z))	C45H81O13P	M+Na-2H	881.5161	2.0
	HMDB0009810	PI(18/18:3(6Z,9Z,12Z))	C45H81O13P	M+Na-2H	881.5161	2.0
	HMDB0009788	PI(16/:3(8Z,11Z,14Z))	C45H81O13P	M+Na-2H	881.5161	2.0
	HMDB0009879	PI(:3(5Z,8Z,11Z)/16)	C45H81O13P	M+Na-2H	881.5161	2.0

	HMDB0009886	PI(:3(8Z,11Z,14Z)/16)	C45H81O13P	M+Na-2H	881.5161	2.0
	HMDB0009787	PI(16/:3(5Z,8Z,11Z))	C45H81O13P	M+Na-2H	881.5161	2.0
883.5328	HMDB0009786	PI(16/:2(11Z,14Z))	C45H83O13P	M+Na-2H	883.5318	1.1
	HMDB0009809	PI(18/18:2(9Z,12Z))	C45H83O13P	M+Na-2H	883.5318	1.1
	HMDB0009825	PI(18:1(11Z)/18:1(9Z))	C45H83O13P	M+Na-2H	883.5318	1.1
	HMDB0009836	PI(18:1(9Z)/18:1(11Z))	C45H83O13P	M+Na-2H	883.5318	1.1
	HMDB0009837	PI(18:1(9Z)/18:1(9Z))	C45H83O13P	M+Na-2H	883.5318	1.1
	HMDB0009847	PI(18:2(9Z,12Z)/18)	C45H83O13P	M+Na-2H	883.5318	1.1
	HMDB0009875	PI(:2(11Z,14Z)/16)	C45H83O13P	M+Na-2H	883.5318	1.1
	HMDB0009824	PI(18:1(11Z)/18:1(11Z))	C45H83O13P	M+Na-2H	883.5318	1.1
	HMDB0009845	PI(18:1(9Z)/:4(8Z,11Z,14Z,17Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009795	PI(16/22:5(4Z,7Z,Z,13Z,16Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009916	PI(22:5(4Z,7Z,Z,13Z,16Z)/16)	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009918	PI(22:5(7Z,Z,13Z,16Z,19Z)/16)	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009908	PI(22:3(Z,13Z,16Z)/16:2(9Z,12Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009902	PI(:4(8Z,11Z,14Z,17Z)/18:1(9Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009901	PI(:4(8Z,11Z,14Z,17Z)/18:1(11Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009896	PI(:4(5Z,8Z,11Z,14Z)/18:1(9Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009895	PI(:4(5Z,8Z,11Z,14Z)/18:1(11Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009890	PI(:3(8Z,11Z,14Z)/18:2(9Z,12Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009883	PI(:3(5Z,8Z,11Z)/18:2(9Z,12Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009854	PI(18:2(9Z,12Z)/:3(5Z,8Z,11Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009833	PI(18:1(11Z)/:4(8Z,11Z,14Z,17Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009832	PI(18:1(11Z)/:4(5Z,8Z,11Z,14Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009804	PI(16:2(9Z,12Z)/22:3(Z,13Z,16Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009796	PI(16/22:5(7Z,Z,13Z,16Z,19Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009855	PI(18:2(9Z,12Z)/:3(8Z,11Z,14Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0009844	PI(18:1(9Z)/:4(5Z,8Z,11Z,14Z))	C47H81O13P	M-H	883.5342	-1.6
	HMDB0062586	[(2R)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]({[(2R,3R,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid	C47H81O13P	M-H	883.5342	-1.6
	HMDB0240667	1-stearoyl-2-oleoyl-sn-glycero-3-phospho-1D-myo-inositol	C45H85O13P	M+Na-2H	885.5474	1.2
	HMDB0009794	PI(16/22:4(7Z,Z,13Z,16Z))	C47H83O13P	M-H	885.5499	-1.5

885.5485	HMDB0009793	PI(16/22:4(Z,13Z,16Z,19Z))	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009881	PI(:3(5Z,8Z,11Z)/18:1(11Z))	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009877	PI(:2(11Z,14Z)/18:2(9Z,12Z))	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009853	PI(18:2(9Z,12Z):2(11Z,14Z))	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009843	PI(18:1(9Z):3(8Z,11Z,14Z))	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009842	PI(18:1(9Z):3(5Z,8Z,11Z))	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009831	PI(18:1(11Z):3(8Z,11Z,14Z))	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009830	PI(18:1(11Z):3(5Z,8Z,11Z))	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009816	PI(18/:4(8Z,11Z,14Z,17Z))	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009882	PI(:3(5Z,8Z,11Z)/18:1(9Z))	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009894	PI(:4(5Z,8Z,11Z,14Z)/18)	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009900	PI(:4(8Z,11Z,14Z,17Z)/18)	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009912	PI(22:4(Z,13Z,16Z,19Z)/16)	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009889	PI(:3(8Z,11Z,14Z)/18:1(9Z))	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009914	PI(22:4(7Z,Z,13Z,16Z)/16)	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009888	PI(:3(8Z,11Z,14Z)/18:1(11Z))	C47H83O13P	M-H	885.5499	-1.5
	HMDB0009815	PI(18/:4(5Z,8Z,11Z,14Z))	C47H83O13P	M-H	885.5499	-1.5
887.5639	HMDB0009785	PI(16/)	C45H87O13P	M+Na-2H	887.5631	0.9
	HMDB0009866	PI(/16)	C45H87O13P	M+Na-2H	887.5631	0.9
	HMDB0009808	PI(18/18)	C45H87O13P	M+Na-2H	887.5631	0.9
	HMDB0009852	PI(18:2(9Z,12Z):1(11Z))	C47H85O13P	M-H	887.5655	-1.8
	HMDB0009792	PI(16/22:3(Z,13Z,16Z))	C47H85O13P	M-H	887.5655	-1.8
	HMDB0009813	PI(18/:3(5Z,8Z,11Z))	C47H85O13P	M-H	887.5655	-1.8
	HMDB0009814	PI(18/:3(8Z,11Z,14Z))	C47H85O13P	M-H	887.5655	-1.8
	HMDB0009872	PI(:1(11Z)/18:2(9Z,12Z))	C47H85O13P	M-H	887.5655	-1.8
	HMDB0009880	PI(:3(5Z,8Z,11Z)/18)	C47H85O13P	M-H	887.5655	-1.8
	HMDB0009887	PI(:3(8Z,11Z,14Z)/18)	C47H85O13P	M-H	887.5655	-1.8
	HMDB0009907	PI(22:3(Z,13Z,16Z)/16)	C47H85O13P	M-H	887.5655	-1.8
	HMDB0009815	PI(18/:4(5Z,8Z,11Z,14Z))	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009888	PI(:3(8Z,11Z,14Z)/18:1(11Z))	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009889	PI(:3(8Z,11Z,14Z)/18:1(9Z))	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009894	PI(:4(5Z,8Z,11Z,14Z)/18)	C47H83O13P	M+Na-2H	907.5318	1.5

907.5332	HMDB0009900	PI(:4(8Z,11Z,14Z,17Z)/18)	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009912	PI(22:4(Z,13Z,16Z,19Z)/16)	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009914	PI(22:4(7Z,Z,13Z,16Z)/16)	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009882	PI(:3(5Z,8Z,11Z)/18:1(9Z))	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009793	PI(16/22:4(Z,13Z,16Z,19Z))	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009881	PI(:3(5Z,8Z,11Z)/18:1(11Z))	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009794	PI(16/22:4(7Z,Z,13Z,16Z))	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009816	PI(18/:4(8Z,11Z,14Z,17Z))	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009830	PI(18:1(11Z)/:3(5Z,8Z,11Z))	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009842	PI(18:1(9Z)/:3(5Z,8Z,11Z))	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009843	PI(18:1(9Z)/:3(8Z,11Z,14Z))	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009853	PI(18:2(9Z,12Z)/:2(11Z,14Z))	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009877	PI(:2(11Z,14Z)/18:2(9Z,12Z))	C47H83O13P	M+Na-2H	907.5318	1.5
	HMDB0009831	PI(18:1(11Z)/:3(8Z,11Z,14Z))	C47H83O13P	M+Na-2H	907.5318	1.5
909.5485	HMDB0009813	PI(18/:3(5Z,8Z,11Z))	C47H85O13P	M+Na-2H	909.5474	1.2
	HMDB0009814	PI(18/:3(8Z,11Z,14Z))	C47H85O13P	M+Na-2H	909.5474	1.2
	HMDB0009852	PI(18:2(9Z,12Z)/:1(11Z))	C47H85O13P	M+Na-2H	909.5474	1.2
	HMDB0009872	PI(:1(11Z)/18:2(9Z,12Z))	C47H85O13P	M+Na-2H	909.5474	1.2
	HMDB0009880	PI(:3(5Z,8Z,11Z)/18)	C47H85O13P	M+Na-2H	909.5474	1.2
	HMDB0009887	PI(:3(8Z,11Z,14Z)/18)	C47H85O13P	M+Na-2H	909.5474	1.2
	HMDB0009907	PI(22:3(Z,13Z,16Z)/16)	C47H85O13P	M+Na-2H	909.5474	1.2
	HMDB0009792	PI(16/22:3(Z,13Z,16Z))	C47H85O13P	M+Na-2H	909.5474	1.2
	HMDB0009865	PI(18:3(9Z,12Z,15Z)/22:3(Z,13Z,16Z))	C49H83O13P	M-H	909.5499	-1.5
	HMDB0009891	PI(:3(8Z,11Z,14Z)/:3(5Z,8Z,11Z))	C49H83O13P	M-H	909.5499	-1.5
	HMDB0009861	PI(18:3(6Z,9Z,12Z)/22:3(Z,13Z,16Z))	C49H83O13P	M-H	909.5499	-1.5
	HMDB0009911	PI(22:3(Z,13Z,16Z)/18:3(9Z,12Z,15Z))	C49H83O13P	M-H	909.5499	-1.5
	HMDB0009910	PI(22:3(Z,13Z,16Z)/18:3(6Z,9Z,12Z))	C49H83O13P	M-H	909.5499	-1.5
	HMDB0009892	PI(:3(8Z,11Z,14Z)/:3(8Z,11Z,14Z))	C49H83O13P	M-H	909.5499	-1.5
	HMDB0009885	PI(:3(5Z,8Z,11Z)/:3(8Z,11Z,14Z))	C49H83O13P	M-H	909.5499	-1.5
	HMDB0009821	PI(18/22:6(4Z,7Z,Z,13Z,16Z,19Z))	C49H83O13P	M-H	909.5499	-1.5
	HMDB0009884	PI(:3(5Z,8Z,11Z)/:3(5Z,8Z,11Z))	C49H83O13P	M-H	909.5499	-1.5
	HMDB0009920	PI(22:6(4Z,7Z,Z,13Z,16Z,19Z)/18)	C49H83O13P	M-H	909.5499	-1.5

911.5638	HMDB0009791	PI(16/22:2(13Z,16Z))	C47H87O13P	M+Na-2H	911.5631	0.8
	HMDB0009812	PI(18:2(11Z,14Z))	C47H87O13P	M+Na-2H	911.5631	0.8
	HMDB0009829	PI(18:1(11Z)/:1(11Z))	C47H87O13P	M+Na-2H	911.5631	0.8
	HMDB0009841	PI(18:1(9Z)/:1(11Z))	C47H87O13P	M+Na-2H	911.5631	0.8
	HMDB0009851	PI(18:2(9Z,12Z)/)	C47H87O13P	M+Na-2H	911.5631	0.8
	HMDB0009867	PI(/18:2(9Z,12Z))	C47H87O13P	M+Na-2H	911.5631	0.8
	HMDB0009870	PI(:1(11Z)/18:1(11Z))	C47H87O13P	M+Na-2H	911.5631	0.8
	HMDB0009871	PI(:1(11Z)/18:1(9Z))	C47H87O13P	M+Na-2H	911.5631	0.8
	HMDB0009876	PI(:2(11Z,14Z)/18)	C47H87O13P	M+Na-2H	911.5631	0.8
	HMDB0009905	PI(22:2(13Z,16Z)/16)	C47H87O13P	M+Na-2H	911.5631	0.8
	HMDB0009917	PI(22:5(4Z,7Z,Z,13Z,16Z)/18)	C49H85O13P	M-H	911.5655	-1.9
	HMDB0009919	PI(22:5(7Z,Z,13Z,16Z,19Z)/18)	C49H85O13P	M-H	911.5655	-1.9
	HMDB0009909	PI(22:3(Z,13Z,16Z)/18:2(9Z,12Z))	C49H85O13P	M-H	911.5655	-1.9
	HMDB0009904	PI(:4(8Z,11Z,14Z,17Z)/:1(11Z))	C49H85O13P	M-H	911.5655	-1.9
	HMDB0009898	PI(:4(5Z,8Z,11Z,14Z)/:1(11Z))	C49H85O13P	M-H	911.5655	-1.9
	HMDB0009874	PI(:1(11Z)/:4(8Z,11Z,14Z,17Z))	C49H85O13P	M-H	911.5655	-1.9
	HMDB0009873	PI(:1(11Z)/:4(5Z,8Z,11Z,14Z))	C49H85O13P	M-H	911.5655	-1.9
	HMDB0009857	PI(18:2(9Z,12Z)/22:3(Z,13Z,16Z))	C49H85O13P	M-H	911.5655	-1.9
	HMDB0009819	PI(18/22:5(4Z,7Z,Z,13Z,16Z))	C49H85O13P	M-H	911.5655	-1.9
	HMDB0009820	PI(18/22:5(7Z,Z,13Z,16Z,19Z))	C49H85O13P	M-H	911.5655	-1.9
913.5797	HMDB0009817	PI(18/22:4(Z,13Z,16Z,19Z))	C49H87O13P	M-H	913.5812	-1.6
	HMDB0009915	PI(22:4(7Z,Z,13Z,16Z)/18)	C49H87O13P	M-H	913.5812	-1.6
	HMDB0009818	PI(18/22:4(7Z,Z,13Z,16Z))	C49H87O13P	M-H	913.5812	-1.6
	HMDB0009856	PI(18:2(9Z,12Z)/22:2(13Z,16Z))	C49H87O13P	M-H	913.5812	-1.6
	HMDB0009868	PI(/:3(8Z,11Z,14Z))	C49H87O13P	M-H	913.5812	-1.6
	HMDB0009869	PI(/:4(5Z,8Z,11Z,14Z))	C49H87O13P	M-H	913.5812	-1.6
	HMDB0009878	PI(:2(11Z,14Z)/:2(11Z,14Z))	C49H87O13P	M-H	913.5812	-1.6
	HMDB0009897	PI(:4(5Z,8Z,11Z,14Z)/)	C49H87O13P	M-H	913.5812	-1.6
	HMDB0009903	PI(:4(8Z,11Z,14Z,17Z)/)	C49H87O13P	M-H	913.5812	-1.6
	HMDB0009906	PI(22:2(13Z,16Z)/18:2(9Z,12Z))	C49H87O13P	M-H	913.5812	-1.6
	HMDB0009913	PI(22:4(Z,13Z,16Z,19Z)/18)	C49H87O13P	M-H	913.5812	-1.6

920.2191	HMDB0143215	6-{[(3S)-3,12-dihydroxy-1-({5-hydroxy-6-methyl-4-[(2,2,2-trifluoro-1-hydroxyethylidene)amino]oxan-2-yl}oxy)--methoxy-6,11-dioxo-3-[2-(pentanoyloxy)acetyl]-1,2,3,4,6,11-hexahydrotetracen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H44F3NO19	M+Na-2H	920.2206	-1.7
	HMDB0143214	6-{[(2R)-2,12-dihydroxy-4-({5-hydroxy-6-methyl-4-[(2,2,2-trifluoro-1-hydroxyethylidene)amino]oxan-2-yl}oxy)-7-methoxy-6,11-dioxo-2-[2-(pentanoyloxy)acetyl]-1,2,3,4,6,11-hexahydrotetracen-5-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid	C40H44F3NO19	M+Na-2H	920.2206	-1.7
971.1033	HMDB0136080	4,5,5',6,6'-pentahydroxy-4'-[2,3,4-trihydroxy-6-({5-hydroxy-6-(hydroxymethyl)-3,4-bis(3,4,5-trihydroxybenzoyloxy)oxan-2-yl]oxy}carbonyl)phenoxy]-[1,1'-biphenyl]-2,2'-dicarboxylic acid	C41H32O28	M-H	971.1007	2.6
981.4185	HMDB0169434	3,4,5-trihydroxy-6-[(3-hydroxy-5-{[(2Z,6Z,Z)-4-hydroxy-2,6,,14-tetramethyl-14-{{3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}hexadeca-2,6,,15-tetraenoyl]oxy}-2-methyl-6-[(3,4,5,6-tetrahydroxyoxan-2-yl)methoxy]oxan-4-yl)oxy]oxane-2-carboxylic acid	C44H70O24	M-H	981.4184	0.1
	HMDB0169433	3,4,5-trihydroxy-6-[(4-hydroxy-5-{[(2Z,Z)-4-hydroxy-2,6,,14-tetramethyl-14-{{3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}hexadeca-2,6,,15-tetraenoyl]oxy}-2-methyl-6-[(3,4,5,6-tetrahydroxyoxan-2-yl)methoxy]oxan-3-yl)oxy]oxane-2-carboxylic acid	C44H70O24	M-H	981.4184	0.1