

[illegible]

Met_057	Medelamine A	C14 H31 N	-0.14	213.24562	214.2529	2.578	24	NA
Met_058	7-Methyl-2,6,9,12-tetraoxahexadecane	C13 H28 O4	0.08	248.19878	249.20598	2.594	30	CCCCOCCOCC(C)OCCOCC
Met_059	TG(17:1(9Z)/17:2(9Z,12Z)/18:0)[iso6]	C55 H100 O6	-0.47	856.75159	857.75926	14.256	59	CCCC(C=C\C/C=C\C\CCCCCCCC(=O)O)COC(=O)CCCCCCC/C=C\C\CCCCC)COC(=O)CCCCCCCCCCCCCCCC
Met_060	1-Methylnicotinamide	C7 H8 N2 O	0.53	136.06373	137.07101	1.907	97	C[N+]=CC=CC(=C1)C(N)=O
Met_061	Cholacalcioic acid	C24 H36 O3	-0.25	373.26635	373.27363	2.578	45	C[C@H](CCC(=O)O)[C@H]1CC[C@H]2[C@@]1(CCC/C2=C\C=C/3[C\C@H](CCCC3=C)O)C
Met_062	Cer(m18:1(4E)/24:0)	C42 H83 N O2	0.08	633.64243	634.64971	11.88	65	CCCCCCCCCCCCC/C=C/O)[C]NC(=O)CCCCCCCCCCCCCCCCCCCC
Met_063	20-oxo-heneicosanoic acid	C21 H40 O3	-0.71	340.2975	341.30478	10.786	65	C(CCCCCCCCCCCCCCCCCC(=O)C)(=O)O
Met_064	N-Stearoyl Glutamic acid	C23 H43 N O5	-0.19	413.31404	414.32132	3.357	30	OC(=O)CC[C@]([H])([H])(NC(CCCCCCCCCCCCCCCC(=O)C)=O)O
Met_065	N-(3-Hydroxy-92-octadecenoyl) glycine	N-3 H37 N O4	-0.53	355.27207	356.27935	3.163	35	C(CC(O)CCCCC/C=C\C\CCCCC)C(=O)NCC(=O)O
Met_066	N-arachidonylethanolamine	C22 H37 N O2	-1.47	347.28192	348.28919	3.204	78	CCCCC/C=C\C/C=C\C/C=C/C=C\C\CCCC(=O)NCCO
Met_067	3,5-Tetradecadiencarnitine	C21 H37 N O4	-0.57	367.27205	368.27933	2.48	NA	CCCCCCCC/C=C/C=C/CC(=O)O[C@H](CCC(=O)[O-])[N+](C)(C)C
Met_068	TG(17:2(9Z,12Z)/17:2(9Z,12Z)/20:1(11Z))[iso3]	C57 H100 O6	-0.15	880.75186	881.75925	13.828	49	CCCCCCCCC/C=C\CCCCCCCCC(=O)OC[C@H](COC(=O)CCCCC/C=C\C/C=C\C\CCCC)OC(=O)CCCCCCC/C=C\C/C=C\C\CCCC
Met_069	PE(18:0/18:3(6Z,9Z,12Z))	C41 H76 N O8 P	0.1	741.53093	742.5382	8.241	75	CCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)(O)OCCN)OC(=O)CCCC/C=C\C/C=C\C/C=C\C\CCCC
Met_070	Glycyl Oleate	C21 H38 O3	-0.76	338.28184	339.28911	10.791	53	NA
Met_071	Tryglyceride OPO	C55 H102 O6	-0.35	858.76734	859.77486	14.691	63	[H]C(COC(=O)CCCCCCC/C=C\CCCCCCC)COC(=O)CCCCCCC/C=C\CCCCCCC)OC(=O)CCCCCCCCCCCCCCC
Met_072	2-Geranylphenol	C16 H22 O	-0.01	230.16706	231.17434	2.963	64	CC(=CCC/C(=C/CC1=CC=CC=C1O))/C/C
Met_073	Cer(m18:1(4E)/24:1(15Z))	C42 H81 N O2	0.25	631.62689	632.63418	11.078	58	CCCCCCCC/C=C\CCCCCCCCCCCCC(=O)N(C)(O)/C=C/C\CCCCCCCCCCCC
Met_074	PE(18:3(6Z,9Z,12Z)/22:4(7Z,10Z,13Z,16Z))	C45 H76 N O8 P	-0.74	789.53027	790.53752	7.672	61	[C@](COP(=O)(O)OCCN)([H])[O](CCCCC/C=C\C/C=C\C/C=C\C\CCCC(=O)COC(CCCC/C=C\C/C=C\C/C=C\C\CCCC)C(=O)OCCN)C(=O)OCCN
Met_075	Patulin	C26 H42 N2 O	-0.35	398.32957	399.33685	7.165	33	OC1OCC=C2OC(=O)C=C12
Met_076	PE(18:1(9E)/18:1(9E))	C41 H78 N O8 P	0.28	743.54671	744.55399	11.175	32	[C@](COP(=O)(O)OCCN)([H])[O](CCCCCCC/C=C\CCCCCCC(=O)COC(CCCCCC/C=C\CCCCCCC)C(=O)OCCN)C(=O)OCCN
Met_077	Pelretin	C23 H28 O2	-1.2	336.20853	337.2158	3.325	44	CC1=C(C(CCC1)C)C/C=C/C/C=C/C=C/C=C/C=C=C(C(C=C2)C(=O)O)/C
Met_078	9-(3,5-dimethylfuran-2-yl)-nonanoic acid	C15 H24 O3	-0.07	252.17253	253.1798	2.762	82	CC1=CC(=C(O1)CCCCCCCCC(=O)O)C
Met_079	Tropeolin	C8 H7 N S	0.11	149.02994	150.03721	2.534	12	C1=CC=C(C=C1)CSC#N
Met_080	cis-5-Tetradecenoylcarnitine	C21 H39 N O4	-0.34	369.28778	370.29506	3.413	NA	[N+](C)(C)(C)CC(OC(=O)CCC/C=C\CCCCCCC)CC(=O)[O-]
Met_081	Docosanamide	C22 H45 N O	-0.49	339.34995	340.35723	2.458	36	O=C(CCCCCCCCCCCCCCCCCC)CN
Met_082	Oxaloterpin E	C21 H33 N O2	-0.29	331.25103	332.25831	2.964	24	C[C@]12CC[C@H]C([C@H]1CC[C@H]3C2=CC[C@]1(C3)C=C(C)(C)C)OC(=O)N
Met_083	Calcimycin	C29 H37 N3 O6	-1.04	523.26769	524.27496	3.335	28	C[C@H]1CCC2[C@H]([C@H]1[C@H](O)2)C(C)(=O)C3=CC=CN3)C)O[C@H]1CC4=NC5=C(O4)C=CC(=C5C(=O)O)NC
Met_084	(3aR,4R,6S,6aS,9bR)-4-hydroxy-6,9-dimethyl-3-methylidene-4,5,6,6a,7,9b-hexahydro-3aH-azuleno[4,5-b]furan-2,8-dione	C15 H18 O4	-0.19	262.12046	263.12773	3.412	70	C[C@H]1C[C@H]([C@H]2[C@H](C3=C(C(=O)C[C@H]13)C)OC(=O)C2=C)O
Met_085	Albaflovenone	C15 H22 O	0.11	218.16709	219.17437	5.119	53	C[C@H]1CCCC2[C@H]([C@H]1[C@H](O)2)C(C)(=O)C3=CC=CN3)C)O[C@H]1CC4=NC5=C(O4)C=CC(=C5C(=O)O)NC
Met_086	Aphidicol-16-ene	C20 H32 O	-1.26	272.25006	273.25733	4.442	28	C1CC[C@]2(C)[C@]34C[C@H](C=C)CC3[C@H]4([H])CC[C

Met_112	Fukiic acid
Met_113	Undecylic acid
Met_114	Temanogrel
Met_115	9'-carboxy-gamma-tocotrienol
Met_116	4-vinylphenol sulfate
Met_117	Protulactone A
Met_118	7-heptadecynoic acid
Met_119	2-methyl-2-dodecenoic acid
Met_120	5-Hydroxy-1-(4-hydroxyphenyl)-3-decanone
Met_121	2,4-dimethyl-5-vinylthiazole

C11 H12 O8	-0.13	272.05318	271.04601	1.751
C11 H22 O2	0.29	186.16203	417.3223	4.943
C24 H28 N4 O4	-3.13	436.20969	435.20241	2.06
C23 H32 O4	0.03	372.23007	371.2228	2.444
C8 H8 O4 S	-3.26	200.01368	199.00632	1.798
C10 H14 O6	-2.2	230.07853	229.07122	1.77
C17 H30 O2	-0.12	266.22455	265.21727	3.566
C13 H24 O2	-2.3	212.17714	211.16987	2.97
C16 H24 O3	-0.11	264.17251	263.16524	2.943
C7 H9 N S	-3.89	139.04503	138.03775	1.86

45	<chem>O[C@H](C(O)=O)[C@](O)(CC1=CC(O)=C(O)C=C1)C(O)=O</chem>
67	<chem>CCCCCCCCCCC(=O)O</chem>
0	<chem>CN1C(=CC=N1)C2=C(C=CC(=C2)NC(=O)C3=CC(=CC=C3)OC)OCCN4CCOCC4</chem>
7	<chem>CC1=C(C=C2CC[C@@](OC2=C1C)(C)CC/C=C(\C)/CC/C=C(\C)/C(=O)O)O</chem>
58	<chem>OS(=O)(=O)OC1=CC=C(C=C)C=C1</chem>
3	<chem>C[C@@H]([C@H]1[C@@H]([C@@H]([C@@H]2[C@H](O1)CC(=O)O2)O)OC(=O)C</chem>
25	<chem>CCCCCCCCC#CCCCCCC(=O)O</chem>
0	<chem>CCCCCCCCC/C=C(\C)/C(=O)O</chem>
63	<chem>CCCCC/C=C/C=C/C(O)C/C=C/C=C/C(=O)O</chem>
	<chem>CC1=NC(C)=C(S1)C=C</chem>