

A1-A2

ID	Metabolite	Metab ID	Kingdom	Superclass	Class	Subclass
pos_1007	Thymyl ac	metab_10	Organic	α	Lipids and Prenol lipi	Monoterpenoids
pos_1075	3,5,7-Trim	metab_84	Organic	α	Phenylpro	Flavonoid: Flavans
pos_115	(3S,5R,6R,	metab_16	Organic	α	Lipids and Prenol lipi	Sesquiterpenoids
pos_1210	Indoleacet	metab_23	Organic	α	Organohe	Indoles an Indoles
pos_1428	Glycyl-Me	metab_47	Organic	α	Organic α	Carboxylic Amino acids, peptides, and anal
pos_1500	Morph	metab_54	Organic	α	Organohe	Oxazinane Morpholines
pos_152	3-Hydroxy	metab_56	Organic	α	Lipids and Prenol lipi	Sesterterpenoids
pos_160	DG(8:0/0:0	metab_65	Not Availa	Not Availa	Not Availa	Not Available
pos_163	Mosinone	metab_68	Organic	α	Lipids and Fatty Acyl	Fatty alcohols
pos_1630	N2-(gamn	metab_68	Organic	α	Organic α	Carboxylic Amino acids, peptides, and anal
pos_1690	SN38 gluc	metab_75	Organic	α	Alkaloids α	Camptoth
pos_1725	Gibberellir	metab_78	Organic	α	Lipids and Prenol lipi	Diterpenoids
pos_173	Norethind	metab_79	Organic	α	Lipids and Steroids α	Estrane steroids
pos_1751	Diosmetin	metab_81	Organic	α	Phenylpro	Flavonoid: Flavonoid glycosides
pos_1755	Diazoetha	metab_82	Organic	α	Organic 1, Propargyl	Diazo compounds
pos_1784	3-Methyl	metab_85	Organic	α	Organohe	Indoles an Indoles
pos_1834	Tyrosyl-Le	metab_90	Organic	α	Organic α	Carboxylic Amino acids, peptides, and anal
pos_1887	Oryzalide	metab_96	Organic	α	Lipids and Prenol lipi	Terpene lactones
pos_1997	Minocyclir	metab_10	Organic	α	Phenylpro	Tetracyclir
pos_2080	Dihydrocu	metab_11	Organic	α	Lipids and Prenol lipi	Terpene lactones
pos_2197	Glucoliqui	metab_12	Organic	α	Phenylpro	Flavonoid: Flavonoid glycosides
pos_2216	Methionyl	metab_13	Organic	α	Organic α	Carboxylic Amino acids, peptides, and anal
pos_2233	Kuwanol E	metab_13	Organic	α	Phenylpro	Diarylhept
pos_2234	Jasmonic α	metab_13	Organic	α	Lipids and Fatty Acyl	Lineolic acids and derivatives
pos_2236	(Z)-3-Met	metab_13	Organic	α	Organic o	Organoox
pos_2268	Leukotrier	metab_13	Organic	α	Organic α	Carboxylic Amino acids, peptides, and anal
pos_2281	Cortolone	metab_13	Organic	α	Lipids and Steroids α	Steroidal glycosides
pos_24	Dinotefurα	metab_15	Organic	α	Organic ni	Organonit
pos_2507	1-(9Z-No	metab_16	Organic	α	Lipids and Glyceroph	Glycerophosphoethanolamines
pos_2530	DG(16:0/0	metab_16	Not Availa	Not Availa	Not Availa	Not Available
pos_2531	PS(22:5(4Z	metab_16	Organic	α	Lipids and Glyceroph	Glycerophosphoserines
pos_2560	DG(18:3(9	metab_16	Organic	α	Lipids and Fatty Acyl	Lineolic acids and derivatives
pos_2623	PC(16:1(9Z	metab_17	Organic	α	Lipids and Glyceroph	Glycerophosphocholines
pos_3058	DG(20:5(7	metab_21	Not Availa	Not Availa	Not Availa	Not Available
pos_3060	DG(18:4(6	metab_21	Organic	α	Lipids and Fatty Acyl	Lineolic acids and derivatives
pos_3110	PE(22:0/2C	metab_22	Organic	α	Lipids and Glyceroph	Glycerophosphoethanolamines
pos_3140	Docosahe	metab_22	Organic	α	Lipids and Fatty Acyl	Fatty acids and conjugates
pos_3184	Phoenicox	metab_23	Organic	α	Lipids and Prenol lipi	Tetraterpenoids
pos_3236	Furanodie	metab_23	Organic	α	Lipids and Prenol lipi	Sesquiterpenoids
pos_3261	DG(16:0/P	metab_23	Not Availa	Not Availa	Not Availa	Not Available
pos_3272	Barringtoç	metab_23	Organic	α	Lipids and Prenol lipi	Triterpenoids
pos_3458	Persicachr	metab_25	Organic	α	Lipids and Prenol lipi	Diterpenoids
pos_3462	Guaiazule	metab_25	Organic	α	Lipids and Prenol lipi	Sesquiterpenoids
pos_3478	3-Phenylp	metab_25	Organic	α	Benzenoic	Benzene α
pos_3553	12-oxo-PI	metab_26	Organic	α	Lipids and Fatty Acyl	Eicosanoids
pos_3578	9-Hydroxy	metab_26	Organic	α	Lipids and Prenol lipi	Sesquiterpenoids
pos_3587	LysoPE(20	metab_26	Organic	α	Lipids and Glyceroph	Glycerophosphoethanolamines
pos_3664	MG(PGD2	metab_27	Not Availa	Not Availa	Not Availa	Not Available
pos_3731	Dicycloper	metab_28	Organic	α	Hydrocarb	Polycyclic
pos_3773	F1alpha	metab_28	Organic	α	Organic o	Organoox
pos_3808	(S)-3-Hyd	metab_29	Organic	α	Lipids and Fatty Acyl	Fatty acyl thioesters
pos_3873	2-Methyl-	metab_29	Organic	α	Organic o	Organoox
pos_3929	Leukotrier	metab_30	Organic	α	Lipids and Fatty Acyl	Eicosanoids
pos_3994	2-Methyl-	metab_31	Organic	α	Organic o	Organoox
pos_4027	Cuminalde	metab_31	Organic	α	Lipids and Prenol lipi	Monoterpenoids
pos_4045	Gibberellir	metab_31	Organic	α	Lipids and Prenol lipi	Diterpenoids

pos_4048 Arlatin metab_31: Organic α Lipids and Prenol lipi: Terpene lactones

pos_4120 Chrysospl metab_32: Organic α Phenylpro Flavonoid: O-methylated flavonoids

pos_4167 Kainic acid metab_33: Organic α Organic α : Carboxylic Amino acids, peptides, and anal

pos_4233 Linalool 3, metab_33: Organic α Organic o: Organoox: Carbohydrates and carbohydrat

pos_4235 Isofraxidin metab_33: Organic α Phenylpro Coumarin: Hydroxycoumarins

pos_4306 17 α -E metab_34: Organic α Lipids and Steroids a: Estrane steroids

pos_4310 (7'R,8'R)-4 metab_34: Organic α Phenylpro 2-arylben: Not Available

pos_4311 Resolvin E metab_34: Organic α Lipids and Fatty Acyl: Eicosanoids

pos_4324 S-Lactoyl metab_34: Organic α Organic α : Carboxylic Amino acids, peptides, and anal

pos_4483 N'-Hydrox metab_36: Organic α Organohe Pyridines ϵ Pyrrolidinylpyridines

pos_4521 17-AAG metab_36: Organic α Phenylpro Macrolact: Not Available

pos_4601 Oryzalide metab_37: Organic α Lipids and Prenol lipi: Terpene lactones

pos_4667 Sterigmat metab_38: Organic α Phenylpro Sterigmat: Not Available

pos_4668 1-Naphth metab_38: Organic α Benzenoic Naphthale: Not Available

pos_4692 Dauricine metab_38: Organic α Organohe Isoquinolir: Benzylisoquinolines

pos_4703 Subaphylli metab_38: Organic α Phenylpro Cinnamic: Hydroxycinnamic acids and deri

pos_4713 2-Hydroxy metab_38: Organic α Organic o: Organoox: Carbonyl compounds

pos_4721 9-Oxo-no metab_39: Organic α Lipids and Fatty Acyl: Fatty acids and conjugates

pos_4831 Aucubin metab_40: Organic α Lipids and Prenol lipi: Terpene glycosides

pos_4882 Gynocardi metab_40: Organic α Organic o: Organoox: Carbohydrates and carbohydrat

pos_4976 Hydroxypr metab_41: Organic α Organic α : Carboxylic Amino acids, peptides, and anal

pos_501 Secologan metab_42: Organic α Lipids and Prenol lipi: Terpene glycosides

pos_5147 1-Ethyl-2- metab_43: Organic α Organohe Pyrrolidine: N-alkylpyrrolidines

pos_5188 Luteone 7 metab_44: Organic α Phenylpro Isoflavono: Isoflavonoid O-glycosides

pos_5200 Trigonellir metab_44: Organic α Alkaloids ϵ : Not Availa: Not Available

pos_53 Delta-12- metab_45: Organic α Lipids and Fatty Acyl: Eicosanoids

pos_59 6-beta-D- metab_48: Organic α Phenylpro Flavonoid: Flavonoid glycosides

pos_63 Estradiol 1 metab_48: Organic α Lipids and Steroids a: Sulfated steroids

pos_802 DG(20:5(7- metab_50: Not Availa: Not Availa: Not Availa: Not Available

pos_860 Androsta- metab_51: Organic α Lipids and Steroids a: Androstane steroids

pos_863 Tenuazoni metab_51: Organic α Organohe Pyrrolines: Not Available

pos_869 Indoxacarl metab_51: Organic α Benzenoic Benzene α Phenylcarbamic acid esters

pos_874 7 α -Hydrox metab_51: Organic α Lipids and Steroids a: Androstane steroids

pos_940 Pregnanet metab_51: Organic α Lipids and Steroids a: Steroidal glycosides

pos_995 5(6)-Epox metab_52: Organic α Lipids and Fatty Acyl: Eicosanoids

pos_301 Aspartic A metab_52: Organic α Organic α : Carboxylic Amino acids, peptides, and anal

neg_1040 Betonicine metab_53: Organic α Organic α : Carboxylic Amino acids, peptides, and anal

neg_1045 Succinic A metab_53: Organic α Organic α : Carboxylic Dicarboxylic acids and derivative

neg_1059 2-Aminoh metab_53: Organic α Organic α : Carboxylic Amino acids, peptides, and anal

neg_1068 3',4',5'-Tri metab_53: Organic α Phenylpro Flavonoid: Flavonoid glycosides

neg_1082 LL-2,6-Di metab_53: Organic α Organic α : Carboxylic Amino acids, peptides, and anal

neg_1138 8-Hydroxy metab_54: Organic α Organohe Imidazopy: Purines and purine derivatives

neg_1207 (R)-Pantot metab_55: Organic α Lipids and Fatty Acyl: Fatty acyl glycosides

neg_1341 Fleroxacin metab_56: Organic α Organic o: Organoox: Carbonyl compounds

neg_1353 5-Hydroxy metab_56: Organic α Benzenoic Phenols: Methoxyphenols

neg_1519 Prenyl glu metab_58: Organic α Lipids and Fatty Acyl: Fatty acyl glycosides

neg_1611 (S)-2-Acet metab_59: Organic α Organic α : Keto acids: Short-chain keto acids and deri

neg_1613 Fursultiam metab_59: Organic α Organohe Diazines: Pyrimidines and pyrimidine deri

neg_1677 Ethyl 7-ep metab_60: Organic α Lipids and Fatty Acyl: Fatty acyl glycosides

neg_1707 3'-(2''-Gal metab_60: Organic α Organic o: Organoox: Carbohydrates and carbohydrat

neg_1745 Scopoletir metab_61: Organic α Phenylpro Coumarin: Hydroxycoumarins

neg_1872 4-Hydroxy metab_62: Organic α Lipids and Fatty Acyl: Fatty alcohols

neg_1912 Undecane metab_62: Organic α Lipids and Fatty Acyl: Fatty acids and conjugates

neg_1977 Leurubicin metab_63: Organic α Phenylpro Anthracycl: Not Available

neg_2013 LysoPA(22 metab_63: Organic α Lipids and Glyceroph: Glycerophosphates

neg_2074 Capsiate metab_64: Organic α Benzenoic Phenols: Methoxyphenols

neg_2094 20-carbox metab_64: Organic α Lipids and Fatty Acyl: Fatty acids and conjugates

neg_2146 Apramycir metab_65: Organic α Organic o: Organoox: Carbohydrates and carbohydrat

neg_2162 3-Methoxy metab_65: Organic α Benzenoic Benzene a Benzoic acids and derivatives
 neg_2188 11beta,17l metab_65: Organic α Lipids and Steroids a Androstane steroids
 neg_2228 Testosterone metab_66: Organic α Lipids and Steroids a Sulfated steroids
 neg_2255 4-Androst metab_66: Organic α Lipids and Steroids a Androstane steroids
 neg_2271 MG(20:3(6 metab_66: Not Availa Not Availa Not Availa Not Available
 neg_228 (S)-2,3-Di metab_66: Organic α Organic o: Organoox Carbohydrates and carbohydrat
 neg_2280 9-Hydroxy metab_66: Organic α Lipids and Fatty Acyl: Lineolic acids and derivatives
 neg_2316 Ineketone metab_67: Organic α Lipids and Prenol lipi: Diterpenoids
 neg_2349 Pheophorl metab_67: Not Availa Not Availa Not Availa Not Available
 neg_2350 Enalapril metab_67: Organic α Organic a: Carboxylic Amino acids, peptides, and anal
 neg_2384 Soyasapor metab_67: Organic α Lipids and Prenol lipi: Terpene glycosides
 neg_2418 Ouabain metab_68: Organic α Lipids and Steroids a Steroid lactones
 neg_277 L-Hypogly metab_71: Organic α Organic a: Carboxylic Amino acids, peptides, and anal
 neg_300 Solerol metab_74: Organic α Organohe Lactones Not Available
 neg_3190 Triton X-1 metab_76: Organic α Benzenoic Benzene a Phenylpropanes
 neg_3219 15H-11,12 metab_76: Organic α Organic a: Hydroxy a Medium-chain hydroxy acids ar
 neg_3301 Prostaglar metab_77: Organic α Lipids and Fatty Acyl: Eicosanoids
 neg_3304 Nandrolor metab_77: Organic α Lipids and Steroids a Estrane steroids
 neg_3316 19-Oxote metab_77: Organic α Lipids and Steroids a Androstane steroids
 neg_3341 Octinoxate metab_77: Organic α Phenylpro Cinnamic : Cinnamic acid esters
 neg_3361 12S-HHT metab_78: Organic α Lipids and Fatty Acyl: Fatty acids and conjugates
 neg_3366 DG(20:5(7 metab_78: Not Availa Not Availa Not Availa Not Available
 neg_3386 Estriol metab_78: Organic α Lipids and Steroids a Estrane steroids
 neg_3399 11-Dehyd metab_78: Organic α Lipids and Fatty Acyl: Eicosanoids
 neg_3404 Ubiquinol metab_78: Organic α Lipids and Prenol lipi: Quinone and hydroquinone lipi
 neg_3451 Lysophosph metab_79: Organic α Lipids and Glyceroph Glycerophosphoinositols
 neg_3509 Cinnacasic metab_79: Organic α Lipids and Prenol lipi: Sesquiterpenoids
 neg_3511 (x)-2-Hep metab_79: Organic α Lipids and Fatty Acyl: Fatty acyl glycosides
 neg_3549 Cinnacasic metab_80: Organic α Lipids and Prenol lipi: Terpene lactones
 neg_3577 1-[2-Amir metab_80: Organic α Organohe Pyridines : Phenylpyridines
 neg_3591 1,5-Diphe metab_80: Organic α Benzenoic Benzene a Phenylhydrazines
 neg_3611 4-p-Coun metab_80: Organic α Organic o: Organoox Alcohols and polyols
 neg_3625 2-Decarbo metab_80: Organic α Organic o: Organoox Carbohydrates and carbohydrat
 neg_3678 Aromader metab_81: Organic α Phenylpro Flavonoid: Flavans
 neg_3680 Traumatic metab_81: Organic α Lipids and Fatty Acyl: Fatty acids and conjugates
 neg_3728 (2r)-1,1,1- metab_82: Organic α Organohe Diazinane: Piperazines
 neg_3836 3,3',4'-Tri metab_83: Organic α Phenylpro Flavonoid: Flavonoid glycosides
 neg_3872 Kanokosid metab_83: Organic α Organic o: Organoox Carbonyl compounds
 neg_3875 Kaempfer metab_83: Organic α Lignans, n Furanoid l Tetrahydrofuran lignans
 neg_3885 Sucrose 1' metab_83: Organic α Phenylpro Stilbenes Stilbene glycosides
 neg_3924 15-Hydro metab_84: Organic α Lipids and Steroids a Steroidal glycosides
 neg_4033 (ent-6alpl metab_85: Organic α Lipids and Prenol lipi: Diterpenoids
 neg_4060 Lofepami metab_85: Organic α Organohe Benzazepi Dibenzazepines
 neg_4120 N-Acetyl- metab_86: Organic α Organic a: Carboxylic Amino acids, peptides, and anal
 neg_4175 3,4-Methy metab_86: Organic α Organohe Benzodiox Not Available
 neg_4195 6-methylt metab_87: Organic α Organic o: Organoox Carbohydrates and carbohydrat
 neg_4198 2-dehydra metab_87: Organic α Organic a: Keto acids Short-chain keto acids and deri
 neg_4205 Trifluoroa metab_87: Organic α Organic a: Carboxylic Amino acids, peptides, and anal
 neg_423 5,7-Dihyd metab_87: Organic α Phenylpro Flavonoid: Flavonoid glycosides
 neg_4281 4-O-Meth metab_88: Organic α Organic o: Organoox Carbohydrates and carbohydrat
 neg_4340 Adipic acid metab_88: Organic α Lipids and Fatty Acyl: Fatty acids and conjugates
 neg_4411 Geniposid metab_89: Organic α Lipids and Prenol lipi: Terpene glycosides
 neg_4583 Asparagin metab_91: Organic α Organic a: Carboxylic Amino acids, peptides, and anal
 neg_4613 Tuliposide metab_91: Organic α Organic o: Organoox Carbohydrates and carbohydrat
 neg_4615 Lippioside metab_91: Organic α Lipids and Prenol lipi: Terpene glycosides
 neg_4658 Gamma-G metab_92: Organic α Organic a: Carboxylic Amino acids, peptides, and anal
 neg_4716 Phaseic ac metab_92: Organic α Lipids and Prenol lipi: Sesquiterpenoids
 neg_4752 1-(beta-D metab_93: Organic α Organic o: Organoox Carbohydrates and carbohydrat

neg_513 9-Hydroxy metab_97: Organic α Lipids and Fatty Acyl: Fatty alcohols
neg_5186 2-Amino- metab_97: Organic α Organic α: Carboxylic Amino acids, peptides, and anal
neg_579 Carbopros metab_99: Organic α Lipids and Fatty Acyl: Eicosanoids
neg_637 (4R,5S,7R, metab_10: Organic α Lipids and Prenol lipi: Terpene glycosides
neg_968 D-Digitox metab_10: Organic α Organic o: Organoox: Carbohydrates and carbohydrat
neg_4912 Isocitric Ac metab_10: Organic α Organic α: Carboxylic Tricarboxylic acids and derivativ
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ID	Metabolite	Metab ID	Kingdom	Superclass	Class	Subclass
pos_1063	Scoparin 2	metab_71	Organic α	Phenylpro	Flavonoid	Flavonoid glycosides
pos_1065	Cosmosiin	metab_73	Organic α	Phenylpro	Flavonoid	Flavonoid glycosides
pos_1071	Capsicum	metab_80	Organic α	Organoh	Tetrapyrro	Not Available
pos_1087	4,4'-Dihydro	metab_97	Organic α	Lignans, n	Furanoid I	Tetrahydrofuran lignans
pos_1088	(7'R)-(+)-l	metab_98	Organic α	Lignans, n	Lignan gly	Not Available
pos_109	Indoleacry	metab_10	Organic α	Organoh	Indoles an	Indoles
pos_1130	Chrysalo	metab_14	Organic α	Benzenoic	Anthracen	Not Available
pos_1137	3-O-Caffe	metab_15	Organic α	Benzenoic	Benzene a	Anilides
pos_128	6-O-Gall	metab_30	Organic α	Benzenoic	Benzene a	Benzoic acids and derivatives
pos_131	Neocnidol	metab_34	Organic α	Organoh	Isobenzof	Not Available
pos_142	PGB1	metab_46	Organic α	Lipids and Fatty Acyl	Eicosanoids	
pos_16	Blumealac	metab_65	Organic α	Lipids and Prenol lipi	Monoterpenoids	
pos_1630	N2-(gamma	metab_68	Organic α	Organic α	Carboxylic Amino acids, peptides, and anal	
pos_1708	3-Pyridine	metab_77	Organic α	Organoh	Pyridines	Not Available
pos_1724	Ser-Leu	metab_78	Organic α	Organic α	Carboxylic Amino acids, peptides, and anal	
pos_1725	Gibberellir	metab_78	Organic α	Lipids and Prenol lipi	Diterpenoids	
pos_1755	Diazoetha	metab_82	Organic α	Organic 1, Propargyl	Diazo compounds	
pos_1784	3-Methyl	metab_85	Organic α	Organoh	Indoles an	Indoles
pos_1817	Coniferin	metab_88	Organic α	Organic o	Organoox	Carbohydrates and carbohydrat
pos_1861	4-O-p-Cc	metab_93	Organic α	Organic o	Organoox	Alcohols and polyols
pos_1919	Genipin	metab_99	Organic α	Lipids and Prenol lipi	Monoterpenoids	
pos_1934	Trans-cinr	metab_10	Organic α	Phenylpro	Cinnamic	Cinnamic acid esters
pos_2010	1-Aminoc	metab_10	Organic α	Organic α	Carboxylic Amino acids, peptides, and anal	
pos_2020	Trans-Pice	metab_11	Organic α	Phenylpro	Stilbenes	Stilbene glycosides
pos_221	2-Phenyle	metab_13	Organic α	Organic o	Organoox	Carbohydrates and carbohydrat
pos_223	Rothindin	metab_13	Organic α	Phenylpro	Isoflavono	Isoflavonoid O-glycosides
pos_228	Trans-p-F	metab_13	Organic α	Phenylpro	Cinnamic	Hydroxycinnamic acids and deri
pos_233	Kaempfer	metab_14	Organic α	Phenylpro	Flavonoid	Flavonoid glycosides
pos_24	Dinotefur	metab_15	Organic α	Organic ni	Organonit	Guanidines
pos_2420	Methylcell	metab_15	Organic α	Organic o	Organoox	Carbohydrates and carbohydrat
pos_2527	FAHFA(16	metab_16	Organic α	Lipids and Fatty Acyl	Fatty acids and conjugates	
pos_2687	DG(18:3(6	metab_17	Organic α	Lipids and Fatty Acyl	Lineolic acids and derivatives	
pos_3039	2-Hydroxy	metab_21	Organic α	Lipids and Prenol lipi	Monoterpenoids	
pos_325	L-2-Amino	metab_23	Organic α	Organic α	Carboxylic Amino acids, peptides, and anal	
pos_3449	2-Quinolir	metab_25	Organic α	Organoh	Quinoline	Quinoline carboxylic acids
pos_3484	Tebucona	metab_26	Organic α	Benzenoic	Benzene a	Phenylbutylamines
pos_3500	6-Hydroxy	metab_26	Organic α	Lipids and Fatty Acyl	Fatty acids and conjugates	
pos_3560	Dehydroc	metab_26	Organic α	Lipids and Prenol lipi	Sesquiterpenoids	
pos_3653	Octadeca-	metab_27	Not Availa	Not Availa	Not Availa	Not Available
pos_3818	Desmethy	metab_29	Organic α	Organoh	Benzodiaz	1,4-benzodiazepines
pos_4120	Chrysospl	metab_32	Organic α	Phenylpro	Flavonoid	O-methylated flavonoids
pos_4130	Swertiajap	metab_32	Organic α	Phenylpro	Flavonoid	Flavonoid glycosides
pos_4131	Isovitexin	metab_32	Organic α	Lipids and Fatty Acyl	Fatty amides	
pos_4205	Hispidulos	metab_33	Organic α	Phenylpro	Flavonoid	Flavonoid glycosides
pos_4215	4-O,6-O-	metab_33	Organic α	Organoh	Pyranodio	Not Available
pos_4250	Coniferald	metab_34	Organic α	Benzenoic	Phenols	Methoxyphenols
pos_4284	Isoorientir	metab_34	Organic α	Phenylpro	Flavonoid	Flavonoid glycosides
pos_4327	13-Hydro	metab_34	Organic α	Lipids and Prenol lipi	Sesquiterpenoids	
pos_4333	Kaempfer	metab_34	Organic α	Phenylpro	Flavonoid	Flavonoid glycosides
pos_4337	Aminodex	metab_34	Organic α	Lipids and Fatty Acyl	Fatty acyl	glycosides

pos_4397 Vanilloyl g metab_35: Organic α Phenylpro Tannins Hydrolyzable tannins

pos_4405 Hypoglyci metab_35: Organic α Organic α Carboxylic Amino acids, peptides, and anal

pos_4426 N-succiny metab_35: Organic α Organic o: Organoox Carbohydrates and carbohydrat

pos_4476 7-Hydroxy metab_36: Organic α Organohe Benzopyr ϵ 1-benzopyrans

pos_4549 Gamma-G metab_37: Organic α Organic α Carboxylic Amino acids, peptides, and anal

pos_4585 Cefetamet metab_37: Organic α Organohe Lactams Beta lactams

pos_4667 Sterigmat metab_38: Organic α Phenylpro Sterigmat Not Available

pos_4668 1-Naphth metab_38: Organic α Benzenoic Naphthale Not Available

pos_4682 Fasoracet metab_38: Organic α Organic α Carboxylic Amino acids, peptides, and anal

pos_470 1,4-Ipome metab_38: Organic α Organohe Heteroar Not Available

pos_4713 2-Hydroxy metab_38: Organic α Organic o: Organoox Carbonyl compounds

pos_4721 9-Oxo-no metab_39: Organic α Lipids and Fatty Acyl: Fatty acids and conjugates

pos_4737 Glycyl-leu metab_39: Organic α Organic α Carboxylic Amino acids, peptides, and anal

pos_478 Isoorientir metab_39: Organic α Lignans, n Lignan gly Not Available

pos_481 7-Oxomat metab_40: Organic α Lignans, n Furanoid I Tetrahydrofuran lignans

pos_4882 Gynocardi metab_40: Organic α Organic o: Organoox Carbohydrates and carbohydrat

pos_5147 1-Ethyl-2- metab_43: Organic α Organohe Pyrrolidine N-alkylpyrrolidines

pos_5152 Pipecolic / metab_43: Organic α Organic α Carboxylic Amino acids, peptides, and anal

pos_53 Delta-12- metab_45: Organic α Lipids and Fatty Acyl: Eicosanoids

pos_5416 N-Methyl metab_46: Organic α Organic α Carboxylic Amino acids, peptides, and anal

pos_5452 Putrescine metab_46: Organic α Organic ni Organonit Amines

pos_57 Glycitin metab_47: Organic α Phenylpro Isoflavono Isoflavonoid O-glycosides

pos_59 6-beta-D- metab_48: Organic α Phenylpro Flavonoid: Flavonoid glycosides

pos_6 Neocarlin metab_48: Organic α Phenylpro Flavonoid: Flavonoid glycosides

pos_860 Androsta- metab_51: Organic α Lipids and Steroids α Androstane steroids

pos_863 Tenuazoni metab_51: Organic α Organohe Pyrrolines Not Available

pos_869 Indoxacarl metab_51: Organic α Benzenoic Benzene α Phenylcarbamic acid esters

pos_874 7a-Hydro metab_51: Organic α Lipids and Steroids α Androstane steroids

pos_888 Pentametl metab_51: Organic α Organohe Benzopyr ϵ 1-benzopyrans

pos_668 LysoPC(18 metab_52: Organic α Lipids and Glyceroph Glycerophosphocholines

neg_1019 L-Gulonol metab_53: Organic α Organohe Lactones Gamma butyrolactones

neg_1040 Betonicine metab_53: Organic α Organic α Carboxylic Amino acids, peptides, and anal

neg_1082 LL-2,6-Di metab_53: Organic α Organic α Carboxylic Amino acids, peptides, and anal

neg_1138 8-Hydroxy metab_54: Organic α Organohe Imidazopy Purines and purine derivatives

neg_1160 8-Epiloga metab_54: Organic α Lipids and Prenol lipi: Terpene glycosides

neg_1223 Gentiopicr metab_55: Organic α Organic o: Organoox Carbohydrates and carbohydrat

neg_1269 ALA-ILE metab_55: Organic α Organic α Carboxylic Amino acids, peptides, and anal

neg_1473 Feruloylqu metab_58: Organic α Organic o: Organoox Carbohydrates and carbohydrat

neg_1597 Diosbulbir metab_59: Organic α Lipids and Prenol lipi: Terpene glycosides

neg_1648 (2S,4S,6S)- metab_59: Organic α Phenylpro Diarylhept Linear diarylheptanoids

neg_1666 Secoisolar metab_60: Organic α Lignans, n Dibenzylb Dibenzylbutanediol lignans

neg_1698 2-(3-Hydr metab_60: Organic α Organic o: Organoox Carbohydrates and carbohydrat

neg_17 Shikimic a metab_60: Organic α Organic o: Organoox Alcohols and polyols

neg_1707 3'-(2''-Gal metab_60: Organic α Organic o: Organoox Carbohydrates and carbohydrat

neg_1742 Berberine metab_61: Organic α Alkaloids ϵ Protoberb Not Available

neg_1765 8-(2-Dietl metab_61: Organic α Organohe Quinolizin Not Available

neg_1771 Frangulosi metab_61: Organic α Benzenoic Anthracen Anthraquinones

neg_1863 Pratenol A metab_62: Organic α Organohe Benzopyr ϵ 1-benzopyrans

neg_2013 LysoPA(22 metab_63: Organic α Lipids and Glyceroph Glycerophosphates

neg_2014 2,4-Dinitr metab_63: Organic α Benzenoic Phenols Nitrophenols

neg_2074 Capsiate metab_64: Organic α Benzenoic Phenols Methoxyphenols

neg_2094 20-carbox metab_64: Organic α Lipids and Fatty Acyl: Fatty acids and conjugates

neg_2146 Apramycir metab_65: Organic α Organic o: Organoox Carbohydrates and carbohydrat

neg_2147 Perilloside metab_65: Organic α Lipids and Prenol lipi: Terpene glycosides

neg_2188 11beta,17l metab_65: Organic α Lipids and Steroids α Androstane steroids

neg_2228 Testosterc metab_66: Organic α Lipids and Steroids α Sulfated steroids

neg_2255 4-Androst metab_66: Organic α Lipids and Steroids α Androstane steroids

neg_2316 Ineketone metab_67: Organic α Lipids and Prenol lipi: Diterpenoids

neg_249 4-Hydroxy metab_68! Organic α Organic o; Organoox Carbohydrates and carbohydrat
 neg_3190 Triton X-1 metab_76! Organic α Benzenoic Benzene a Phenylpropanes
 neg_3219 15H-11,12 metab_76! Organic α Organic a; Hydroxy a Medium-chain hydroxy acids ar
 neg_3301 Prostaglar metab_77! Organic α Lipids and Fatty Acyl; Eicosanoids
 neg_3304 Nandrolor metab_77! Organic α Lipids and Steroids a; Estrane steroids
 neg_3316 19-Oxote; metab_77! Organic α Lipids and Steroids a; Androstane steroids
 neg_3317 19-Noran; metab_77! Organic α Lipids and Steroids a; Estrane steroids
 neg_3330 Pinometo; metab_77! Organic α Nucleosid; 5''-deoxyr Not Available
 neg_3341 Octinoxat; metab_77! Organic α Phenylpro Cinnamic ; Cinnamic acid esters
 neg_3366 DG(20:5(7; metab_78; Not Availa Not Availa Not Availa Not Available
 neg_3386 Estriol metab_78; Organic α Lipids and Steroids a; Estrane steroids
 neg_3399 11-Dehyd metab_78! Organic α Lipids and Fatty Acyl; Eicosanoids
 neg_3404 Ubiquinon metab_78! Organic α Lipids and Prenol lipi; Quinone and hydroquinone lipi
 neg_3419 [6]-Ginger metab_78! Organic α Benzenoic Phenols Methoxyphenols
 neg_3472 Fexaramin metab_79; Organic α Benzenoic Benzene a Biphenyls and derivatives
 neg_349 Kaempfer; metab_79; Organic α Phenylpro Flavonoid; Flavonoid glycosides
 neg_3509 Cinnassic metab_79! Organic α Lipids and Prenol lipi; Sesquiterpenoids
 neg_3549 Cinnassic metab_80! Organic α Lipids and Prenol lipi; Terpene lactones
 neg_3625 2-Decarb; metab_80! Organic α Organic o; Organoox Carbohydrates and carbohydrat
 neg_3684 Chlorazine metab_81! Organic α Organohe Benzothia; Phenothiazines
 neg_3895 Moracin P metab_83! Organic α Phenylpro 2-arylben; Not Available
 neg_3945 Etoposide metab_84; Organic α Organohe Diazines Pyrimidines and pyrimidine deri
 neg_3981 Cichoriosi; metab_84! Organic α Organic o; Organoox Carbohydrates and carbohydrat
 neg_4011 Luteolin-6 metab_85; Organic α Phenylpro Flavonoid; Flavonoid glycosides
 neg_4015 Eriojaposi; metab_85; Organic α Lipids and Fatty Acyl; Fatty acyl glycosides
 neg_4037 Sinapyl alc metab_85; Organic α Benzenoic Phenols Methoxyphenols
 neg_405 Isorhamne metab_85! Organic α Phenylpro Flavonoid; Flavonoid glycosides
 neg_4085 Parasorbic metab_85! Organic α Organohe Pyrans Pyranones and derivatives
 neg_4120 N-Acetyl- metab_86; Organic α Organic a; Carboxylic Amino acids, peptides, and anal
 neg_4121 Vicenin metab_86; Organic α Phenylpro Flavonoid; Flavonoid glycosides
 neg_4141 Paeoniflor metab_86! Organic α Lipids and Prenol lipi; Terpene glycosides
 neg_4165 MURABUT metab_86! Organic α Organic a; Carboxylic Amino acids, peptides, and anal
 neg_418 (10S,11R)- metab_86! Organic α Organic o; Organoox Carbohydrates and carbohydrat
 neg_4211 Kievitone metab_87; Organic α Phenylpro Isoflavono Isoflavans
 neg_423 5,7-Dihyd metab_87; Organic α Phenylpro Flavonoid; Flavonoid glycosides
 neg_4274 4-Hydroxy metab_87! Organic α Phenylpro Cinnamic ; Hydroxycinnamic acids and deri
 neg_4294 DIBOA di; metab_88; Organic α Organohe Benzoxazi Benzoxazinones
 neg_4296 Homovani metab_88; Organic α Benzenoic Phenols Methoxyphenols
 neg_4355 Pamapimc metab_88! Organic α Organic o; Organoox Ethers
 neg_4420 P-Toluene metab_89! Organic α Benzenoic Benzene a Benzenesulfonic acids and deriv
 neg_4490 Isoliquiritir metab_90; Organic α Phenylpro Flavonoid; Flavonoid glycosides
 neg_4507 5,6-Dihyd metab_90! Organic α Phenylpro Kavalactor Not Available
 neg_4516 Thr-Leu metab_90! Organic α Organic a; Carboxylic Amino acids, peptides, and anal
 neg_4583 Asparagin; metab_91; Organic α Organic a; Carboxylic Amino acids, peptides, and anal
 neg_4716 Phaseic ac metab_92! Organic α Lipids and Prenol lipi; Sesquiterpenoids
 neg_4752 1-(beta-D metab_93; Organic α Organic o; Organoox Carbohydrates and carbohydrat
 neg_5078 L-Histidin; metab_96! Organic α Organic a; Carboxylic Amino acids, peptides, and anal
 neg_5186 2-Amino- metab_97! Organic α Organic a; Carboxylic Amino acids, peptides, and anal
 neg_55 (+)-Lyonir metab_99; Organic α Lignans, n Lignan gly Not Available
 neg_626 Pinolidoxir metab_10! Organic α Organohe Oxocins Not Available
 neg_963 D-4-Hydr metab_10; Organic α Organic a; Keto acids Gamma-keto acids and derivati
 neg_4207 3-Methyl- metab_10; Organic α Organic a; Keto acids Short-chain keto acids and deri
 neg_4912 Isocitric Ac metab_10; Organic α Organic a; Carboxylic Tricarboxylic acids and derivativ
 neg_4073 Lamprant; metab_10; Organic α Phenylpro Flavonoid; Flavonoid glycosides

A3-A2

ID	Metabolite	Metab ID	Kingdom	Superclass	Class	Subclass
pos_1007	Thymyl ac	metab_10	Organic α	Lipids and Prenol lipi	Monoterpenoids	
pos_1028	3-Propylic	metab_32	Organic α	Organohe	Isocoumar	Isobenzofuranones

pos_1029 Icariside E metab_33 Organic α Phenylpro Stilbenes Stilbene glycosides
 pos_1087 4,4'-Dihydroxy metab_97 Organic α Lignans, n Furanoid I Tetrahydrofuran lignans
 pos_1137 3-O-Caffe metab_15 Organic α Benzenoid Benzene a Anilides
 pos_115 (3S,5R,6R,7S) metab_16 Organic α Lipids and Prenol lipi Sesquiterpenoids
 pos_1184 6-Hydroxy metab_20 Organic α Organohetero Indoles an Hydroxyindoles
 pos_1210 Indoleacet metab_23 Organic α Organohetero Indoles an Indoles
 pos_125 Ingenol metab_27 Organic α Lipids and Prenol lipi Diterpenoids
 pos_1306 Spermidin metab_33 Organic α Organic nitrogen Organonit Amines
 pos_141 7-Epi-12-metab_45 Organic α Lipids and Fatty Acyls Lineolic acids and derivatives
 pos_1428 Glycyl-Me metab_47 Organic α Organic ac Carboxylic Amino acids, peptides, and anal
 pos_152 3-Hydroxy metab_56 Organic α Lipids and Prenol lipi Sesterterpenoids
 pos_1520 Glycyl-Tyr metab_56 Organic α Organic ac Carboxylic Amino acids, peptides, and anal
 pos_160 DG(8:0/0) metab_65 Not Available Not Available Not Available Not Available
 pos_163 Mosinone metab_68 Organic α Lipids and Fatty Acyls Fatty alcohols
 pos_1708 3-Pyridine metab_77 Organic α Organohetero Pyridines ϵ Not Available
 pos_173 Norethind metab_79 Organic α Lipids and Steroids a Estrane steroids
 pos_1743 Panthenol metab_80 Organic α Lipids and Fatty Acyls Fatty amides
 pos_176 1-Lyso-2-metab_82 Organic α Lipids and Glyceroph Glycerophosphates
 pos_1834 Tyrosyl-Le metab_90 Organic α Organic ac Carboxylic Amino acids, peptides, and anal
 pos_1938 Netilmicin metab_10 Organic α Organic o; Organoox Carbohydrates and carbohydrat
 pos_1988 Metabolite metab_10 Organic α Benzenoid Indanes Not Available
 pos_1997 Minocyclir metab_10 Organic α Phenylpro Tetracyclir Not Available
 pos_2080 Dihydrocuc metab_11 Organic α Lipids and Prenol lipi Terpene lactones
 pos_2087 2-O-alpha-metab_11 Organic α Organic o; Organoox Carbohydrates and carbohydrat
 pos_211 7-Epijasmin metab_12 Organic α Lipids and Fatty Acyls Lineolic acids and derivatives
 pos_212 Trans-Jasr metab_12 Organic α Organic o; Organoox Carbonyl compounds
 pos_2201 Perilloside metab_13 Organic α Lipids and Prenol lipi Terpene glycosides
 pos_2216 Methionyl metab_13 Organic α Organic ac Carboxylic Amino acids, peptides, and anal
 pos_2234 Jasmonic ϵ metab_13 Organic α Lipids and Fatty Acyls Lineolic acids and derivatives
 pos_2236 (Z)-3-Met metab_13 Organic α Organic o; Organoox Carbonyl compounds
 pos_2268 Leukotriene metab_13 Organic α Organic ac Carboxylic Amino acids, peptides, and anal
 pos_2276 Concanam metab_13 Organic α Phenylpro Macrolide Not Available
 pos_2281 Cortolone metab_13 Organic α Lipids and Steroids a Steroidal glycosides
 pos_2288 Oxyglutinic metab_13 Organic α Organic o; Organoox Carbonyl compounds
 pos_233 Kaempferol metab_14 Organic α Phenylpro Flavonoid Flavonoid glycosides
 pos_234 Tuberose l metab_14 Organic α Organohetero Lactones Gamma butyrolactones
 pos_2420 Methylcell metab_15 Organic α Organic o; Organoox Carbohydrates and carbohydrat
 pos_2507 1-(9Z)-Nol metab_16 Organic α Lipids and Glyceroph Glycerophosphoethanolamines
 pos_2530 DG(16:0/0) metab_16 Not Available Not Available Not Available Not Available
 pos_2531 PS(22:5(4Z) metab_16 Organic α Lipids and Glyceroph Glycerophosphoserines
 pos_2560 DG(18:3(9Z) metab_16 Organic α Lipids and Fatty Acyls Lineolic acids and derivatives
 pos_2644 DG(16:1(9Z) metab_17 Organic α Lipids and Fatty Acyls Lineolic acids and derivatives
 pos_3058 DG(20:5(7Z) metab_21 Not Available Not Available Not Available Not Available
 pos_3060 DG(18:4(6Z) metab_21 Organic α Lipids and Fatty Acyls Lineolic acids and derivatives
 pos_3078 Cer(t18:0) metab_22 Not Available Not Available Not Available Not Available
 pos_3079 Squamoxil metab_22 Organic α Lipids and Fatty Acyls Fatty alcohols
 pos_3080 Glabranin metab_22 Organic α Lipids and Fatty Acyls Fatty alcohols
 pos_3092 Muconin metab_22 Organic α Lipids and Fatty Acyls Fatty alcohols
 pos_3140 Docosahe metabolite metab_22 Organic α Lipids and Fatty Acyls Fatty acids and conjugates
 pos_3142 DG(16:0/P) metab_22 Not Available Not Available Not Available Not Available
 pos_3184 Phoenicos metab_23 Organic α Lipids and Prenol lipi Tetraterpenoids
 pos_32 Pisumionin metab_23 Organic α Lipids and Prenol lipi Terpene glycosides
 pos_3261 DG(16:0/P) metab_23 Not Available Not Available Not Available Not Available
 pos_3266 Pachymic metab_23 Organic α Lipids and Prenol lipi Triterpenoids
 pos_3272 Barrington metab_23 Organic α Lipids and Prenol lipi Triterpenoids
 pos_3320 DG(22:4(7Z) metab_24 Organic α Lipids and Glycerolip Diradylglycerols
 pos_3380 DG(22:6(4Z) metab_25 Not Available Not Available Not Available Not Available
 pos_3387 Quinceoxal metab_25 Organic α Organic o; Organoox Ethers

pos_3449 2-Quinolir metab_25! Organic α Organohe Quinolines; Quinoline carboxylic acids
 pos_3484 Tebucona; metab_26! Organic α Benzenoic Benzene a Phenylbutylamines
 pos_3553 12-oxo-PI metab_26! Organic α Lipids and Fatty Acyl; Eicosanoids
 pos_3664 MG(PGD2; metab_27! Not Availa Not Availa Not Availa Not Available
 pos_3704 Gibberellir metab_28! Organic α Lipids and Prenol lipi; Diterpenoids
 pos_371 4-Hydroxy metab_28! Organic α Benzenoic Benzene a Not Available
 pos_3731 Dicyclopei metab_28! Organic α Hydrocarb; Polycyclic Not Available
 pos_3732 Tfllr-NH2 metab_28! Organic α Organic a; Carboxylic Amino acids, peptides, and anal
 pos_3796 2,6-Dimet metab_29! Organic α Benzenoic Naphthale Not Available
 pos_3808 (S)-3-Hyd metab_29! Organic α Lipids and Fatty Acyl; Fatty acyl thioesters
 pos_3873 2-Methyl- metab_29! Organic α Organic o; Organoox; Carbonyl compounds
 pos_3883 6'-Sialylla; metab_30! Organic α Organic o; Organoox; Carbohydrates and carbohydrat
 pos_3918 Glyceryl 5- metab_30! Organic α Lipids and Fatty Acyl; Fatty alcohols
 pos_3954 Kurarinon; metab_30! Organic α Phenylpro Flavonoid; Flavans
 pos_3961 3alpha-Hy metab_30! Organic α Organohe Naphthof; Not Available
 pos_3964 4,5-Dihyd metab_30! Organic α Organohe Benzoxepi Not Available
 pos_3994 2-Methyl- metab_31! Organic α Organic o; Organoox; Carbonyl compounds
 pos_4027 Cuminalde; metab_31! Organic α Lipids and Prenol lipi; Monoterpenoids
 pos_4045 Gibberellir metab_31! Organic α Lipids and Prenol lipi; Diterpenoids
 pos_4048 Arlatin metab_31! Organic α Lipids and Prenol lipi; Terpene lactones
 pos_4059 Loliolide metab_31! Organic α Organohe Benzofura Not Available
 pos_4094 Eugenol metab_32! Organic α Benzenoic Phenols Methoxyphenols
 pos_4115 Arginyl-G; metab_32! Organic α Organic a; Carboxylic Amino acids, peptides, and anal
 pos_4122 (1beta,2be metab_32! Organic α Lipids and Prenol lipi; Monoterpenoids
 pos_4147 Vomifoliol metab_32! Organic α Organic o; Organoox; Carbohydrates and carbohydrat
 pos_4167 Kainic acic metab_33! Organic α Organic a; Carboxylic Amino acids, peptides, and anal
 pos_4233 Linalool 3, metab_33! Organic α Organic o; Organoox; Carbohydrates and carbohydrat
 pos_4284 Isoorientir metab_34! Organic α Phenylpro Flavonoid; Flavonoid glycosides
 pos_4306 17alpha-E metab_34! Organic α Lipids and Steroids a; Estrane steroids
 pos_4311 Resolvin E metab_34! Organic α Lipids and Fatty Acyl; Eicosanoids
 pos_440 N-OCTAN metab_35! Organic α Organic a; Carboxylic Amino acids, peptides, and anal
 pos_4405 Hypoglyci; metab_35! Organic α Organic a; Carboxylic Amino acids, peptides, and anal
 pos_4440 Gardenosi metab_36! Organic α Lipids and Prenol lipi; Terpene glycosides
 pos_4445 Trans-Chl; metab_36! Organic α Organic o; Organoox; Alcohols and polyols
 pos_4483 N'-Hydro; metab_36! Organic α Organohe Pyridines ; Pyrrolidinylpyridines
 pos_4521 17-AAG metab_36! Organic α Phenylpro Macrolact; Not Available
 pos_4671 Butyl 4-an metab_38! Organic α Benzenoic Benzene a Benzoic acids and derivatives
 pos_4692 Dauricine metab_38! Organic α Organohe Isoquinolir Benzylisoquinolines
 pos_4703 Subaphylli metab_38! Organic α Phenylpro Cinnamic ; Hydroxycinnamic acids and deri
 pos_478 Isoorientir metab_39! Organic α Lignans, n Lignan gly Not Available
 pos_4976 Hydroxypr metab_41! Organic α Organic a; Carboxylic Amino acids, peptides, and anal
 pos_50 PERILLIC A metab_42! Organic α Lipids and Prenol lipi; Monoterpenoids
 pos_509 3,4-Dihyd metab_43! Organic α Benzenoic Phenols Benzenediols
 pos_515 Senkyunol metab_43! Organic α Organohe Isobenzof; Not Available
 pos_6 Neocarlin; metab_48! Organic α Phenylpro Flavonoid; Flavonoid glycosides
 pos_657 (6AR,10AR metab_48! Organic α Organohe Benzopyr; 1-benzopyrans
 pos_802 DG(20:5(7; metab_50! Not Availa Not Availa Not Availa Not Available
 pos_807 DG(9D3/9 metab_50! Organic α Lipids and Fatty Acyl; Fatty acids and conjugates
 pos_821 FAHFA(22; metab_50! Organic α Lipids and Fatty Acyl; Fatty acids and conjugates
 pos_863 Tenuazoni metab_51! Organic α Organohe Pyrrolines Not Available
 pos_869 Indoxacarl metab_51! Organic α Benzenoic Benzene a Phenylcarbamic acid esters
 pos_9 Linalool o; metab_51! Organic α Organic o; Organoox; Carbohydrates and carbohydrat
 pos_913 Phe-Phe-l metab_51! Organic α Organic a; Carboxylic Amino acids, peptides, and anal
 pos_940 Pregnanet metab_51! Organic α Lipids and Steroids a; Steroidal glycosides
 pos_961 Thymulin metab_52! Organic α Organic P; Polypeptic Not Available
 pos_966 Dihydroac metab_52! Organic α Organohe Benzofura Not Available
 pos_988 (Z)-3-Oxo metab_52! Organic α Organic o; Organoox; Carbonyl compounds
 pos_995 5(6)-Epox; metab_52! Organic α Lipids and Fatty Acyl; Eicosanoids

pos_996 Tributyrilc metab_52: Organic α Lipids and Fatty Acyl: Fatty alcohols

pos_301 Aspartic A metab_52: Organic α Organic α: Carboxylic Amino acids, peptides, and anal

pos_3590 Estradiol metab_52: Organic α Lipids and Steroids α Steroid esters

pos_1114 Lawsone metab_52: Organic α Benzenoic Naphthale Naphthoquinones

neg_1045 Succinic A metab_53: Organic α Organic α: Carboxylic Dicarboxylic acids and derivative

neg_1207 (R)-Pantot metab_55: Organic α Lipids and Fatty Acyl: Fatty acyl glycosides

neg_1461 Stachyosic metab_57: Organic α Lipids and Prenol lipi: Terpene glycosides

neg_1519 Prenyl glu metab_58: Organic α Lipids and Fatty Acyl: Fatty acyl glycosides

neg_1677 Ethyl 7-ep metab_60: Organic α Lipids and Fatty Acyl: Fatty acyl glycosides

neg_1759 Lysyltryptc metab_61: Organic α Organic α: Carboxylic Amino acids, peptides, and anal

neg_1797 3-beta-D- metab_61: Organic α Lipids and Glycerolip: Glycosylglycerols

neg_1872 4-Hydroxy metab_62: Organic α Lipids and Fatty Acyl: Fatty alcohols

neg_1912 Undecane metab_62: Organic α Lipids and Fatty Acyl: Fatty acids and conjugates

neg_1982 (1S,4S)-Di metab_63: Organic α Lipids and Prenol lipi: Monoterpenoids

neg_2003 Phaseolic metab_63: Organic α Organic α: Keto acids Medium-chain keto acids and d

neg_2049 Luteolin metab_64: Organic α Phenylpro Flavonoid: Flavones

neg_2129 Panaxytric metab_65: Organic α Lipids and Fatty Acyl: Fatty alcohols

neg_2189 DG(2:0/0:0 metab_65: Not Availa Not Availa Not Availa Not Available

neg_2271 MG(20:3(6 metab_66: Not Availa Not Availa Not Availa Not Available

neg_2280 9-Hydroxy metab_66: Organic α Lipids and Fatty Acyl: Lineolic acids and derivatives

neg_2350 Enalapril metab_67: Organic α Organic α: Carboxylic Amino acids, peptides, and anal

neg_2384 Soyasapor metab_67: Organic α Lipids and Prenol lipi: Terpene glycosides

neg_3046 PA(15:0/2:0 metab_74: Not Availa Not Availa Not Availa Not Available

neg_3190 Triton X-1 metab_76: Organic α Benzenoic Benzene α Phenylpropanes

neg_3361 12S-HHT metab_78: Organic α Lipids and Fatty Acyl: Fatty acids and conjugates

neg_3402 (3S)-3-hy metab_78: Organic α Organic o: Organoox Alcohols and polyols

neg_3419 [6]-Ginger metab_78: Organic α Benzenoic Phenols Methoxyphenols

neg_344 Linocinnar metab_78: Organic α Organic o: Organoox Carbohydrates and carbohydrat

neg_349 Kaempferc metab_79: Organic α Phenylpro Flavonoid: Flavonoid glycosides

neg_3491 Jasmolone metab_79: Organic α Organic o: Organoox Alcohols and polyols

neg_3511 (x)-2-Hep metab_79: Organic α Lipids and Fatty Acyl: Fatty acyl glycosides

neg_3577 1-[2-Amir metab_80: Organic α Organohe Pyridines α Phenylpyridines

neg_3591 1,5-Diphe metab_80: Organic α Benzenoic Benzene α Phenylhydrazines

neg_3680 Traumatic metab_81: Organic α Lipids and Fatty Acyl: Fatty acids and conjugates

neg_3687 3,5,5-Trim metab_81: Organic α Organic o: Organoox Carbonyl compounds

neg_3691 Arphamer metab_81: Organic α Organic α: Carboxylic Amino acids, peptides, and anal

neg_3747 Hexyl gluc metab_82: Organic α Lipids and Fatty Acyl: Fatty acyl glycosides

neg_3762 1-Methox metab_82: Organic α Benzenoic Benzene α Phenylpropanes

neg_3772 (+/-)-2-H metab_82: Organic α Lipids and Prenol lipi: Monoterpenoids

neg_3782 Polyethyle metab_82: Organic α Organic α: Keto acids Medium-chain keto acids and d

neg_3858 Exo,exo-1 metab_83: Organic α Organohe Oxanes Not Available

neg_3921 Mirificin metab_84: Organic α Lipids and Prenol lipi: Terpene glycosides

neg_3924 15-Hydro metab_84: Organic α Lipids and Steroids α Steroidal glycosides

neg_3945 Etoposide metab_84: Organic α Organohe Diazines Pyrimidines and pyrimidine deri

neg_4011 Luteolin-6 metab_85: Organic α Phenylpro Flavonoid: Flavonoid glycosides

neg_4033 (ent-6alpl metab_85: Organic α Lipids and Prenol lipi: Diterpenoids

neg_4060 Lofepami metab_85: Organic α Organohe Benzazepi Dibenzazepines

neg_4121 Vicenin metab_86: Organic α Phenylpro Flavonoid: Flavonoid glycosides

neg_4202 Esculetin metab_87: Organic α Phenylpro Coumarin: Hydroxycoumarins

neg_4281 4-O-Meth metab_88: Organic α Organic o: Organoox Carbohydrates and carbohydrat

neg_4411 Geniposid metab_89: Organic α Lipids and Prenol lipi: Terpene glycosides

neg_4420 P-Toluene metab_89: Organic α Benzenoic Benzene α Benzenesulfonic acids and deriv

neg_4628 Isoglobotr metab_91: Organic α Lipids and Fatty Acyl: Fatty acyl glycosides

neg_4700 (S)-alpha- metab_92: Organic α Organic o: Organoox Carbohydrates and carbohydrat

neg_4928 2'-Fluorot metab_95: Organic α Nucleosid: Pyrimidine Pyrimidine 2"-deoxyribonucleos

neg_498 2-Hydroxy metab_95: Organic α Lipids and Fatty Acyl: Fatty alcohols

neg_5 5-Heptylt metab_95: Organic α Organohe Lactones Gamma butyrolactones

neg_513 9-Hydroxy metab_97: Organic α Lipids and Fatty Acyl: Fatty alcohols

neg_579 Carboprost metab_99 Organic c Lipids and Fatty Acyls Eicosanoids
neg_637 (4R,5S,7R, metab_10 Organic c Lipids and Prenol lipi Terpene glycosides

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