

Supplementary data

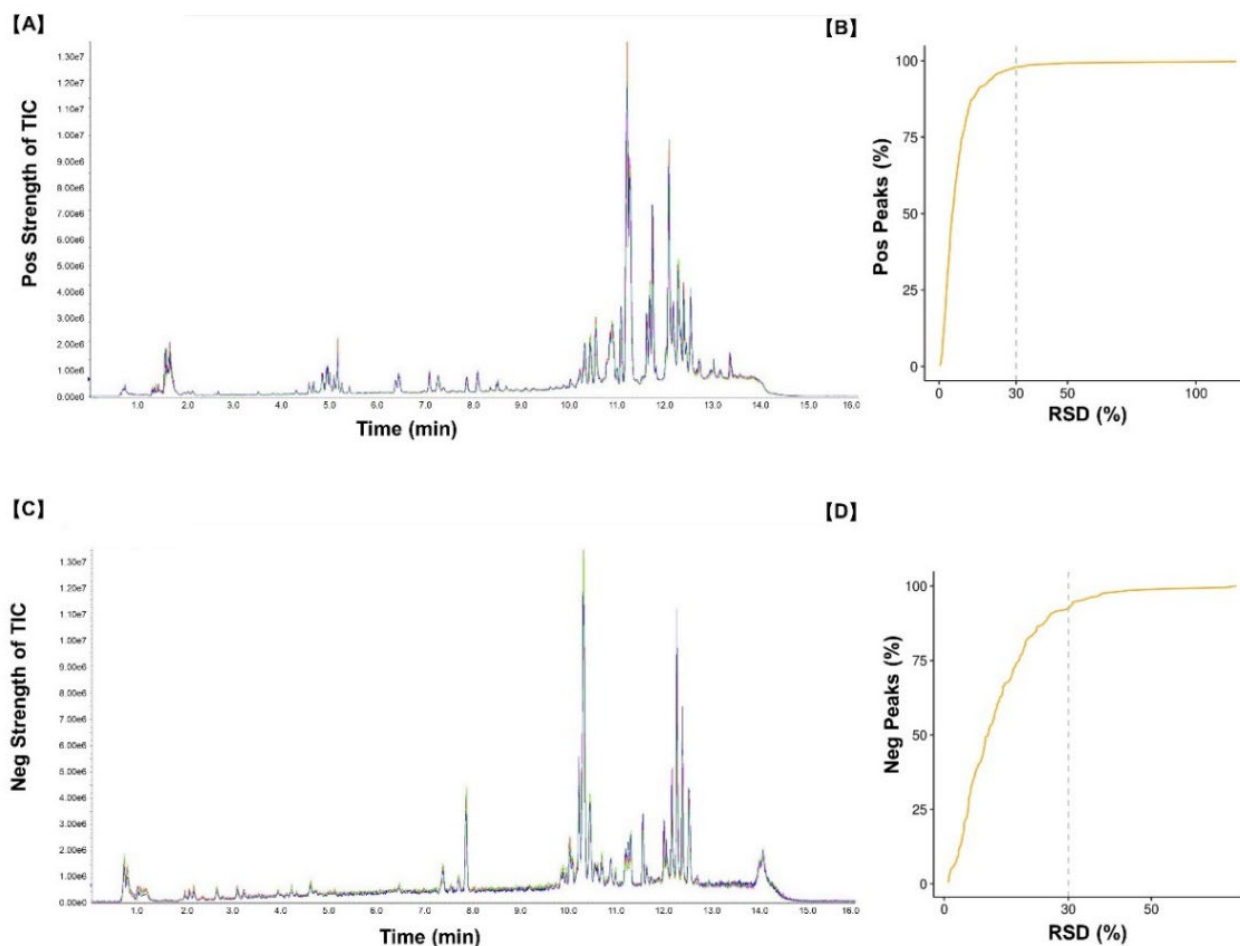


Figure S1. Data quality evaluation of instrument of QC. [A] Positive and [C] Negative sample total ion current (TIC) of QC. [B] Positive and [D] Negative sample relative standard deviation (RSD) of QC.

Table S1. Identified metabolites (624 metabolites were identified in total)

	ID	Name	Superclass
1	POS_5857	10-Hydroxycamptothecin	Alkaloids and derivatives
2	POS_7446	[1,14-Dihydroxy-8-(hydroxymethyl)-4,12,12,15-tetramethyl-5-oxo-13-tetracyclo[8.5.0.02,6.011,13]pentadeca-3,8-dienyl] acetate	Lipids and lipid-like molecules
3	POS_3991	11-(Phenylcarbonyl)-7,11-diazatricyclo[7.3.1.0<2,7>]trideca-2,4-dien-6-one	Organoheterocyclic compounds
4	POS_5143	12,19,20-Trihydroxy-14-methylenegeranylnerol	Undefined

5	POS_1389	1-(2-Chlorophenyl)piperazine	Organoheterocyclic compounds
6	POS_12445	1,2-Dipalmitoylphosphatidylcholine	Lipids and lipid-like molecules
7	POS_4493	(12Z)-9,10-Dihydroxyoctadec-12-enoic acid	Lipids and lipid-like molecules
8	POS_6662	[1,3-Dihydroxy-1-(7-methoxy-2-oxochromen-6-yl)-3-methylbutan-2-yl] (E)-2-methylbut-2-enoate	Phenylpropanoids and polyketides
9	POS_1641	1,3-Diphenylguanidine	Benzenoids
10	POS_7382	13'-Hydroxy-alpha-tocopherol	Undefined
11	POS_253	1,4-Cyclohexanedione	Organic oxygen compounds
12	POS_5482	1-(4-Hydroxyphenyl)-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxypropan-1-one	Lipids and lipid-like molecules
13	POS_2965	1,9-Heptadecadiene-4,6-diyne-3,8-diol	Lipids and lipid-like molecules
14	POS_1012	1-(Aminomethyl)cyclohexaneacetate	Organic acids and derivatives
15	POS_1481	1-Decanamine, N,N-dimethyl-, N-oxide	Organic nitrogen compounds
16	POS_9130	1-Heptadecanoyl-sn-glycero-3-phosphocholine	Lipids and lipid-like molecules
17	POS_7980	1-Hexadecanoyl-sn-glycero-3-phosphoethanolamine	Lipids and lipid-like molecules
18	POS_497	1-Methylnicotinamide	Organoheterocyclic compounds
19	POS_569	1-Naphthylamine	Benzenoids
20	POS_12045	1-O-[(2alpha,3beta,5xi,6beta,9xi,18xi,19alpha)-2,3,6,19,23-pentahydroxy-28-oxoolean-12-en-28-yl]-beta-D-glucopyranose	Lipids and lipid-like molecules
21	POS_9572	1-O-linoleoyl-3-O-beta-D-galactopyranosyl-syn-glycerol	Undefined
22	POS_8592	1-Pentadecanoyl-sn-glycero-3-phosphocholine	Lipids and lipid-like molecules
23	POS_8329	[(1S,5R)-6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl]methyl 6-O-alpha-L-arabinopyranosyl-beta-D-glucopyranoside	Lipids and lipid-like molecules
24	POS_9395	1-Stearoyl-sn-glycero-3-phosphocholine	Lipids and lipid-like molecules
25	POS_4597	1-(Tert-butylamino)-3-{[4-(morpholin-4-yl)-1,2,5-thiadiazol-3-yl]oxy}propan-2-ol	Organic nitrogen compounds
26	POS_2907	1-Tetradecanamine, N,N-dimethyl-, N-oxide	Organic nitrogen compounds
27	POS_750	2,2,6,6-Tetramethyl-4-piperidone	Organoheterocyclic compounds
28	POS_888	2-(2-Butoxyethoxy)ethanol	Organic oxygen compounds
29	POS_3041	2',2'-Difluorodeoxyuridine	Nucleosides, nucleotides, and analogues
30	POS_589	2,2-Dimethylsuccinic acid	Lipids and lipid-like molecules
31	POS_7702	22-Hydroxy-6-hopanone	Lipids and lipid-like molecules
32	POS_9539	2-[(2R,4As,8S,8aS)-8-[2-[(4aS,7R,8aR)-7-(1-carboxyethenyl)-1-hydroxy-4a-methyl-2-oxo-6,7,8,8a-tetrahydro-5H-naphthalen-1-yl]ethyl]-4a-methyl-7-oxo-1,2,3,4,8,8a-hexahydronaphthalen-2-yl]prop-2-enoic acid	Lipids and lipid-like molecules
33	POS_8328	2-[[3,4-Dihydroxy-4-(hydroxymethyl)oxolan-2-	Lipids and lipid-like molecules

		yl]oxymethyl]-6-[(6,6-dimethyl-4-bicyclo[3.1.1]hept-3-enyl)methoxy]oxane-3,4,5-triol	
34	POS_6719	[2,3-Dihydroxy-1-(7-methoxy-2-oxochromen-6-yl)-3-methylbutyl] 3-methylbutanoate	Phenylpropanoids and polyketides
35	POS_3731	2,3-Dihydroxypropyl tetradecanoate	Lipids and lipid-like molecules
36	POS_4501	2,4-Dihydroxyheptadecyl acetate	Lipids and lipid-like molecules
37	POS_5481	2',5,6-Trimethoxyflavone	Phenylpropanoids and polyketides
38	POS_5547	(2,6,6-Trimethyl-4-oxo-2-cyclohexen-1-yl)methyl beta-D-glucopyranoside	Organic oxygen compounds
39	POS_3110	2-(6-Aminopurin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol	Nucleosides, nucleotides, and analogues
40	POS_322	2,6-Dimethylaniline	Benzenoids
41	POS_1562	2,6-DI-Tert-butylphenol	Benzenoids
42	POS_7250	2-{[6-O-(6-Deoxy-alpha-L-mannopyranosyl)-beta-D-glucopyranosyl]oxy}-3-methylbutanenitrile	Organic oxygen compounds
43	POS_6966	2-Acetoxy-4-pentadecylbenzoic acid	Benzenoids
44	POS_4632	2-Aminooctadecane-1,3,4-triol	Organic nitrogen compounds
45	POS_2013	2'-Deoxycytidine	Nucleosides, nucleotides, and analogues
46	POS_4681	[2-[(E)-3,4-Dihydroxypent-1-enyl]-6-oxooxan-3-yl] (E)-2-methylbut-2-enoate	Organoheterocyclic compounds
47	POS_2728	(2E,4E)-N-(2-Methylpropyl)dodeca-2,4-dienamide	Lipids and lipid-like molecules
48	POS_9758	2-(Hydroxymethyl)-6-[5-[3-(hydroxymethyl)-5-(3-hydroxypropyl)-7-methoxy-2,3-dihydro-1-benzofuran-2-yl]-2-methoxyphenoxy]oxane-3,4,5-triol	Phenylpropanoids and polyketides
49	POS_5609	2-(Hydroxymethyl)-6-(6-hydroxy-6-methyl-3-propan-2-ylcyclohex-3-en-1-yl)oxyoxane-3,4,5-triol	Lipids and lipid-like molecules
50	POS_5832	2-Methoxy-4-pentadecylbenzoic acid	Benzenoids
51	POS_10280	2-Methoxy-4-[tetrahydro-3a,6a-dihydroxy-4-(4-hydroxy-3-methoxyphenyl)-1H,3H-furo[3,4-c]furan-1-yl]phenyl-beta-D-glucopyranoside	Lignans, neolignans and related compounds
52	POS_4207	2-Monomyristin	Lipids and lipid-like molecules
53	POS_4978	2-Palmitoylglycerol	Lipids and lipid-like molecules
54	POS_1791	2-Phenyl-2-piperidin-1-ium-2-ylacetate	Organic nitrogen compounds
55	POS_486	2-Phenylacetamide	Benzenoids
56	POS_2893	2-(((R)-2,3-Dihydroxypropyl)phosphoryloxy)-N,N,N-trimethylethanaminium	Lipids and lipid-like molecules
57	POS_12640	(2R,3S,4R,5R,8R,10R,11R,13S,14R)-11-[(2S,3R,4S,6R)-4-(Dimethylamino)-3-hydroxy-6-	Organic oxygen compounds

		methyloxan-2-yl]oxy-2-ethyl-3,4,10-trihydroxy-13-[(2R,4R,5S,6S)-5-hydroxy-4-methoxy-4,6-dimethyloxan-2-yl]oxy-3,5,6,8,10,12,14-heptamethyl-1-oxa-6-azacyclopentadecan-15-one	
58	POS_8605	(2R,3S,4S,5R,6R)-2-[[[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxymethyl]-6-[4-(4-hydroxyphenyl)butan-2-yloxy]oxane-3,4,5-triol	Lipids and lipid-like molecules
59	POS_5608	(2R,3S,4S,5R,6S)-2-(hydroxymethyl)-6-[4-(hydroxymethyl)-1-propan-2-ylcyclohex-3-en-1-yl]oxyoxane-3,4,5-triol	Lipids and lipid-like molecules
60	POS_5511	(2R,3S,5R)-2-[6-[[[(1S,2S)-2-Hydroxycyclopentyl]amino]-9-purinyl]-5-(hydroxymethyl)oxolane-3,4-diol	Nucleosides, nucleotides, and analogues
61	POS_4193	3,3',4',5,5',7-Hexahydroxyflavylium	Phenylpropanoids and polyketides
62	POS_3892	3-(3,4-Dimethoxyphenyl)-2-methyl-6-methylaminohexane-3-carbonitrile	Benzenoids
63	POS_6065	3,4-Dihydro-6,8-dihydroxy-3-(10-hydroxyundecyl)isocoumarin	Benzenoids
64	POS_5544	3-(4-Hydroxyphenyl)propanoic acid 3-(4-hydroxy-3-methoxyphenyl)propyl ester	Benzenoids
65	POS_6617	3,5,5-Trimethyl-4-[3-[(beta-D-glucopyranosyl)oxy]butyl]-3-cyclohexen-1-ol	Lipids and lipid-like molecules
66	POS_7129	3-[5,7-Dihydroxy-4-(4-hydroxyphenyl)-2-oxo-3,4-dihydrochromen-3-yl]-5,6,7,8-tetrahydroxy-4-(4-hydroxyphenyl)-3,4-dihydrochromen-2-one	Phenylpropanoids and polyketides
67	POS_3880	3,6-Diphenylcyclohexan-1,2-diol	Organic oxygen compounds
68	POS_10263	3-{7-[5-(1-hydroxyhenicosa-4,8-dien-1-yl)oxolan-2-yl]heptyl}-5-methyl-5H-furan-2-one	
69	POS_6670	3-[(Acetyloxy)methyl]-5-[(1R,4aR,8aR)-decahydro-5,5,8a-trimethyl-2-methylene-1-naphthalenyl]-, methyl ester, (2Z)-2-pentenoic acid	Lipids and lipid-like molecules
70	POS_3958	3alpha,17beta-Dihydroxy-5alpha-androstane	Lipids and lipid-like molecules
71	POS_9584	3-Deoxo-3-beta-Acetoxydeoxydihydrogedunin	Organoheterocyclic compounds
72	POS_8182	3-Ethyl-4-hydroxy-4-methylpentyl 6-O-[(2S,3R,4R)-tetrahydro-3,4-dihydroxy-4-(hydroxymethyl)-2-furanyl]-beta-D-glucopyranoside	Lipids and lipid-like molecules
73	POS_7995	[3-Hydroxy-1-(4-methoxy-7-oxofuro[3,2-g]chromen-9-yl)oxy-3-methylbutan-2-yl] (E)-2-methylbut-2-enoate	Phenylpropanoids and polyketides
74	POS_8225	3-Hydroxy-3-(hydroxymethyl)-4-methylpentyl 6-O-[(2S,3R,4R)-3,4-dihydroxy-4-	Lipids and lipid-like molecules

		(hydroxymethyl)tetrahydro-2-furanyl]-beta-D-glucopyranoside	
75	POS_1125	3-Methoxycinnamic acid	Phenylpropanoids and polyketides
76	POS_5367	3-(Toluene-4-sulfonyl)-1,2,3,4,5,6-hexahydro-1,5-methano-pyrido[1,2-a][1,5]diazocin-8-one	Alkaloids and derivatives
77	POS_6864	4-(1,3-Benzodioxol-5-ylmethyl)-3-[(3,4-dimethoxyphenyl)methyl]oxolan-2-one	Lignans, neolignans and related compounds
78	POS_7520	4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxypentan-2-yl (E)-3-(4-hydroxyphenyl)prop-2-enoate	Lipids and lipid-like molecules
79	POS_6922	4-[3-(Beta-D-glucopyranosyloxy)-4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl]-2-butanone	Lipids and lipid-like molecules
80	POS_9406	4,4,8,10,14-Pentamethyl-17-(4,5,6-trihydroxy-6-methylheptan-2-yl)-2,5,6,7,9,15-hexahydro-1H-cyclopenta[a]phenanthrene-3,16-dione	Lipids and lipid-like molecules
81	POS_8517	4-[5-[[4-[5-[Acetyl(hydroxy)amino]pentylamino]-4-oxobutanoyl]-hydroxyamino]pentylamino]-4-oxobutanoic acid	Lipids and lipid-like molecules
82	POS_5620	[4,6-diethyl-6-(4-ethyl-2-methyloctyl)-3H-1,2-dioxin-3-yl]acetic acid	Undefined
83	POS_602	4-Acetamidobutyric acid	Organic acids and derivatives
84	POS_4200	4-[Formyl(6-methoxyquinolin-8-yl)amino]pentanoic acid	Organoheterocyclic compounds
85	POS_1479	4-Hydroxy-1-(2-hydroxyethyl)-2,2,6,6-tetramethylpiperidine	Organoheterocyclic compounds
86	POS_1880	4-Hydroxybenzoylcholine	Benzenoids
87	POS_7889	4'-Methoxyflavone	Phenylpropanoids and polyketides
88	POS_8403	4''-Methylepigallocatechin gallate	Phenylpropanoids and polyketides
89	POS_7996	5-(1-benzofuran-2-yl)-N,N-dimethyl-2-[4-(piperazin-1-yl)phenyl]-1,3-thiazole-4-carboxamide	Organoheterocyclic compounds
90	POS_5008	5-[(1S,4aS,8aS)-Decahydro-5,5,8a-trimethyl-2-methylene-1-naphthalenyl]-3-methyl-, (2E)-2-penten-1-ol	Lipids and lipid-like molecules
91	POS_2303	5-Cyclohexadecen-1-one	Organic oxygen compounds
92	POS_4067	5'-Deoxy-5'-methylthioadenosine	Nucleosides, nucleotides, and analogues
93	POS_3022	5-dodecyl-4-hydroxy-4-methylcyclopent-2-en-1-one	Undefined
94	POS_8079	5-Hydroxy-7-[4-hydroxy-2-methoxy-3-(3-methylbut-2-enyl)phenyl]-2,2-dimethyl-7,8-dihydropyrano[3,2-g]chromen-6-one	Phenylpropanoids and polyketides
95	POS_3082	5-Methyl-7-methoxyisoflavone	Undefined
96	POS_2892	5-Methylcytidine	Nucleosides, nucleotides, and analogues

97	POS_7037	6-[3-[(3,4-Dimethoxyphenyl)methyl]-4-methoxy-2-(methoxymethyl)butyl]-4-methoxy-1,3-benzodioxole	Lignans, neolignans and related compounds
98	POS_6634	6-{9a,11a-dimethyl-1H,2H,3H,3aH,3bH,4H,8H,9H,9bH,10H,11H-cyclopenta[a]phenanthren-1-yl}-3-ethyl-2-methylheptane	Undefined
99	POS_7321	(6beta,22E)-6-Hydroxystigmasta-4,22-dien-3-one	Undefined
100	POS_7948	6-(beta-D-Glucopyranosyloxy)-4,5,6,7,8,8a-hexahydro-5-hydroxy-5-(1-hydroxy-1-methylethyl)-3,8-dimethyl-2(1H)-azulenone	Lipids and lipid-like molecules
101	POS_2791	7,2'-Dihydroxyflavone	Phenylpropanoids and polyketides
102	POS_7213	7alpha-Hydroxy-4-cholesten-3-one	Lipids and lipid-like molecules
103	POS_5859	(7E,13E)-9,15-Dihydroxy-4,10,16-trimethyl-1,5,11-trioxacyclohexadeca-7,13-diene-2,6,12-trione	Phenylpropanoids and polyketides
104	POS_2957	7-Hydroxyflavone	Phenylpropanoids and polyketides
105	POS_6730	7-Ketocholesterol	Lipids and lipid-like molecules
106	POS_7240	8-(2,3-Dihydroxy-3-methylbutyl)-5,7-dimethoxy-2-phenyl-2,3-dihydrochromen-4-one	Phenylpropanoids and polyketides
107	POS_4602	8-(2,6-Diethyl-4-methylphenyl)tetrahydropyrazolo(1,2-d)(1,4,5)oxadiazepine-7,9-dione	Benzenoids
108	POS_6666	8-Hydroxy-2,7,7,11,15-pentamethyl-5,12,16-trioxapentacyclo[9.8.0.0(2),.0,.0(1)(3),(1)]nonadec-13(18)-ene-3,17-dione	Organoheterocyclic compounds
109	POS_5141	8-Hydroxy-9,10-epoxystearic acid	Lipids and lipid-like molecules
110	POS_5250	8-Prenylnaringenin	Phenylpropanoids and polyketides
111	POS_4008	9-Oxo-octadeca-10,12-dienoic acid	Lipids and lipid-like molecules
112	POS_693	Acenaphthylene	Benzenoids
113	POS_1503	Acetyl-d-carnitine	Lipids and lipid-like molecules
114	POS_7309	Acetyl-Leu-Leu-Arg-al	Organic acids and derivatives
115	POS_1378	Acridinone	Organoheterocyclic compounds
116	POS_1490	Ala-Ile	Organic acids and derivatives
117	POS_9192	Alisol A	Lipids and lipid-like molecules
118	POS_10542	Alkergot	Alkaloids and derivatives
119	POS_9903	(all-E)-beta-Cryptoxanthin	Lipids and lipid-like molecules
120	POS_489	Allopurinol	Organoheterocyclic compounds
121	POS_3244	alpha-Naphthoflavone	Phenylpropanoids and polyketides
122	POS_7997	Amethopterin	Organoheterocyclic compounds
123	POS_3055	Ammothamnine	Undefined
124	POS_5549	Anileridine	Organoheterocyclic compounds
125	POS_120	Aniline	Benzenoids

126	POS_10472	Anthranoyllycoctonine	Lipids and lipid-like molecules
127	POS_1081	Arginine	Organic acids and derivatives
128	POS_8346	Aspergamid B	Organoheterocyclic compounds
129	POS_8361	Astragalin	Phenylpropanoids and polyketides
130	POS_12340	Atazanavir	Organic acids and derivatives
131	POS_4423	Avocadene 2-acetate	Lipids and lipid-like molecules
132	POS_4479	Benzyl butyl phthalate	Benzenoids
133	POS_3926	Benzylidiphenylphosphine oxide	Benzenoids
134	POS_7324	beta-Amyrin	Lipids and lipid-like molecules
135	POS_285	Betaine	Organic acids and derivatives
136	POS_7416	Bidwillon A	Phenylpropanoids and polyketides
137	POS_2054	Bisphenol A	Benzenoids
138	POS_6563	Brucine	Alkaloids and derivatives
139	POS_8906	Bryodulcosigenin	Lipids and lipid-like molecules
140	POS_6876	Bufalin	Lipids and lipid-like molecules
141	POS_5356	Bullatine A	Undefined
142	POS_3846	Bupivacaine	Organic acids and derivatives
143	POS_1154	Caffeic acid	Phenylpropanoids and polyketides
144	POS_1344	Caffeine	Organoheterocyclic compounds
145	POS_5451	Camptothecin	Alkaloids and derivatives
146	POS_1298	Carbendazim	Organic acids and derivatives
147	POS_7684	(-)-Catechin gallate	Phenylpropanoids and polyketides
148	POS_9366	Catechin pentaacetate	Phenylpropanoids and polyketides
149	POS_9578	Cer 34:3;2O Cer 18:2;2O/16:1	Undefined
150	POS_9470	Chaetoglobosin C	Alkaloids and derivatives
151	POS_13838	Chlorophyll b from Chlorella	Organoheterocyclic compounds
152	POS_6319	Cholest-4,6-Dien-3-One	Lipids and lipid-like molecules
153	POS_6875	Cholic acid	Lipids and lipid-like molecules
154	POS_180	Choline	Organic nitrogen compounds
155	POS_4298	Cimifugin	Organoheterocyclic compounds
156	POS_5127	Cirsimaritin	Phenylpropanoids and polyketides
157	POS_4132	Clobazam	Organoheterocyclic compounds
158	POS_4861	Clozapine	Organic oxygen compounds
159	POS_399	Coniine	Alkaloids and derivatives
160	POS_2720	Cordycepin	Nucleosides, nucleotides, and analogues
161	POS_3685	Crotonoside	Nucleosides, nucleotides, and analogues
162	POS_9664	Cucurbitacin D	Lipids and lipid-like molecules
163	POS_7831	Cyanidin-3-O-glucoside chloride	Undefined
164	POS_4955	Cyclic AMP	Nucleosides, nucleotides, and analogues
165	POS_729	Cyclo-prolylglycine	Organic acids and derivatives
166	POS_6516	Cylindrol B	Organic oxygen compounds
167	POS_7830	Cynaroside	Undefined
168	POS_1926	Cyprodinil	Benzenoids

169	POS_2531	Cytidine	Nucleosides, nucleotides, and analogues
170	POS_8575	Decaethylene glycol	Organic oxygen compounds
171	POS_1249	Deethylatrazine	Organoheterocyclic compounds
172	POS_4172	Dehydroevodiamine	Organoheterocyclic compounds
173	POS_4705	Dehydrohistidyltryptophyldiketopiperazine	Organic acids and derivatives
174	POS_10444	Dehydroxynocardamine	Phenylpropanoids and polyketides
175	POS_4555	delta9-Tetrahydrocannabinol	Organoheterocyclic compounds
176	POS_11202	Demethoxycentaureidin 7-O-rutinoside	Phenylpropanoids and polyketides
177	POS_10560	Deoxykhivorin	Organoheterocyclic compounds
178	POS_1556	Dexibuprofen	Phenylpropanoids and polyketides
179	POS_10676	DG(18:2(9Z,12Z)/18:2(9Z,12Z))	Undefined
180	POS_11129	DG 36:5 DG 18:2_18:3	Undefined
181	POS_11104	DG 36:6 DG 18:3_18:3	Undefined
182	POS_1155	D(+)-Glucose	Organic oxygen compounds
183	POS_3424	Dibutyl phthalate	Benzenoids
184	POS_1178	Dicyclohexylamine	Organic nitrogen compounds
185	POS_1853	Diethyl phthalate	Benzenoids
186	POS_1315	Diethyltoluamide	Benzenoids
187	POS_940	Dihydrojasnone	Undefined
188	POS_4489	Dihydroxyoctadecadienoic acid	Lipids and lipid-like molecules
189	POS_2481	Diocetylamine	Organic nitrogen compounds
190	POS_6477	Diocetyl phthalate	Benzenoids
191	POS_11105	Diosmetin-7-O-rutinoside	Phenylpropanoids and polyketides
192	POS_2680	Diphenyl phosphate	Organic acids and derivatives
193	POS_4039	Disulfiram	Organic nitrogen compounds
194	POS_443	DL-Isoleucine	Organic acids and derivatives
195	POS_4626	Drofenine	Benzenoids
196	POS_7298	(E)-3-[3-Methoxy-4-[1-(3,4,5-trimethoxyphenyl)propan-2-yloxy]phenyl]prop-2-en-1-ol	Phenylpropanoids and polyketides
197	POS_9002	Ecdysterone	Lipids and lipid-like molecules
198	POS_9872	Echinenone	Lipids and lipid-like molecules
199	POS_10545	Edpetiline	Undefined
200	POS_11492	Enniatin B	Organic acids and derivatives
201	POS_3875	Epicatechin	Phenylpropanoids and polyketides
202	POS_4296	Epigallocatechin	Phenylpropanoids and polyketides
203	POS_4566	(E)-Piperolein A	Organoheterocyclic compounds
204	POS_10305	Ergocryptinine	Alkaloids and derivatives
205	POS_5185	Erucamide	Lipids and lipid-like molecules
206	POS_1335	Ethyl-4-dimethylaminobenzoate	Benzenoids
207	POS_6683	Fecosterol	Undefined
208	POS_4244	Fenpropimorph	Benzenoids
209	POS_3771	Fisetin	Phenylpropanoids and polyketides

210	POS_4519	Flubendazole	Benzenoids
211	POS_5603	Flumioxazin	Organoheterocyclic compounds
212	POS_928	Fluorene	Benzenoids
213	POS_7480	Forskolin	Lipids and lipid-like molecules
214	POS_1484	Fructose (Generic Ketohexose)	Organic oxygen compounds
215	POS_6584	Fucosterol	Lipids and lipid-like molecules
216	POS_3256	Galaxolidone	Organoheterocyclic compounds
217	POS_4726	Gelsemine	Alkaloids and derivatives
218	POS_6042	Gentian violet cation	Benzenoids
219	POS_7634	Ginkgolide C	Undefined
220	POS_13062	Ginsenoside Rk1	Undefined
221	POS_5128	Glabrone	Phenylpropanoids and polyketides
222	POS_622	Glutamic acid	Organic acids and derivatives
223	POS_614	Glutamine Analogue, 1	Organic acids and derivatives
224	POS_5658	Glyceryl monooleate	Lipids and lipid-like molecules
225	POS_5717	Glyceryl monostearate	Lipids and lipid-like molecules
226	POS_5436	Glyceryl palmitate	Lipids and lipid-like molecules
227	POS_689	Guanine	Organoheterocyclic compounds
228	POS_3680	Guanosine	Nucleosides, nucleotides, and analogues
229	POS_6960	Hexa(methoxymethyl)melamine	Organic nitrogen compounds
230	POS_12168	HexCer 34:2;3O HexCer 18:2;2O/16:0;O	Undefined
231	POS_11914	HexCer 34:3;2O HexCer 18:2;2O/16:1	Undefined
232	POS_1363	Hexylresorcinol	Benzenoids
233	POS_5391	Himbacine	Organoheterocyclic compounds
234	POS_5907	Hirsuteine	Alkaloids and derivatives
235	POS_5950	Hirsutine	
236	POS_748	Histidine	Organic acids and derivatives
237	POS_325	Hydron;benzoate	Benzenoids
238	POS_338	Hydron;pyridine-3-carboxylate	Organoheterocyclic compounds
239	POS_225	Hydroquinone	Benzenoids
240	POS_8681	Hyperoside	Phenylpropanoids and polyketides
241	POS_7238	Icariside F2	Organic oxygen compounds
242	POS_14	Imidazole	Organoheterocyclic compounds
243	POS_5455	Imidocarb	Benzenoids
244	POS_7395	Imperialine	Lipids and lipid-like molecules
245	POS_3002	Indigo	Undefined
246	POS_599	Indole-3-carboxaldehyde	Organoheterocyclic compounds
247	POS_3126	Inosine	Nucleosides, nucleotides, and analogues
248	POS_107	Isobutyric acid	Organic acids and derivatives
249	POS_13449	Isobutyryl CoA	Lipids and lipid-like molecules
250	POS_9865	Isogomphrenin I	Organic oxygen compounds
251	POS_2597	Isoleucylaspartic acid	Organic acids and derivatives
252	POS_1777	Isoleucylserine	Organic acids and derivatives

253	POS_512	Isophorone	Organic oxygen compounds
254	POS_8222	Isoquercitin	Phenylpropanoids and polyketides
255	POS_5926	Jacobine N-oxide	Alkaloids and derivatives
256	POS_6248	Junipediol B 8-O-glucoside	Organic oxygen compounds
257	POS_7475	Kaempferol 7-O-rhamnoside	Phenylpropanoids and polyketides
258	POS_6200	Karakoline	Lipids and lipid-like molecules
259	POS_12265	Khasianine	Undefined
260	POS_109	Lactamide	Organic oxygen compounds
261	POS_5328	Lauramidopropylbetaine	Organic acids and derivatives
262	POS_3818	Lauryl diethanolamide	Lipids and lipid-like molecules
263	POS_9946	[Leu]enkephalin	Organic acids and derivatives
264	POS_10870	L-Glutathione (oxidized form)	Organic acids and derivatives
265	POS_309	L-Homoserine	Organic acids and derivatives
266	POS_5398	Limocitrin	Phenylpropanoids and polyketides
267	POS_501	Limonene	Lipids and lipid-like molecules
268	POS_442	L-Norleucine	Organic acids and derivatives
269	POS_6300	Loratadine	Organoheterocyclic compounds
270	POS_7300	Lovastatin	Organoheterocyclic compounds
271	POS_8833	LPC 16:1	Undefined
272	POS_7272	Lupenone	Undefined
273	POS_979	Lupinine	Alkaloids and derivatives
274	POS_3770	Luteolin	Phenylpropanoids and polyketides
275	POS_10283	Lyoniside	Lignans, neolignans and related compounds
276	POS_6008	MEF-Glu	Organic acids and derivatives
277	POS_377	Melamine	Organoheterocyclic compounds
278	POS_1126	Methyl 4-hydroxycinnamate	Undefined
279	POS_4010	Methyl linoleate	Undefined
280	POS_299	Methylmalonic acid	Organic acids and derivatives
281	POS_3073	Mirtazapine	Organoheterocyclic compounds
282	POS_12386	MMPE 34:2 MMPE 16:0_18:2	Undefined
283	POS_4591	Mucorisocoumarin B	Phenylpropanoids and polyketides
284	POS_8490	Mundulone acetate	Phenylpropanoids and polyketides
285	POS_6027	Myristamidopropyl betaine	Organic acids and derivatives
286	POS_5645	N-(2-Hydroxyethyl)icosanamide	Organic nitrogen compounds
287	POS_5751	N-(2-Phenylethyl)hexadecanamide	Lipids and lipid-like molecules
288	POS_5543	N(4)-Acetylsulfadimethoxine	Benzenoids
289	POS_3567	N6-Methyladenosine	Nucleosides, nucleotides, and analogues
290	POS_1272	N6,N6,N6-Trimethyl-L-lysine	Organic acids and derivatives
291	POS_12594	Naadp	Nucleosides, nucleotides, and analogues
292	POS_3302	Nandrolone	Lipids and lipid-like molecules
293	POS_392	Naphthalene	Benzenoids
294	POS_10713	Naringin	Undefined
295	POS_3070	N-Benzylloxycarbonyl-L-leucine	Organic acids and derivatives

296	POS_394	N-Cyclohexylformamide	Organic acids and derivatives
297	POS_1583	Neocuproine	Organoheterocyclic compounds
298	POS_6212	Neotame	Organic acids and derivatives
299	POS_1458	N-Methyldodecylamine	Organic nitrogen compounds
300	POS_1493	N,N-Dimethylarginine	Organic acids and derivatives
301	POS_1235	N,N-Dimethyldecylamine	Organic nitrogen compounds
302	POS_1692	N,N-Dimethyldodecylamine	Organic nitrogen compounds
303	POS_2083	N,N-Dimethyldodecylamine N-oxide	Organic nitrogen compounds
304	POS_4447	N,N-Dimethylguanosine	Nucleosides, nucleotides, and analogues
305	POS_7563	Nonaethylene glycol	Organic oxygen compounds
306	POS_7001	Norbuprenorphine	Benzenoids
307	POS_3925	Norcimifugin	Undefined
308	POS_4477	Norclozapine	Organoheterocyclic compounds
309	POS_5074	Nor-Dentatin	Phenylpropanoids and polyketides
310	POS_2162	Norfentanyl	Benzenoids
311	POS_975	Npi-methyl-L-histidine	Organic acids and derivatives
312	POS_1502	O-Acetylcarnitine	Lipids and lipid-like molecules
313	POS_3710	Octadecanamide	Organic acids and derivatives
314	POS_6517	Octaethylene glycol	Organic oxygen compounds
315	POS_3890	Octyl methoxycinnamate	Phenylpropanoids and polyketides
316	POS_7346	O-Stearoylcarnitine	Lipids and lipid-like molecules
317	POS_7818	Oxaline	Organoheterocyclic compounds
318	POS_455	Oxindole	Organoheterocyclic compounds
319	POS_8603	Paeonolide	Undefined
320	POS_2857	Palmitic amide	Undefined
321	POS_1790	Pantothenic acid	Organic acids and derivatives
322	POS_12421	PC 32:1 PC 16:0_16:1	Undefined
323	POS_12334	PC 32:4 PC 14:1_18:3	Undefined
324	POS_12602	PC 33:1 PC 15:0_18:1	Undefined
325	POS_12586	PC 33:2 PC 15:0_18:2	Undefined
326	POS_12561	PC 33:3 PC 15:0_18:3	Undefined
327	POS_12776	PC 34:1 PC 16:0_18:1	Undefined
328	POS_12720	PC 34:3 PC 16:0_18:3	Undefined
329	POS_12692	PC 34:4 PC 16:1_18:3	Undefined
330	POS_13036	PC 36:2 PC 18:1_18:1	Undefined
331	POS_13016	PC 36:3 PC 18:1_18:2	Undefined
332	POS_13001	PC 36:4 PC 18:2_18:2	Undefined
333	POS_13211	PC 38:6 PC 18:3_20:3	Undefined
334	POS_12197	PE 34:2 PE 16:0_18:2	Undefined
335	POS_1052	Peganine	Organoheterocyclic compounds
336	POS_7981	Peimine	Lipids and lipid-like molecules
337	POS_7396	Peiminine	Undefined
338	POS_7339	Peimisine	Undefined

339	POS_10591	Pelargonin	Phenylpropanoids and polyketides
340	POS_5954	Perindopril	Organic acids and derivatives
341	POS_1888	Phenazine-1-carboxylic acid	Organoheterocyclic compounds
342	POS_918	Phenylalanine	Organic acids and derivatives
343	POS_1075	Phenyl dihydrogen phosphate	Organic acids and derivatives
344	POS_369	Phloroglucinol	Benzenoids
345	POS_1192	Phosphocholine	Organic nitrogen compounds
346	POS_1191	Phosphorylcholine	Organic nitrogen compounds
347	POS_923	Phthalic acid	Benzenoids
348	POS_626	Phthalic anhydride	Undefined
349	POS_4635	Phytosphingosine	Organic nitrogen compounds
350	POS_421	Pipecolic acid	Organic acids and derivatives
351	POS_87	Piperidine	Organoheterocyclic compounds
352	POS_7937	Polygalatenoside A	Organic oxygen compounds
353	POS_10372	Procyanidin B2	Phenylpropanoids and polyketides
354	POS_279	Proline	Organic acids and derivatives
355	POS_1275	Propamocarb	Benzenoids
356	POS_2947	Propranolol	Benzenoids
357	POS_1776	Pterosin B	Benzenoids
358	POS_2207	Pterosin G	Benzenoids
359	POS_1626	Pyocyanine	Organoheterocyclic compounds
360	POS_4807	Quinidine	Alkaloids and derivatives
361	POS_419	Quinoline	Organoheterocyclic compounds
362	POS_6720	Reserpine acid	Alkaloids and derivatives
363	POS_6168	Riboflavin	Organoheterocyclic compounds
364	POS_2968	Ropinirole	Organoheterocyclic compounds
365	POS_4095	Roquefortine A	Alkaloids and derivatives
366	POS_7595	Sayaendoside	Organic oxygen compounds
367	POS_10380	Sciadopitysin	Phenylpropanoids and polyketides
368	POS_1928	Secbumeton	Organoheterocyclic compounds
369	POS_13627	Solamargine	Lipids and lipid-like molecules
370	POS_7011	Solasodine	Undefined
371	POS_13731	Solasonine	Lipids and lipid-like molecules
372	POS_7122	Solvent green 3	Benzenoids
373	POS_5670	Songorine	Lipids and lipid-like molecules
374	POS_2635	Sophoridine	Undefined
375	POS_14112	Soyasaponin Ba	Lipids and lipid-like molecules
376	POS_2236	Sparteine sulfate	Undefined
377	POS_4129	Sphingosine	Organic nitrogen compounds
378	POS_4077	Spiroxamine	Organic oxygen compounds
379	POS_926	(S)-Suspensaside	Organic oxygen compounds
380	POS_6934	STIGMASTA-4,22-DIEN-3-ONE	Undefined
381	POS_6984	Stigmasterol	Lipids and lipid-like molecules

382	POS_5078	Strychnine	Alkaloids and derivatives
383	POS_2553	Suberosin	Phenylpropanoids and polyketides
384	POS_4398	Sulfadimethoxine	Benzenoids
385	POS_7738	Tetracycline	Phenylpropanoids and polyketides
386	POS_6051	Tetradecanoylcarnitine	Lipids and lipid-like molecules
387	POS_5833	Tetraethylene glycol monododecyl ether	Organic oxygen compounds
388	POS_10999	Thalsimidine	Lignans, neolignans and related compounds
389	POS_1156	Theobromine	Organoheterocyclic compounds
390	POS_2149	Threonylleucine	Organic acids and derivatives
391	POS_4917	Tiapride	Benzenoids
392	POS_3029	Tramadol	Benzenoids
393	POS_7687	Trichoverrol A	Lipids and lipid-like molecules
394	POS_8803	Tricin 5-glucoside	Phenylpropanoids and polyketides
395	POS_671	Triethanolamine	Organic nitrogen compounds
396	POS_6866	Trifloxystrobin	Benzenoids
397	POS_503	Trigonelline HCl	Undefined
398	POS_3093	Triisobutyl phosphate	Organic acids and derivatives
399	POS_0	Trimethylamine	Organic nitrogen compounds
400	POS_4858	Triphenyl phosphate	Organic acids and derivatives
401	POS_3394	Triphenylphosphine oxide	Benzenoids
402	POS_5699	Triptonide	Undefined
403	POS_4856	Tris(1-chloro-2-propyl)phosphate	Organic acids and derivatives
404	POS_4636	Tsitsikammamine B	Organoheterocyclic compounds
405	POS_6146	Tuberostemonine	Undefined
406	POS_317	Tyramine	Benzenoids
407	POS_1172	Tyrosine	Organic acids and derivatives
408	POS_12916	Unguisin E	Organic acids and derivatives
409	POS_249	Uracil	Organoheterocyclic compounds
410	POS_2551	Uridine	Nucleosides, nucleotides, and analogues
411	POS_5489	Vinpocetine	Alkaloids and derivatives
412	POS_6167	Xanthohumol	Phenylpropanoids and polyketides
413	POS_9499	Xolegel	Organoheterocyclic compounds
414	POS_5254	Yohimbic Acid	Alkaloids and derivatives
415	NEG_1394	14-(3-Ethylloxiran-2-yl)tetradeca-9,12-dienoic acid	Lipids and lipid-like molecules
416	NEG_1841	(15Z)-9,12,13-Trihydroxy-15-octadecenoic acid	Lipids and lipid-like molecules
417	NEG_6920	16-Hydroxy-3-(beta-D-xylopyranosyloxy)-, (3beta,5xi,9xi,16alpha)-olean-12-ene-23,28-dioic acid	Lipids and lipid-like molecules
418	NEG_5504	1-Palmitoylphosphatidylcholine	Lipids and lipid-like molecules
419	NEG_5820	2-[4-[4-[Hydroxy-(4-hydroxy-3-methoxyphenyl)methyl]-3-(hydroxymethyl)oxolan-2-yl]-2-	Lignans, neolignans and related compounds

		methoxyphenoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	
420	NEG_4441	2-Azaniumylethyl (2-hydroxy-3-octadec-9-enoyloxypropyl) phosphate	Lipids and lipid-like molecules
421	NEG_3887	2-Azaniumylethyl (3-hexadecanoyloxy-2-hydroxypropyl) phosphate	Lipids and lipid-like molecules
422	NEG_1573	2-Dodecoxyethyl hydrogen sulfate	Organic acids and derivatives
423	NEG_7992	[2-Hydroxy-3-[3,4,5-trihydroxy-6-[[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxan-2-yl]oxypropyl] octadeca-9,12,15-trienoate	Lipids and lipid-like molecules
424	NEG_5835	[2-Hydroxy-3-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxypropyl] octadeca-9,12-dienoate	Lipids and lipid-like molecules
425	NEG_5922	(2-Hydroxy-3-octadec-9-enoyloxypropyl) 2-(trimethylazaniumyl)ethyl phosphate	Lipids and lipid-like molecules
426	NEG_5855	(2-Hydroxy-3-octadeca-9,12,15-trienoyloxypropyl) 2-(trimethylazaniumyl)ethyl phosphate	Lipids and lipid-like molecules
427	NEG_5889	(2-Hydroxy-3-octadeca-9,12-dienoyloxypropyl) 2-(trimethylazaniumyl)ethyl phosphate	Lipids and lipid-like molecules
428	NEG_2482	2-Hydroxy-4-methoxy-3,5-bis(3-methylbut-2-enyl)-6-pentylbenzoic acid	Benzenoids
429	NEG_5883	2-Oahsa	Lipids and lipid-like molecules
430	NEG_4389	[3-[2-Aminoethoxy(hydroxy)phosphoryl]oxy-2-hydroxypropyl] octadeca-9,12-dienoate	Lipids and lipid-like molecules
431	NEG_2096	3(2'-Chlorophenyl)-7-hydroxy-4-phenylcoumarin	Phenylpropanoids and polyketides
432	NEG_671	3-(4-Hydroxy-3-methoxyphenyl)-2-propenoic acid	Phenylpropanoids and polyketides
433	NEG_5793	3-(Hexopyranosyloxy)-2-hydroxypropyl ester, (9Z,12Z,15Z)-9,12,15-octadecatrienoic acid	Lipids and lipid-like molecules
434	NEG_240	3-Hydroxybenzoic acid	Benzenoids
435	NEG_1726	(3S)-5-[(1R,2R,8aS)-2-hydroxy-2,5,5,8a-tetramethyl-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl]-3-methylpentanoic acid	Lipids and lipid-like molecules
436	NEG_156	4-Hydroxybenzaldehyde	Organic oxygen compounds
437	NEG_1453	4-Hydroxybenzoic acid 4-O-glucoside	Organic oxygen compounds
438	NEG_437	4-Hydroxycinnamic acid	Phenylpropanoids and polyketides
439	NEG_273	4-Hydroxyquinoline	Organoheterocyclic compounds
440	NEG_248	4-Nitrophenol	Benzenoids
441	NEG_2128	5-(5-Methoxycarbonyl-5,8a-dimethyl-2-methylidene-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl)-3-methylpentanoic acid	Lipids and lipid-like molecules

442	NEG_4952	5,7-Dihydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-3-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	Phenylpropanoids and polyketides
443	NEG_4732	(6,6-Dimethylbicyclo[3.1.1]hept-2-yl)methyl 6-O-[(2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)tetrahydro-2-furanyl]-beta-D-glucopyranoside	Lipids and lipid-like molecules
444	NEG_2755	7-Ethyl-10-Hydroxy-Camptothecin	Undefined
445	NEG_1362	8-(2-Oxo-5-pent-2-enylcyclopent-3-en-1-yl)octanoic acid	Lipids and lipid-like molecules
446	NEG_1838	9,12,13-Trihydroxyoctadec-10-enoic acid	Lipids and lipid-like molecules
447	NEG_1800	9,12,13-Trihydroxyoctadeca-10,15-dienoic acid	Lipids and lipid-like molecules
448	NEG_1074	9-Hexadecenoic acid	Lipids and lipid-like molecules
449	NEG_1600	9-Hydroperoxyoctadeca-10,12-dienoic acid	Lipids and lipid-like molecules
450	NEG_1408	9-Hydroxy-10E,12Z-octadecadienoic acid	Lipids and lipid-like molecules
451	NEG_2524	9-Methoxycamptothecin	Alkaloids and derivatives
452	NEG_1502	Abietic acid	Lipids and lipid-like molecules
453	NEG_216	Adenine	Organoheterocyclic compounds
454	NEG_3446	Afzelin	Phenylpropanoids and polyketides
455	NEG_8365	alpha-Hederin	Undefined
456	NEG_9545	alpha-Solanine	Undefined
457	NEG_7928	Amatain	Alkaloids and derivatives
458	NEG_1789	Androsin	Organic oxygen compounds
459	NEG_8232	Apigenin 7-O-(2G-rhamnosyl)gentiobioside	Undefined
460	NEG_1522	Arachidonic acid	Lipids and lipid-like molecules
461	NEG_4606	Asiatic acid	Undefined
462	NEG_4670	Aurantio-obtusin beta-D-glucoside	Benzenoids
463	NEG_4605	Bayogenin	Undefined
464	NEG_3968	Betulinic acid	Lipids and lipid-like molecules
465	NEG_674	Butylparaben	Benzenoids
466	NEG_1996	Caffeic acid hexoside	Phenylpropanoids and polyketides
467	NEG_829	Calcium pantothenate	Undefined
468	NEG_1963	Canrenone	Lipids and lipid-like molecules
469	NEG_498	cis-Aconitic acid	Organic acids and derivatives
470	NEG_547	cis-Caffeic acid	Phenylpropanoids and polyketides
471	NEG_2939	Corynanthine	Alkaloids and derivatives
472	NEG_1307	Cyanidin	Phenylpropanoids and polyketides
473	NEG_8422	Cyanidin 3-(2G-glucosylrutinoside)	Undefined
474	NEG_3760	Cyanidin 3-O-glucoside	Phenylpropanoids and polyketides
475	NEG_6983	Decahydrogambogic acid	Organoheterocyclic compounds
476	NEG_1460	Dehydroabietic acid	Lipids and lipid-like molecules
477	NEG_4287	Deoxynivalenol 3-glucuronide	Lipids and lipid-like molecules

478	NEG_2982	Desoxyrhaponticin	Undefined
479	NEG_552	D-Glucose	Organic oxygen compounds
480	NEG_2753	Digoxigenin	Lipids and lipid-like molecules
481	NEG_2257	Dinoprost	Lipids and lipid-like molecules
482	NEG_1805	Docosahexaenoic acid	Lipids and lipid-like molecules
483	NEG_1980	Docosanoic acid	Lipids and lipid-like molecules
484	NEG_1744	Dodecylbenzenesulfonic acid	Benzenoids
485	NEG_5733	Dronedarone	Organic oxygen compounds
486	NEG_2386	(E)-3-(3,4-Dihydroxyphenyl)acrylic acid (1R,2R,3R)-2,3,5-trihydroxy-5-(methoxycarbonyl)cyclohexyl ester	Organic oxygen compounds
487	NEG_6923	Echinocystic acid-3-O-glucoside	Undefined
488	NEG_3633	(-)-Epicatechin gallate	Phenylpropanoids and polyketides
489	NEG_3984	(-)-Epigallocatechin gallate	Phenylpropanoids and polyketides
490	NEG_8171	Erythromycin	Organic oxygen compounds
491	NEG_3124	FA 26:0;2O	Lipids and lipid-like molecules
492	NEG_3093	FA 27:0	Lipids and lipid-like molecules
493	NEG_3624	Folic acid	Organic acids and derivatives
494	NEG_138	Fumaric acid	Organic acids and derivatives
495	NEG_461	Gallic acid	Benzenoids
496	NEG_479	gamma-Aminobutyrate	Organic acids and derivatives
497	NEG_1255	gamma-Linolenic acid	Lipids and lipid-like molecules
498	NEG_1383	Gingerol	Benzenoids
499	NEG_6987	Ginsenoside F1	Undefined
500	NEG_9161	Ginsenoside F2	Undefined
501	NEG_8585	Ginsenoside F3	Undefined
502	NEG_9937	Ginsenoside Rb1	Undefined
503	NEG_8904	Ginsenoside Rf	Undefined
504	NEG_8724	Ginsenoside Rg2	Undefined
505	NEG_8723	Ginsenoside Rg3(R-FORM)	Undefined
506	NEG_8532	Ginsenoside Rg5	Undefined
507	NEG_7551	Ginsenoside Rh1	Undefined
508	NEG_7353	Ginsenoside Rh2 (S-FORM)	Undefined
509	NEG_1141	Glucose 6-phosphate	Organic oxygen compounds
510	NEG_670	Glucuronic acid	Undefined
511	NEG_4166	Glycocholic acid	Lipids and lipid-like molecules
512	NEG_7236	Gypsogenin-3-O-glucuronide	Undefined
513	NEG_1756	Heneicosanoic acid	Lipids and lipid-like molecules
514	NEG_1200	Heptadecanoic acid	Lipids and lipid-like molecules
515	NEG_1452	Hispidulin	Phenylpropanoids and polyketides
516	NEG_661	Hydron;2-hydroxypropane-1,2,3-tricarboxylate	Organic acids and derivatives
517	NEG_1389	Hydron;tetradecyl sulfate	Organic acids and derivatives
518	NEG_2342	Indapamide	Benzenoids

519	NEG_4126	Isoquercitrin	Phenylpropanoids and polyketides
520	NEG_1642	Isorhamnetin	Phenylpropanoids and polyketides
521	NEG_6804	Isorhamnetin-3-O-galactoside-6"-rhamnoside	Undefined
522	NEG_4400	Isorhamnetin-3-O-glucoside	Phenylpropanoids and polyketides
523	NEG_3236	Isorhapontin	Phenylpropanoids and polyketides
524	NEG_1877	Isoxaben	Benzenoids
525	NEG_6075	Kaempferitrin	Undefined
526	NEG_1306	Kaempferol	Phenylpropanoids and polyketides
527	NEG_6614	Kaempferol 3,7-diglucoside	Phenylpropanoids and polyketides
528	NEG_6357	Kaempferol-3-O-glucoside-6"-p-coumaroyl	Undefined
529	NEG_6360	Kaempferol-3-O-glucoside-7-O-rhamnoside	Phenylpropanoids and polyketides
530	NEG_6609	Kaempferol 3-O-sophoroside	Undefined
531	NEG_5323	Kukoamine A	Undefined
532	NEG_1164	Lauryl sulfate	Organic acids and derivatives
533	NEG_4771	Leukotriene D4	Lipids and lipid-like molecules
534	NEG_1267	Linoleic acid	Lipids and lipid-like molecules
535	NEG_1257	Linolenic acid	Lipids and lipid-like molecules
536	NEG_211	L-Malic acid	Organic acids and derivatives
537	NEG_1310	Loureirin A	Undefined
538	NEG_4363	LPE 18:3	Undefined
539	NEG_4555	LPG 16:0	Undefined
540	NEG_4513	LPG 16:1	Undefined
541	NEG_4963	LPG 18:2	Undefined
542	NEG_4917	LPG 18:3	Undefined
543	NEG_5988	LPI 16:0	Undefined
544	NEG_6399	LPI 18:2	Undefined
545	NEG_5167	LPS 18:2	Undefined
546	NEG_5134	LPS 18:3	Undefined
547	NEG_175	L-Pyroglutamic acid	Organic acids and derivatives
548	NEG_3762	Luteolin-7-O-glucoside	Undefined
549	NEG_6359	Luteolin 7-O-rutinoside	Phenylpropanoids and polyketides
550	NEG_4883	Madecassic acid	Undefined
551	NEG_4851	Medicagenic acid	Lipids and lipid-like molecules
552	NEG_1641	Methoxyluteolin	Phenylpropanoids and polyketides
553	NEG_5067	Methyl (3R,4R,5R)-5-[(2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(E)-3-phenylprop-2-enoyl]oxyoxan-2-yl]oxy-3,4-dihydroxycyclohexene-1-carboxylate	Lipids and lipid-like molecules
554	NEG_1651	Methyl hexadecanoate	Undefined
555	NEG_8506	Momordin Ic	Undefined
556	NEG_2708	Mycophenolic acid IV	Lipids and lipid-like molecules
557	NEG_4450	Myricetin-3-Galactoside	Phenylpropanoids and polyketides
558	NEG_4124	Myricitrin	Phenylpropanoids and polyketides

559	NEG_1358	N(4)-Acetylsulfadiazine	Benzenoids
560	NEG_2372	Nervonic acid	Lipids and lipid-like molecules
561	NEG_3698	Nonyl glucosinolate	Organic oxygen compounds
562	NEG_6633	Novobiocin	Phenylpropanoids and polyketides
563	NEG_5867	NP-000062(6)	Undefined
564	NEG_3330	Octacosanoic acid	Lipids and lipid-like molecules
565	NEG_1281	Oleic acid	Lipids and lipid-like molecules
566	NEG_7402	PA 34:2 PA 16:0_18:2	Undefined
567	NEG_7377	PA 34:3 PA 16:0_18:3	Undefined
568	NEG_7695	PA 36:4 PA 18:2_18:2	Undefined
569	NEG_7671	PA 36:5 PA 18:2_18:3	Undefined
570	NEG_1090	Palmitic acid	Lipids and lipid-like molecules
571	NEG_9165	PC 36:2 PC 18:0_18:2	Undefined
572	NEG_9119	PC 36:5 PC 18:2_18:3	Undefined
573	NEG_7947	PE 34:1	Undefined
574	NEG_7916	PE 34:2	Undefined
575	NEG_8261	PE 36:3	Undefined
576	NEG_8225	PE 36:4 PE 18:2_18:2	Undefined
577	NEG_8200	PE 36:5 PE 18:2_18:3	Undefined
578	NEG_2604	Pentacosanoic acid	Lipids and lipid-like molecules
579	NEG_960	Pentadecanoic acid	Lipids and lipid-like molecules
580	NEG_4401	Petunidin 3-galactoside	Phenylpropanoids and polyketides
581	NEG_7674	PG 30:0	Undefined
582	NEG_8329	PG 34:2 PG 16:0_18:2	Undefined
583	NEG_8628	PG 36:2	Undefined
584	NEG_8587	PG 36:4	Undefined
585	NEG_8567	PG 36:5 PG 18:2_18:3	Undefined
586	NEG_4899	Phosphatidylcholine lyso 18:2	Lipids and lipid-like molecules
587	NEG_4861	Phosphatidylcholine lyso 18:3	Lipids and lipid-like molecules
588	NEG_5362	Phytolaccagenin	Undefined
589	NEG_9200	PI 34:1	Undefined
590	NEG_9187	PI 34:2	Undefined
591	NEG_9269	PI 35:2	Undefined
592	NEG_9348	PI 36:2	Undefined
593	NEG_9309	PI 36:5	Undefined
594	NEG_7403	PMeOH 33:2 PMeOH 15:0_18:2	Undefined
595	NEG_7602	PMeOH 34:1 PMeOH 16:0_18:1	Undefined
596	NEG_7576	PMeOH 34:2 PMeOH 16:0_18:2	Undefined
597	NEG_7555	PMeOH 34:3 PMeOH 16:0_18:3	Undefined
598	NEG_7528	PMeOH 34:4 PMeOH 16:1_18:3	Undefined
599	NEG_7835	PMeOH 36:4 PMeOH 18:2_18:2	Undefined
600	NEG_4016	(-)-Podophyllotoxin	Undefined
601	NEG_4603	Polygalic acid	Undefined

602	NEG_4805	Poricoic acid A	Undefined
603	NEG_4906	Protohypericin	Undefined
604	NEG_3176	Puerarin	Phenylpropanoids and polyketides
605	NEG_1469	(R)-2-Hydroxystearic acid	Undefined
606	NEG_3615	Roburic acid	Undefined
607	NEG_2176	(S)-7-Hydroxy-2-(4-hydroxyphenyl)-5-methoxy-8-(3-methylbut-2-en-1-yl)chroman-4-one	Phenylpropanoids and polyketides
608	NEG_8680	Saikosaponin a	Undefined
609	NEG_9599	Saikosaponin C	Undefined
610	NEG_241	Salicylic acid	Benzenoids
611	NEG_9563	Solasodine base + 2H, 1O, O-Hex-Hex-Hex	Lipids and lipid-like molecules
612	NEG_3447	Sophoricoside	Undefined
613	NEG_6579	Spinosin	Undefined
614	NEG_1298	Stearic acid	Lipids and lipid-like molecules
615	NEG_2447	Stenophylline A	Organic oxygen compounds
616	NEG_147	Succinic acid	Organic acids and derivatives
617	NEG_2403	Tetracosanoic acid	Lipids and lipid-like molecules
618	NEG_1998	Trehalose	Organic oxygen compounds
619	NEG_2802	Triamcinolone	Lipids and lipid-like molecules
620	NEG_5898	Uridine-5'-diphosphate-glucose	Nucleosides, nucleotides, and analogues
621	NEG_244	Urocanic acid	Organoheterocyclic compounds
622	NEG_3935	Ursonic acid	Undefined
623	NEG_4251	Xyl(b1-6)Glc(b)-O-octyl	Lipids and lipid-like molecules
624	NEG_1840	(Z)-5,8,11-Trihydroxyoctadec-9-enoic acid	Lipids and lipid-like molecules