

**Figure S1.** Visualization of significant differential metabolites. Six comparisons among four groups of samples in each mode. (a–c) are negative ion mode and (d–f) are positive ion mode. Blocks in orange are upregulated metabolites and blocks in blue are downregulated.

**Table S1.** The list of a total of 977 identified metabolites in fermented broccoli samples.

No.	R <sub>t</sub> (min)	m/z	Name	Adduct	Superclass
1	0.565	308.0894	L-Glutathione (reduced form)	[M+H] <sup>+</sup>	Organic acids and derivatives
2	0.569	259.0215	alpha-D-Mannose 1-phosphate	[M-H] <sup>-</sup>	Organic oxygen compounds
3	0.572	276.1169	gamma-Glutamylglutamine	[M+H] <sup>+</sup>	Organic acids and derivatives
4	0.574	134.044	2-Aminobutanedioate;hydron	[M+H] <sup>+</sup>	Organic acids and derivatives
5	0.575	147.1108	Lysine	[M+H] <sup>+</sup>	Organic acids and derivatives
6	0.579	193.0366	2-Dehydro-D-gluconic acid	[M-H] <sup>-</sup>	Organic oxygen compounds
7	0.581	209.0301	Galactaric acid	[M-H] <sup>-</sup>	Organic oxygen compounds
8	0.584	102.0549	1-Azaniumylcyclopropane-1-carboxylate	[M+H] <sup>+</sup>	Organic acids and derivatives
9	0.593	132.0304	Aspartic acid	[M-H] <sup>-</sup>	Organic acids and derivatives
10	0.605	195.0528	Gluconic acid	[M-H] <sup>-</sup>	Organic acids and derivatives
11	0.608	135.0296	Threonic acid	[M-H] <sup>-</sup>	Organic oxygen compounds
12	0.609	146.0459	Glutamic acid	[M-H] <sup>-</sup>	Organic acids and derivatives
13	0.61	104.0354	Serine	[M-H] <sup>-</sup>	Organic acids and derivatives
14	0.611	115.0028	Hexanoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
15	0.613	102.0553	3-Aminoisobutyrate	[M-H] <sup>-</sup>	Organic acids and derivatives
16	0.613	191.0556	Quinic acid	[M-H] <sup>-</sup>	Organic oxygen compounds
17	0.614	131.0454	Asparagine	[M-H] <sup>-</sup>	Organic acids and derivatives
18	0.616	147.075	Glutamine Analogue, 1	[M+H] <sup>+</sup>	Organic acids and derivatives
19	0.617	145.0623	Glutamine	[M-H] <sup>-</sup>	Organic acids and derivatives
20	0.619	75.00932	2-Oxonioacetate	[M-H] <sup>-</sup>	Organic acids and derivatives
21	0.62	154.0626	Histidine	[M-H] <sup>-</sup>	Organic acids and derivatives
22	0.623	203.0515	Fructose (Generic Ketohexose)	[M+Na] <sup>+</sup>	Organic oxygen compounds
23	0.623	227.0759	Mannitol	[M+FA-H] <sup>-</sup>	Organic oxygen compounds
24	0.623	181.0723	Sorbitol	[M-H] <sup>-</sup>	Organic oxygen compounds
25	0.624	351.1208	6a,7,8-Trihydroxy-3-methyl-3,4,5,6,7,12a-hexahydro-2H-benzo[a]anthracene-1,12-dione	[M+Na] <sup>+</sup>	Benzenoids
26	0.625	118.0513	L-Threonine	[M-H] <sup>-</sup>	Organic acids and derivatives
27	0.626	455.1148	[3-Hydroxy-1-(4-methoxy-7-oxofuro[3,2-g]chromen-9-yl)oxy-3-methylbutan-2-yl] (E)-2-methylbut-2-enoate	[M+K] <sup>+</sup>	Phenylpropanoids and polyketides
28	0.627	173.1044	Arginine	[M-H] <sup>-</sup>	Organic acids and derivatives
29	0.629	120.0631	Allo-thr	[M+H] <sup>+</sup>	Organic acids and derivatives
30	0.633	180.0861	D-Glucosamine	[M+H] <sup>+</sup>	Organic oxygen compounds
31	0.633	69.03308	Furan	[M+H] <sup>+</sup>	Undefined

32	0.634	166.051	L-Methionine sulfoxide	[M+H] <sup>+</sup>	Organic acids and derivatives
33	0.636	179.0561	D-Glucose	[M-H] <sup>-</sup>	Organic oxygen compounds
34	0.641	162.0752	O-Acetylhomoserine	[M+H] <sup>+</sup>	Organic acids and derivatives
35	0.641	133.0148	L-Malic acid	[M-H] <sup>-</sup>	Organic acids and derivatives
36	0.643	341.1077	Lactulose	[M-H] <sup>-</sup>	Organic oxygen compounds
37	0.645	360.1496	beta-Gentiobiose	[M+NH <sub>4</sub> ] <sup>+</sup>	Organic oxygen compounds
38	0.645	138.0545	Trigonelline HCl	[M+H] <sup>+</sup>	Undefined
39	0.646	165.0741	1,5-Anhydro-D-glucitol	[2M+H] <sup>+</sup>	Organic oxygen compounds
40	0.646	87.00861	Pyruvic acid	[M-H] <sup>-</sup>	Organic acids and derivatives
41	0.648	503.1569	Raffinose	[M-H] <sup>-</sup>	Organic oxygen compounds
42	0.651	114.0561	Proline	[M-H] <sup>-</sup>	Organic acids and derivatives
43	0.652	104.1074	Choline	[M] <sup>+</sup>	Organic nitrogen compounds
44	0.652	355.1048	Gentiopicroside	[M-H] <sup>-</sup>	Undefined
45	0.653	68.04893	Pyrrole	[M+H] <sup>+</sup>	Organoheterocyclic compounds
46	0.658	322.0431	Cytidine 3'-monophosphate	[M-H] <sup>-</sup>	Organic oxygen compounds
47	0.66	307.0321	2'-Deoxyuridine 5'-monophosphate	[M-H] <sup>-</sup>	Nucleosides, nucleotides, and analogues
48	0.66	177.0408	Gulonic acid	[M-H] <sup>-</sup>	Organic acids and derivatives
49	0.663	128.0348	L-Pyroglutamic acid	[M-H] <sup>-</sup>	Organic acids and derivatives
50	0.664	305.1427	Nopaline	[M+H] <sup>+</sup>	Organic acids and derivatives
51	0.665	304.0345	Cytidine 2',3'-cyclic phosphate	[M-H] <sup>-</sup>	Nucleosides, nucleotides, and analogues
52	0.667	89.02812	L-Lactic acid	[M+FA-H] <sup>-</sup>	Organic acids and derivatives
53	0.668	324.0566	Cytidine-5'-monophosphate	[M+H] <sup>+</sup>	Nucleosides, nucleotides, and analogues
54	0.674	111.0435	2-Acetylfuran	[M+H-H <sub>2</sub> O] <sup>+</sup>	Undefined
55	0.676	129.0197	Citraconic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
56	0.682	243.0637	Pseudouridine	[M-H] <sup>-</sup>	Nucleosides, nucleotides, and analogues
57	0.685	173.0905	Glycyl-L-proline	[M+H] <sup>+</sup>	Organic acids and derivatives
58	0.69	173.0089	cis-Aconitic acid	[M-H] <sup>-</sup>	Organic acids and derivatives
59	0.703	139.0391	3,4-Dihydroxybenzaldehyde	[M+H] <sup>+</sup>	Organic oxygen compounds
60	0.746	130.0859	Pipecolic acid	[M+H] <sup>+</sup>	Organic acids and derivatives
61	0.748	146.0916	4-Guanidinobutyric acid	[M+H] <sup>+</sup>	Organic acids and derivatives
62	0.757	189.1578	N <sub>6</sub> ,N <sub>6</sub> ,N <sub>6</sub> -Trimethyl-L-lysine	[M+H] <sup>+</sup>	Organic acids and derivatives
63	0.758	203.1485	N,N-Dimethylarginine	[M+H] <sup>+</sup>	Organic acids and derivatives
64	0.758	149.0214	Phthalic anhydride	[M+H] <sup>+</sup>	Undefined
65	0.771	146.1177	Acetylcholine	[M] <sup>+</sup>	Organic nitrogen compounds
66	0.787	111.0206	Uracil	[M-H] <sup>-</sup>	Organoheterocyclic compounds
67	0.79	242.0773	Cytidine	[M-H] <sup>-</sup>	Nucleosides, nucleotides, and analogues

68	0.796	371.1555	Arctigenin	[M-H]-	Undefined
69	0.798	187.1096	L-Ala-L-Val	[M-H]-	Organic acids and derivatives
70	0.804	315.0715	Benzoic acid + 2O, O-Hex	[M-H]-	Organic oxygen compounds
71	0.807	148.0438	Methionine	[M-H]-	Organic acids and derivatives
72	0.81	117.0199	Succinic acid	[M-H]-	Organic acids and derivatives
73	0.812	161.0446	Meglutol	[M-H]-	Lipids and lipid-like molecules
74	0.813	399.1409	S-Adenosylmethionine	[M+H]+	Nucleosides, nucleotides, and analogues
75	0.816	180.0664	Tyrosine	[M-H]-	Organic acids and derivatives
76	0.821	243.0633	Uridine	[M-H]-	Nucleosides, nucleotides, and analogues
77	0.826	309.1187	gamma-Glutamyltyrosine	[M-H]-	Organic acids and derivatives
78	0.827	152.0343	Mesalamine	[M-H]-	Benzenoids
79	0.831	175.1185	Glycylvaline	[M+H]+	Organic acids and derivatives
80	0.831	237.0883	Gly-Tyr	[M-H]-	Organic acids and derivatives
81	0.848	322.1391	Codeine	[M+Na]+	Alkaloids and derivatives
82	0.862	132.1015	DL-Isoleucine	[M+H]+	Organic acids and derivatives
83	0.869	130.0876	l-Isoleucine	[M-H]-	Organic acids and derivatives
84	0.871	124.0381	Hydron;pyridine-3-carboxylate	[M+H]+	Organoheterocyclic compounds
85	0.896	202.1785	4-Hydroxy-1-(2-hydroxyethyl)-2,2,6,6-tetramethylpiperidine	[M+H]+	Organoheterocyclic compounds
86	0.911	228.0856	2'-Deoxycytidine	[M+H]+	Nucleosides, nucleotides, and analogues
87	0.943	112.0497	Cytosine	[M+H]+	Organoheterocyclic compounds
88	0.959	188.1755	N8-Acetylspermidine	[M+H]+	Organic acids and derivatives
89	1.005	201.123	Ala-Ile	[M-H]-	Organic acids and derivatives
90	1.016	282.1197	N6-Methyladenosine	[M+H]+	Nucleosides, nucleotides, and analogues
91	1.066	365.1009	Sucrose	[M+Na]+	Organic oxygen compounds
92	1.123	366.0781	(2S)-7-Hydroxy-3-oxo-3,4-dihydro-2H-1,4-benzoxazin-2-yl beta-D-glucopyranoside	[M+Na]+	Organic oxygen compounds
93	1.132	154.0833	Dopamine	[M+H]+	Benzenoids
94	1.166	166.0505	Pyridoxal	[M-H]-	Organoheterocyclic compounds
95	1.169	282.0824	Guanosine	[M-H]-	Nucleosides, nucleotides, and analogues
96	1.228	126.0643	5-Methylcytosine	[M+H]+	Organoheterocyclic compounds
97	1.246	298.1131	2-Methylguanosine	[M+H]+	Nucleosides, nucleotides, and analogues
98	1.246	150.0754	3-Methyladenine	[M+H]+	Organoheterocyclic compounds
99	1.255	138.0543	Trigonelline	[M+H]+	Alkaloids and derivatives
100	1.255	119.0336	Methylmalonic acid	[M+H]+	Organic acids and derivatives
101	1.26	170.0794	Pyridoxine	[M+H]+	Organoheterocyclic compounds
102	1.263	344.0375	Cyclic guanosine monophosphate	[M-H]-	Nucleosides, nucleotides, and analogues

103	1.267	291.1416	Trimethoprim	[M+H] <sup>+</sup>	Benzenoids
104	1.276	118.0844	Betaine	[M+H] <sup>+</sup>	Organic acids and derivatives
105	1.291	145.0505	Monomethyl glutaric acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
106	1.293	203.139	2-[(2-Ammonio-4-methylpentanoyl)amino]propanoate	[M+H] <sup>+</sup>	Organic acids and derivatives
107	1.295	137.0237	4-Hydroxybenzoic acid	[M-H] <sup>-</sup>	Benzenoids
108	1.364	127.0498	Thymine	[M+H] <sup>+</sup>	Organoheterocyclic compounds
109	1.375	217.1547	H-DL-Val-DL-Val-OH	[M+H] <sup>+</sup>	Organic acids and derivatives
110	1.402	158.0797	1-Acetylproline	[M+H] <sup>+</sup>	Organic acids and derivatives
111	1.421	312.0677	2-(1-Chlorocyclopropyl)-1-(2-chlorophenyl)-3-(1H-1,2,4-triazol-1-yl)propan-2-ol	[M+H] <sup>+</sup>	Benzenoids
112	1.43	488.2412	Methyl (2E,8E)-9-[3a-hydroxy-6,7-dimethyl-1-(2-methylpropyl)-3-oxo-2,4,7,7a-tetrahydro-1H-isoindol-4-yl]-4,5-dihydroxy-8-methylnona-2,8-dienoate	[M+K] <sup>+</sup>	Lipids and lipid-like molecules
113	1.462	258.1071	2'-O-Methylcytidine	[M+H] <sup>+</sup>	Nucleosides, nucleotides, and analogues
114	1.462	112.0498	Pyrrole-2-carboxylic acid	[M+H] <sup>+</sup>	Organoheterocyclic compounds
115	1.462	130.0866	Leucine	[M-H] <sup>-</sup>	Organic acids and derivatives
116	1.463	131.034	Methylsuccinic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
117	1.468	150.0419	Guanine	[M-H] <sup>-</sup>	Organoheterocyclic compounds
118	1.471	332.1328	Pyridoxine + O-Hex	[M+H] <sup>+</sup>	Organoheterocyclic compounds
119	1.473	138.0556	4-Nitrophenol	[M-H] <sup>-</sup>	Benzenoids
120	1.473	176.0377	N-Formylmethionine	[M-H] <sup>-</sup>	Organic acids and derivatives
121	1.526	155.0804	Cyclo-prolylglycine	[M+H] <sup>+</sup>	Organic acids and derivatives
122	1.526	381.1353	Fumiquinazoline F	[M+Na] <sup>+</sup>	Organoheterocyclic compounds
123	1.535	123.0543	Nicotinamide	[M+H] <sup>+</sup>	Organoheterocyclic compounds
124	1.574	80.04843	Pyridine	[M+H] <sup>+</sup>	Organoheterocyclic compounds
125	1.576	233.1484	Threonylleucine	[M+H] <sup>+</sup>	Organic acids and derivatives
126	1.604	261.1433	h-gamma-Glu-leu-oh	[M+H] <sup>+</sup>	Organic acids and derivatives
127	1.635	266.0904	2'-Deoxyguanosine	[M-H] <sup>-</sup>	Nucleosides, nucleotides, and analogues
128	1.651	131.1287	Agmatine	[M+H] <sup>+</sup>	Organic nitrogen compounds
129	1.666	163.0397	3-Hydroxycinnamic acid	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
130	1.671	117.0549	3-Hydroxypentanoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
131	1.689	295.1279	H-Asp-Phe-OMe	[M+H] <sup>+</sup>	Organic acids and derivatives
132	1.711	203.1391	Ala-Leu	[M+H] <sup>+</sup>	Organic acids and derivatives
133	1.715	187.1087	Gly-Leu	[M-H] <sup>-</sup>	Organic acids and derivatives
134	1.717	328.0457	Adenosine 2',3'-cyclic phosphate	[M-H] <sup>-</sup>	Nucleosides, nucleotides, and analogues
135	1.759	308.1553	Tebuconazole	[M+H] <sup>+</sup>	Benzenoids
136	1.772	191.0181	Hydron;2-hydroxypropane-1,2,3-tricarboxylate	[M-H] <sup>-</sup>	Organic acids and derivatives
137	1.774	116.0695	Pyrrolidin-1-ium-2-carboxylate	[M+H] <sup>+</sup>	Organic acids and derivatives

138	1.779	367.0968	(E)-3-(3,4-Dihydroxyphenyl)acrylic acid (1R,2R,3R)-2,3,5-trihydroxy-5-(methoxycarbonyl)cyclohexyl ester	[M-H]-	Organic oxygen compounds
139	1.78	353.085	N(4)-Acetylsulfadimethoxine	[M+H]+	Benzenoids
140	1.787	138.0529	Anthranilic acid	[M+H]+	Benzenoids
141	1.806	296.1007	2'-O-Methylguanosine	[M-H]-	Nucleosides, nucleotides, and analogues
142	1.822	129.0189	Hydron;2-methylidenebutanedioate	[M-H]-	Lipids and lipid-like molecules
143	1.822	343.1282	Tyr-Tyr	[M-H]-	Organic acids and derivatives
144	1.833	181.0506	2-Hydroxy-3-(4-hydroxyphenyl)propanoic acid	[M-H]-	Phenylpropanoids and polyketides
145	1.852	329.2177	17alpha-Hydroxypregn-4-ene-3,20-dione	[M-H]-	Lipids and lipid-like molecules
146	1.877	210.0484	Dimethirimol	[M+H]+	Undefined
147	1.877	310.0027	5-Hydroxydiclofenac	[M-H]-	Benzenoids
148	1.878	149.0578	p-Coumaraldehyde	[M+H]+	Phenylpropanoids and polyketides
149	1.888	244.13	Leu-Gly-Gly	[M-H]-	Organic acids and derivatives
150	1.892	182.0449	4-Pyridoxic acid	[M-H]-	Organoheterocyclic compounds
151	1.894	337.1524	alpha-Cyclopiazonic acid	[M+H]+	Organoheterocyclic compounds
152	1.914	218.1029	Calcium pantothenate	[M-H]-	Undefined
153	1.925	353.0873	Neochlorogenic acid	[M-H]-	Organic oxygen compounds
154	1.927	355.0989	Cryptochlorogenic acid	[M+H]+	Organic oxygen compounds
155	1.932	163.038	4-Hydroxycoumarin	[M+H]+	Phenylpropanoids and polyketides
156	1.936	364.1209	9-Aminocamptothecin	[M+H]+	Undefined
157	1.947	180.0862	D-(+)-Glucosamine	[M+H]+	Undefined
158	1.956	296.0986	3'-O-Methylguanosine	[M-H]-	Nucleosides, nucleotides, and analogues
159	1.964	137.0452	Hypoxanthine	[M+H]+	Organoheterocyclic compounds
160	1.979	237.1232	Carbetamide	[M+H]+	Undefined
161	1.981	285.1559	L-Ornithine	[M-H]-	Organic acids and derivatives
162	1.99	225.0742	2-(2-Acetyl-3-hydroxy-5-methoxyphenyl)acetic acid	[M+H]+	Organic oxygen compounds
163	1.992	183.0642	Syringaldehyde	[M+H]+	Benzenoids
164	2.018	312.1532	Leonurine	[M+H]+	Undefined
165	2.026	302.11	Flutriafol	[M+H]+	Benzenoids
166	2.031	220.1184	Pantothenic acid	[M+H]+	Organic acids and derivatives
167	2.032	242.0984	D-Pantothenic acid	[M+Na]+	Organic acids and derivatives
168	2.048	279.0989	L-Aspartyl-L-phenylalanine	[M-H]-	Organic acids and derivatives
169	2.064	190.054	N-Acetyl-DL-methionine	[M-H]-	Organic acids and derivatives
170	2.068	164.0725	Phenylalanine	[M-H]-	Organic acids and derivatives
171	2.069	122.0584	Benzamide	[M+H]+	Benzenoids
172	2.079	268.1025	2-(6-Aminopurin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol	[M+H]+	Nucleosides, nucleotides, and analogues

173	2.084	546.2625	Homoharringtonine	[M+H] <sup>+</sup>	Undefined
174	2.084	353.0876	3-[3-(3,4-Dihydroxyphenyl)prop-2-enoyloxy]-1,4,5-trihydroxycyclohexane-1-carboxylic acid	[M-H] <sup>-</sup>	Organic oxygen compounds
175	2.085	257.0768	2'-O-Methyluridine	[M-H] <sup>-</sup>	Nucleosides, nucleotides, and analogues
176	2.089	304.1281	Imazamox	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
177	2.098	231.1706	H-DL-xille-DL-Val-OH	[M+H] <sup>+</sup>	Organic acids and derivatives
178	2.118	262.0909	Flumequine	[M+H] <sup>+</sup>	Organoheterocyclic compounds
179	2.13	659.3348	(2E,6E,10E)-14-[[2-O-(beta-D-Glucopyranosyl)-beta-D-glucopyranosyl]oxy]-4-hydroxy-2,6,10,14-tetramethyl-2,6,10,15-hexadecatetraenoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
180	2.137	116.0715	Valine	[M-H] <sup>-</sup>	Organic acids and derivatives
181	2.142	351.106	1-(4-Hydroxyphenyl)-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxypropan-1-one	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
182	2.16	448.2238	Aspergamid B	[M+H] <sup>+</sup>	Organoheterocyclic compounds
183	2.162	317.1084	(1E,4E)-1,5-Bis(4-methoxyphenyl)penta-1,4-dien-3-one	[M+Na] <sup>+</sup>	Benzenoids
184	2.171	413.2003	Gardneramine	[M+H] <sup>+</sup>	Organoheterocyclic compounds
185	2.173	252.1092	Cordycepin	[M+H] <sup>+</sup>	Nucleosides, nucleotides, and analogues
186	2.182	384.1687	Prazosin	[M+H] <sup>+</sup>	Organoheterocyclic compounds
187	2.195	235.1092	Alanylphenylalanine	[M-H] <sup>-</sup>	Organic acids and derivatives
188	2.247	299.0758	Salicylic acid glucoside	[M-H] <sup>-</sup>	Organic oxygen compounds
189	2.261	259.1294	gamma-Glu-leu	[M-H] <sup>-</sup>	Organic acids and derivatives
190	2.261	353.0906	1-Caffeoylquinic acid	[M-H] <sup>-</sup>	Organic oxygen compounds
191	2.29	342.1589	Naltrexone	[M+H] <sup>+</sup>	Benzenoids
192	2.296	133.9983	Acetanilide	[M-H] <sup>-</sup>	Benzenoids
193	2.309	134.0465	Adenine	[M-H] <sup>-</sup>	Organoheterocyclic compounds
194	2.313	118.004	L-Allothreonine	[M-H] <sup>-</sup>	Organic acids and derivatives
195	2.33	352.182	Retrorsine	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
196	2.338	215.0814	3-Ethyl-4-(methoxyamino)-2,5-dioximidazolidine-4-carboxamide	[M-H] <sup>-</sup>	Organoheterocyclic compounds
197	2.342	295.1256	Glutamylphenylalanine	[M+H] <sup>+</sup>	Organic acids and derivatives
198	2.354	337.0877	Cirsimaritin	[M+Na] <sup>+</sup>	Phenylpropanoids and polyketides
199	2.355	203.0828	Tryptophan	[M-H] <sup>-</sup>	Organoheterocyclic compounds
200	2.357	310.1725	Fluperlapine	[M+H] <sup>+</sup>	Organoheterocyclic compounds
201	2.36	132.0785	2-Methylindole	[M+H] <sup>+</sup>	Organoheterocyclic compounds
202	2.36	144.0798	Tryptophol	[M+H-H <sub>2</sub> O] <sup>+</sup>	Organoheterocyclic compounds
203	2.362	315.0921	Pantoyl lactone glucoside	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
204	2.368	118.0633	Norvaline	[M+H] <sup>+</sup>	Organic acids and derivatives
205	2.434	284.1102	Crotonoside	[M+H] <sup>+</sup>	Nucleosides, nucleotides, and analogues

206	2.458	468.2889	Delsoline	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
207	2.469	433.1441	Bruceine D	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
208	2.476	254.1249	Penciclovir	[M+H] <sup>+</sup>	Organoheterocyclic compounds
209	2.478	178.1212	Phenmetrazine	[M+H] <sup>+</sup>	Organoheterocyclic compounds
210	2.483	261.13	Diaveridine	[M+H] <sup>+</sup>	Benzenoids
211	2.485	151.0398	Benzoylformic acid	[M-H] <sup>-</sup>	Benzenoids
212	2.496	137.0235	Salicylic acid	[M-H] <sup>-</sup>	Benzenoids
213	2.498	743.2994	Ritonavir	[M+Na] <sup>+</sup>	Organic acids and derivatives
214	2.527	310.1146	N,N-Dimethylguanosine	[M-H] <sup>-</sup>	Nucleosides, nucleotides, and analogues
215	2.532	282.1201	2'-O-Methyladenosine	[M+H] <sup>+</sup>	Nucleosides, nucleotides, and analogues
216	2.54	135.0448	Phenylacetic acid	[M-H] <sup>-</sup>	Benzenoids
217	2.547	337.0922	3-p-Coumaroylquinic acid	[M-H] <sup>-</sup>	Organic oxygen compounds
218	2.548	453.1328	Polygalatenoside A	[M+Na] <sup>+</sup>	Organic oxygen compounds
219	2.551	163.0402	4-Hydroxycinnamic acid	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
220	2.553	413.1442	1-[4-[2-(7-Methoxy-1,3-benzodioxol-5-yl)ethyl]phenoxy]-3-methylbutane-2,3-diol	[M+K] <sup>+</sup>	Phenylpropanoids and polyketides
221	2.561	147.0431	Coumarin	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
222	2.565	563.1521	8-[3,4-Dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-5,7-dihydroxy-2-(4-hydroxyphenyl)-6-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]chromen-4-one	[M-H] <sup>-</sup>	Undefined
223	2.567	179.035	Caffeic acid	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
224	2.594	353.0873	4-Caffeoylquinic acid;4-O-Caffeoylquinic acid	[M-H] <sup>-</sup>	Organic oxygen compounds
225	2.606	195.0639	4-Formyl-2-methoxyphenyl acetate	[M+H] <sup>+</sup>	Benzenoids
226	2.625	188.035	Kynurenic acid	[M-H] <sup>-</sup>	Organoheterocyclic compounds
227	2.647	122.0956	Phenethylamine	[M+H] <sup>+</sup>	Benzenoids
228	2.647	105.0698	3-Cyanopyridine	[M+H] <sup>+</sup>	Organoheterocyclic compounds
229	2.653	339.0717	Esculin	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
230	2.654	144.0441	4-Hydroxyquinoline	[M-H] <sup>-</sup>	Organoheterocyclic compounds
231	2.688	413.1418	N6-Carbamoyl-L-threonyladenosine	[M+H] <sup>+</sup>	Nucleosides, nucleotides, and analogues
232	2.69	367.1017	3-Feruloylquinic acids	[M-H] <sup>-</sup>	Undefined
233	2.714	543.3115	Puberanidine	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
234	2.762	229.1543	1-(2-Ammonio-4-methylpentanoyl)pyrrolidine-2-carboxylate	[M+H] <sup>+</sup>	Organic acids and derivatives
235	2.822	271.0827	Arbutin	[M-H] <sup>-</sup>	Undefined
236	2.836	282.1197	1-Methyladenosine	[M+H] <sup>+</sup>	Nucleosides, nucleotides, and analogues
237	2.86	328.0761	Fluazifop	[M+H] <sup>+</sup>	Benzenoids
238	2.863	367.1018	5-O-Feruloylquinic acid	[M-H] <sup>-</sup>	Organic oxygen compounds

239	2.864	431.1287	Nodakenin	[M+Na] <sup>+</sup>	Phenylpropanoids and polyketides
240	2.871	447.0926	Cyanidin 3-O-galactoside	[M-2H] <sup>-</sup>	Phenylpropanoids and polyketides
241	2.875	193.0489	3-(4-Hydroxy-3-methoxyphenyl)-2-propenoic acid	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
242	2.898	641.322	Steviolbioside	[M-H] <sup>-</sup>	Undefined
243	2.906	355.1011	Staphylin	[M+H] <sup>+</sup>	Organic oxygen compounds
244	2.907	639.1675	3-[(2S,3R,4S,5R,6R)-3-[(2S,3S,4R,5R,6S)-3,5-Dihydroxy-4-methoxy-6-methyloxan-2-yl]oxy-4,5-dihydroxy-6-methyloxan-2-yl]oxy-8-hydroxy-15-methyl-11,18-dioxapentacyclo[10.6.2.02,7.09,19.016,20]icosa-1(19),2(7),3,5,8,12(20),13,15-octaene-10,17-dione	[M-H] <sup>-</sup>	Organoheterocyclic compounds
245	2.921	241.1206	Pyroglutamylisoleucine	[M-H] <sup>-</sup>	Organic acids and derivatives
246	2.924	163.0403	2-Hydroxycinnamic acid	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
247	2.94	589.2525	3-[[6-[[1,4a-Dimethyl-6-methylidene-5-[2-(5-oxo-2H-furan-4-yl)ethyl]-3,4,5,7,8,8a-hexahydro-2H-naphthalen-1-yl]methoxy]-3,4,5-trihydroxyoxan-2-yl]methoxy]-3-oxopropanoic acid	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
248	2.944	385.1122	Sinapoylhexoside	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
249	2.952	381.0924	(7E,13E)-9,15-Dihydroxy-4,10,16-trimethyl-1,5,11-trioxacyclohexadeca-7,13-diene-2,6,12-trione	[M+K] <sup>+</sup>	Phenylpropanoids and polyketides
250	2.955	167.0345	Vanillic acid	[M-H] <sup>-</sup>	Benzenoids
251	2.957	245.1848	H-DL-Leu-DL-Leu-OH	[M+H] <sup>+</sup>	Organic acids and derivatives
252	2.963	114.091	2-Imino-1-methylimidazolidin-4-one	[M+H] <sup>+</sup>	Organic acids and derivatives
253	2.966	165.019	Phthalic acid	[M-H] <sup>-</sup>	Benzenoids
254	2.979	179.0362	Aspirin	[M-H] <sup>-</sup>	Benzenoids
255	3.008	537.194	2-[4-[4-[Hydroxy-(4-hydroxy-3-methoxyphenyl)methyl]-3-(hydroxymethyl)oxolan-2-yl]-2-methoxyphenoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	[M-H] <sup>-</sup>	Lignans, neolignans and related compounds
256	3.01	561.1926	3-Hydroxy-1-(3-hydroxy-4-methoxyphenyl)-2-{4-[(1E)-3-hydroxy-1-propen-1-yl]-2-methoxyphenoxy}propyl beta-D-glucopyranoside	[M+Na] <sup>+</sup>	Organic oxygen compounds
257	3.011	418.2258	Protostemonine	[M+H] <sup>+</sup>	Undefined
258	3.017	131.0711	2-Hydroxy-4-methylvaleric acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
259	3.025	191.035	Isoscapoletin	[M-H] <sup>-</sup>	Undefined
260	3.026	399.0926	Scopolin	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
261	3.043	517.1546	Sibiricose A5	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
262	3.057	483.1459	Paeonolide	[M+H] <sup>+</sup>	Undefined
263	3.078	547.1634	[(2R,3S,4S,5R,6R)-6-[(2S,3S,4S,5R)-3,4-Dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-3,4,5-trihydroxyoxan-2-yl]methyl (E)-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enoate	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides

264	3.095	265.1104	Thiamine	[M] <sup>+</sup>	Organoheterocyclic compounds
265	3.114	411.1243	Phenyl 6-O-[(2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)tetrahydro-2-furanyl]-beta-D-glucopyranoside	[M+Na] <sup>+</sup>	Organic oxygen compounds
266	3.115	159.065	3-Methyladipic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
267	3.121	377.1239	Fusarenone X	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
268	3.122	85.06549	3-Methyl-3-buten-2-one	[M-H] <sup>-</sup>	Undefined
269	3.148	697.3439	Cyanidin-3-(6"-malonylglucoside)	[M+NH <sub>4</sub> ] <sup>+</sup>	Undefined
270	3.162	149.0232	2-Carboxybenzaldehyde	[M-H] <sup>-</sup>	Benzenoids
271	3.165	177.0534	7-Methoxycoumarin	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
272	3.172	265.1538	H-DL-Val-DL-Phe-OH	[M+H] <sup>+</sup>	Organic acids and derivatives
273	3.175	477.0618	1-Methoxyindol-3-ylmethyl glucosinolate	[M-H] <sup>-</sup>	Undefined
274	3.21	323.1098	Desmedipham	[M+Na] <sup>+</sup>	Benzenoids
275	3.218	752.4186	Germinaline	[M+H] <sup>+</sup>	Undefined
276	3.219	177.0192	Daphnetin	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
277	3.227	395.1279	Syringin	[M+Na] <sup>+</sup>	Organic oxygen compounds
278	3.23	369.1169	Dimethyl 2-[3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enoyloxy]butanedioate	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
279	3.253	195.0639	Isoferulic acid	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
280	3.258	172.098	N-Acetyl-L-leucine	[M-H] <sup>-</sup>	Organic acids and derivatives
281	3.27	165.0564	L-(-)-3-Phenyllactic acid	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
282	3.284	551.2769	Isogomphrenin I	[M+H] <sup>+</sup>	Organic oxygen compounds
283	3.298	769.221	7-O-Methylquercetin-3-O-galactoside-6"-rhamnoside	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
284	3.321	325.0921	Coumaric acid 4-O-glucoside	[M-H] <sup>-</sup>	Organic oxygen compounds
285	3.323	243.1709	H-DL-xille-DL-xille-OH	[M-H] <sup>-</sup>	Organic acids and derivatives
286	3.326	193.0511	Cinnamic acid	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
287	3.332	495.2563	Leukotriene D4	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
288	3.343	367.1016	Methyl chlorogenate	[M-H] <sup>-</sup>	Organic oxygen compounds
289	3.351	439.1554	Sayaenoside	[M+Na] <sup>+</sup>	Organic oxygen compounds
290	3.367	368.1757	Jacobine N-oxide	[M+H] <sup>+</sup>	Alkaloids and derivatives
291	3.369	121.0288	Hydron;benzoate	[M-H] <sup>-</sup>	Benzenoids
292	3.377	611.1547	Cyanin	[M] <sup>+</sup>	Phenylpropanoids and polyketides
293	3.385	449.1078	Luteolin-4'-o-glucoside	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
294	3.398	349.1173	(13-Methyl-17-oxo-7,8,9,11,12,14,15,16-octahydro-6H-cyclopenta[a]phenanthren-3-yl) hydrogen sulfate	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
295	3.401	321.0925	N(4)-Acetylsulfamethazine	[M+H] <sup>+</sup>	Benzenoids

296	3.401	561.1935	2-Methoxy-4-[(2R,3R,4S)-tetrahydro-4-hydroxy-4-[(4-hydroxy-3-methoxyphenyl)methyl]-3-(hydroxymethyl)-2-furanyl]phenyl-beta-D-glucopyranoside	[M+Na] <sup>+</sup>	Lignans, neolignans and related compounds
297	3.403	305.1109	Diazinon	[M+H] <sup>+</sup>	Organic acids and derivatives
298	3.408	172.098	Acetylleucine	[M-H] <sup>-</sup>	Organic acids and derivatives
299	3.414	605.1809	Methyl (4S,5Z,6S)-5-(2-acetyloxyethylidene)-4-[2-[2-(4-hydroxyphenyl)ethoxy]-2-oxoethyl]-6-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4H-pyran-3-carboxylate	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
300	3.426	309.094	Salicin	[M+H] <sup>+</sup>	Organic oxygen compounds
301	3.438	291.0833	Chloroxuron	[M+H] <sup>+</sup>	Benzenoids
302	3.438	190.0503	5-Hydroxyindole-3-acetic acid	[M-H] <sup>-</sup>	Organoheterocyclic compounds
303	3.446	755.1826	Quercetin 3-O-[2''-O-(6'''-O-p-coumaroyl)-b-D-glucopyranosyl]-a-L-rhamnopyranoside	[M-H] <sup>-</sup>	Undefined
304	3.452	148.038	Isatin	[M+H] <sup>+</sup>	Organoheterocyclic compounds
305	3.453	281.1376	Octyl gallate	[M-H] <sup>-</sup>	Undefined
306	3.47	222.1342	DL-Dihydrozeatin	[M+H] <sup>+</sup>	Organoheterocyclic compounds
307	3.488	492.2446	Imatinib	[M-H] <sup>-</sup>	Benzenoids
308	3.508	342.1438	Sulpiride	[M+H] <sup>+</sup>	Benzenoids
309	3.513	349.1829	Imidocarb	[M+H] <sup>+</sup>	Benzenoids
310	3.516	206.0816	N-Acetyl-L-phenylalanine	[M-H] <sup>-</sup>	Organic acids and derivatives
311	3.527	370.1765	Amisulpride	[M+H] <sup>+</sup>	Benzenoids
312	3.539	669.3503	Goshonoside F5	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
313	3.539	298.0965	5'-Deoxy-5'-methylthioadenosine	[M+H] <sup>+</sup>	Nucleosides, nucleotides, and analogues
314	3.544	163.0398	3-(3-Hydroxy-phenyl)-acrylic acid	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
315	3.549	445.1608	Tetracycline	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
316	3.581	204.066	Indole-3-lactic acid	[M-H] <sup>-</sup>	Organoheterocyclic compounds
317	3.598	609.145	Luteolin-7,3'-di-O-galactoside	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
318	3.603	175.0253	Ascorbic acid	[M-H] <sup>-</sup>	Organoheterocyclic compounds
319	3.603	609.1694	5-Hydroxy-2-(3-hydroxy-4-methoxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxy-2,3-dihydrochromen-4-one	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
320	3.631	421.0742	Mangiferin	[M-H] <sup>-</sup>	Organoheterocyclic compounds
321	3.641	385.1133	1-O-Sinapoyl-beta-D-glucose	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
322	3.647	409.1093	Khelloside	[M+H] <sup>+</sup>	Organoheterocyclic compounds
323	3.66	394.1968	Glutamyl-valyl-phenylalanine	[M+H] <sup>+</sup>	Organic acids and derivatives
324	3.67	245.094	N-Acetyl-D-tryptophan	[M-H] <sup>-</sup>	Organic acids and derivatives

325	3.705	265.1425	Dihydro-3-methylene-4-[(2E)-3-methyl-4-(tetrahydro-4-methyl-5-oxo-2-furanyl)-2-buten-1-yl]-, (4R)-2(3H)-furanone,	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
326	3.724	163.0403	Phenylpyruvic acid	[M-H] <sup>-</sup>	Benzenoids
327	3.726	559.1746	8-Hydroxypinoresinol 4'-glucoside	[M+Na] <sup>+</sup>	Lignans, neolignans and related compounds
328	3.732	411.2184	Risperidone	[M+H] <sup>+</sup>	Organoheterocyclic compounds
329	3.733	406.2314	H-Leu-Leu-Tyr-OH	[M-H] <sup>-</sup>	Organic acids and derivatives
330	3.782	218.1051	trans-Zeatin	[M-H] <sup>-</sup>	Organoheterocyclic compounds
331	3.802	393.2091	Octaethylene glycol	[M+Na] <sup>+</sup>	Organic oxygen compounds
332	3.819	431.2488	Bufalin	[M+FA-H] <sup>-</sup>	Undefined
333	3.823	375.1308	Riboflavin	[M-H] <sup>-</sup>	Organoheterocyclic compounds
334	3.829	357.1333	Pinoresinol	[M-H] <sup>-</sup>	Lignans, neolignans and related compounds
335	3.851	639.161	isorhamnetin-3-glucoside-4'-glucoside (Isorhamnetin 3,4'-diglucoside)	[M-H] <sup>-</sup>	Undefined
336	3.87	455.151	5-(1-benzofuran-2-yl)-N,N-dimethyl-2-[4-(piperazin-1-yl)phenyl]-1,3-thiazole-4-carboxamide	[M+Na] <sup>+</sup>	Organoheterocyclic compounds
337	3.873	575.1696	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	[M+Na] <sup>+</sup>	Lignans, neolignans and related compounds
338	3.883	421.161	3-[(7S,8S)-5-Hydroxy-2,2,7,8-tetramethyl-6-oxo-7,8-dihydropyrano[3,2-g]chromen-10-yl]-3-phenylpropanoic acid	[M-H] <sup>-</sup>	Organoheterocyclic compounds
339	3.884	134.0584	Indoxyl sulfate	[M+H] <sup>+</sup>	Organic acids and derivatives
340	3.9	247.1065	N-(6-Methoxyquinolin-8-yl)alanine	[M+H] <sup>+</sup>	Organoheterocyclic compounds
341	3.932	121.0294	4-Hydroxybenzaldehyde	[M-H] <sup>-</sup>	Organic oxygen compounds
342	3.934	137.0585	Sabinene	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
343	3.94	181.0498	Methyl vanillate	[M-H] <sup>-</sup>	Benzenoids
344	3.941	195.0665	3-(4-Hydroxy-3-methoxyphenyl)propionic acid	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
345	3.967	611.1966	Dihydrohesperetin-7-O-neohesperidoside	[M-H] <sup>-</sup>	Undefined
346	3.975	623.2769	Thalsimidine	[M+H] <sup>+</sup>	Lignans, neolignans and related compounds
347	3.984	114.0372	4-Isothiocyanato-1-butene	[M+2Na-H] <sup>+</sup>	Undefined
348	4	301.0352	Quercetin	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
349	4.003	193.0499	Ferulic acid	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
350	4.005	223.0605	Sinapic acid	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
351	4.006	285.0412	Rhein	[M+H] <sup>+</sup>	Benzenoids
352	4.021	181.0846	Isopropyl 4-Hydroxybenzoate	[M+H] <sup>+</sup>	Undefined
353	4.038	427.1693	[1-(3,4-Dihydroxy-5-methoxyphenyl)-7-(3,4-dihydroxyphenyl)heptan-3-yl] acetate	[M+Na] <sup>+</sup>	Phenylpropanoids and polyketides
354	4.039	593.2589	1,7-Bis(4-hydroxyphenyl)-3-heptanyl 2-O-[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)tetrahydro-2-furanyl]-beta-D-glucopyranoside	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides

355	4.04	177.0544	Hymecromone	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
356	4.047	453.2084	6-(beta-D-Glucopyranosyloxy)-4,5,6,7,8,8a-hexahydro-5-hydroxy-5-(1-hydroxy-1-methylethyl)-3,8-dimethyl-2(1H)-azulenone	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
357	4.055	352.1601	trans-Ribosylzeatin	[M+H] <sup>+</sup>	Nucleosides, nucleotides, and analogues
358	4.059	167.0702	Ethylparaben	[M+H] <sup>+</sup>	Benzenoids
359	4.073	413.1193	2,3,4,9,10-Pentamethoxy-6a,11a-dihydro-6H-[1]benzofuro[3,2-c]chromen-8-ol	[M+Na] <sup>+</sup>	Phenylpropanoids and polyketides
360	4.088	167.0611	9H-Pyrido[3,4-B]indole	[M-H] <sup>-</sup>	Organoheterocyclic compounds
361	4.089	399.1077	4'-Demethylpodophyllotoxin	[M-H] <sup>-</sup>	Lignans, neolignans and related compounds
362	4.089	191.0352	Scopoletin	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
363	4.095	174.057	Indole-3-acetic acid	[M-H] <sup>-</sup>	Organoheterocyclic compounds
364	4.097	575.2067	Lyoniside	[M+Na] <sup>+</sup>	Lignans, neolignans and related compounds
365	4.106	415.1043	Puerarin	[M-H] <sup>-</sup>	Undefined
366	4.112	449.1046	Cyanidin 3-O-glucoside	[M] <sup>+</sup>	Phenylpropanoids and polyketides
367	4.113	609.1448	Panasenoside	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
368	4.116	447.0894	Astragalin	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
369	4.131	229.0861	Resveratrol	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
370	4.142	169.0751	5H-Pyrido[4,3-b]indole	[M+H] <sup>+</sup>	Organoheterocyclic compounds
371	4.171	765.2581	(2S,3R,4S,5S,6R)-2-[4-[(3S,3aR,6S,6aR)-6-[3,5-Dimethoxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]-1,3,3a,4,6,6a-hexahydrofuro[3,4-c]furan-3-yl]-2,6-dimethoxyphenoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	[M+Na] <sup>+</sup>	Lignans, neolignans and related compounds
372	4.18	325.0904	Skimmin	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
373	4.195	646.3165	Aconitine	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
374	4.22	361.1645	Secoisolariciresinol	[M-H] <sup>-</sup>	Undefined
375	4.244	441.1165	Barbaloin	[M+Na] <sup>+</sup>	Benzenoids
376	4.263	399.1398	Ailanthone	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
377	4.268	211.1435	(3S,8As)-3-Isobutylhexahydropyrrolo[1,2-a]pyrazine-1,4-dione	[M+H] <sup>+</sup>	Organic acids and derivatives
378	4.278	345.1873	3-[(4As,12aR)-2-methyl-1,3,4,5,12,12a-hexahydropyrido[3,4-b]acridin-4a-yl]phenol	[M+H] <sup>+</sup>	Organoheterocyclic compounds
379	4.285	217.1074	3-Hydroxysebacic acid	[M-H] <sup>-</sup>	Organic acids and derivatives
380	4.286	303.1186	(3As,6S,7R,8aR)-8-hydroxy-6,8-dimethyl-3-methylidenespiro[4,5,6,8a-tetrahydro-3aH-cyclohepta[b]furan-7,5'-oxolane]-2,2'-dione	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
381	4.306	545.1977	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	[M+Na] <sup>+</sup>	Phenylpropanoids and polyketides
382	4.308	139.11	Isophorone	[M+H] <sup>+</sup>	Organic oxygen compounds
383	4.331	247.129	Santonin	[M+H] <sup>+</sup>	Lipids and lipid-like molecules

384	4.352	395.1754	Veraguensin	[M+Na] <sup>+</sup>	Lignans, neolignans and related compounds
385	4.355	329.1569	Tiapride	[M+H] <sup>+</sup>	Benzenoids
386	4.377	178.0512	(Sulfonatoazaniumyl)cyclohexane	[M-H] <sup>-</sup>	Organic acids and derivatives
387	4.378	307.114	Cimifugin	[M+H] <sup>+</sup>	Organoheterocyclic compounds
388	4.402	501.1581	[3,4,5-Trihydroxy-6-[(3,4,5-trihydroxyoxan-2-yl)oxymethyl]oxan-2-yl] 2,6,6-trimethylcyclohexene-1-carboxylate	[M+K] <sup>+</sup>	Organic oxygen compounds
389	4.427	160.0399	Indole-3-carboxylic acid	[M-H] <sup>-</sup>	Organoheterocyclic compounds
390	4.446	525.2886	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	[M+K] <sup>+</sup>	Lipids and lipid-like molecules
391	4.458	339.1056	(3R,5R)-1,3,5-trihydroxy-4-[(E)-3-(4-hydroxyphenyl)acryloyl]oxy-cyclohexanecarboxylic acid	[M+H] <sup>+</sup>	Organic oxygen compounds
392	4.469	144.0462	Indole-3-carboxaldehyde	[M-H] <sup>-</sup>	Organoheterocyclic compounds
393	4.471	473.1405	[(1S)-5-hydroxy-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-1,4a,5,7a-tetrahydrocyclopenta[c]pyran-7-yl]methyl benzoate	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
394	4.485	177.0557	4-Hydroxy-3-methoxycinnamaldehyde	[M-H] <sup>-</sup>	Benzenoids
395	4.488	209.0788	3,5-Dimethoxycinnamic acid	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
396	4.524	443.1286	Isorhapontin	[M+Na] <sup>+</sup>	Phenylpropanoids and polyketides
397	4.529	285.1669	(4E,6E)-2-(Hydroxymethyl)-3-(3-methoxy-3-oxopropyl)deca-4,6-dienoic acid	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
398	4.541	428.2492	(3R,7R,8R,8aS)-3,4'-Dihydroxy-7'-(2-hydroxyethyl)-4,4,7,8a-tetramethylspiro[2,3,4a,5,6,7-hexahydro-1H-naphthalene-8,2'-3,8-dihydrofuro[2,3-e]isoindole]-6'-one	[M-H] <sup>-</sup>	Organoheterocyclic compounds
399	4.543	197.1177	Lolilide	[M+H] <sup>+</sup>	Organoheterocyclic compounds
400	4.555	631.1605	Diosmetin-7-O-rutinoside	[M+Na] <sup>+</sup>	Phenylpropanoids and polyketides
401	4.556	616.3171	Hypaconitine	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
402	4.575	336.1893	Senecionine	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
403	4.577	535.2325	Methyl 2-[(1R,5R,6R,13S,14S,16S)-14-acetyloxy-6-(furan-3-yl)-1,5,15,15-tetramethyl-8,17-dioxo-7-oxatetracyclo[11.3.1.02,11.05,10]heptadec-10-en-16-yl]acetate	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
404	4.587	486.2569	3',4',4'a,5',6,6',7',8,8',8'a-Decahydro-4,6',7'-trihydroxy-2',5',5',8'a-tetramethyl-6-oxo-, (2R,2'R,6'S,7'R,8'aS)-spiro[2H-furo[2,3-e]isoindole-2,1'(2'H)-naphthalene]-7(3H)-butanoic acid	[M-H] <sup>-</sup>	Organoheterocyclic compounds
405	4.589	312.13	Imazaquin	[M+H] <sup>+</sup>	Organoheterocyclic compounds
406	4.626	179.0348	4-Hydroxyphenylpyruvic acid	[M-H] <sup>-</sup>	Benzenoids
407	4.628	208.1307	Benzoylcholine	[M] <sup>+</sup>	Benzenoids
408	4.634	245.1276	Hexahydro-3-(phenylmethyl)-pyrrolo[1,2-a]pyrazine-1,4-dione	[M+H] <sup>+</sup>	Organic acids and derivatives
409	4.662	405.1538	Neosolaniol	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules

410	4.676	128.1062	N-Cyclohexylformamide	[M+H] <sup>+</sup>	Organic acids and derivatives
411	4.68	653.3216	Isohernandezine	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
412	4.68	359.1452	Triptonide	[M+H] <sup>+</sup>	Undefined
413	4.689	287.0554	Dihydrokaempferol	[M-H] <sup>-</sup>	Undefined
414	4.698	413.2127	Hexa(methoxymethyl)melamine	[M+Na] <sup>+</sup>	Organic nitrogen compounds
415	4.723	182.1886	Dicyclohexylamine	[M+H] <sup>+</sup>	Organic nitrogen compounds
416	4.742	632.3373	Pseudojervine	[M+FA-H] <sup>-</sup>	Undefined
417	4.758	753.2246	Hedysarimcoumestan D	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
418	4.759	487.3043	Polygalic acid	[M-H] <sup>-</sup>	Undefined
419	4.763	531.169	Sibiricose A6	[M-H <sub>2</sub> O+H] <sup>+</sup>	Phenylpropanoids and polyketides
420	4.766	529.3004	Kukoamine A	[M-H] <sup>-</sup>	Undefined
421	4.806	411.1608	2-[(2Z)-5-(Hexopyranosyloxy)-2-penten-1-yl]-3-oxo-, (1R,2R)-cyclopentaneacetic acid	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
422	4.809	213.0303	Mecoprop	[M-H] <sup>-</sup>	Benzenoids
423	4.83	151.0399	4-Methoxybenzoic acid	[M-H] <sup>-</sup>	Benzenoids
424	4.841	225.1457	5-(6-Methyl-7-oxooctyl)furan-2(5H)-one	[M+H] <sup>+</sup>	Organoheterocyclic compounds
425	4.842	292.1889	2-Oxostenine	[M+H] <sup>+</sup>	Alkaloids and derivatives
426	4.842	310.162	Sinapine	[M] <sup>+</sup>	Phenylpropanoids and polyketides
427	4.851	186.2213	Tributylamine	[M+H] <sup>+</sup>	Organic nitrogen compounds
428	4.853	195.0618	Dimethyl phthalate	[M+H] <sup>+</sup>	Benzenoids
429	4.86	331.1175	3-(2,4-Dihydroxypentyl)-6,8-dimethoxyisochromen-1-one	[M+Na] <sup>+</sup>	Phenylpropanoids and polyketides
430	4.885	178.035	Sulforaphane	[M+H] <sup>+</sup>	Organosulfur compounds
431	4.912	723.2134	Ligustroflavone	[M-H] <sup>-</sup>	Undefined
432	4.925	343.0651	(9-Hydroxy-8,8-dimethyl-2-oxo-9,10-dihydropyrano[2,3-f]chromen-10-yl) acetate	[M+K] <sup>+</sup>	Phenylpropanoids and polyketides
433	4.943	213.056	3-Phenoxybenzoic acid	[M-H] <sup>-</sup>	Benzenoids
434	4.966	261.133	9-(2,3-Dihydroxypropoxy)-9-oxononanoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
435	4.978	327.1771	Gelsenicine	[M+H] <sup>+</sup>	Organoheterocyclic compounds
436	4.999	411.1972	gamma-Tocotrienol	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
437	5.022	485.1957	(1R,4S,7S,8S,9R,12E,20R,21R,22S,23S)-7,8,21,22,23-Pentahydroxy-12,16-dimethyl-3,5,10,19,24-pentaoxatricyclo[18.3.1.0 <sub>4,9</sub> ]tetracos-12-en-11-one	[M+Na] <sup>+</sup>	Organic oxygen compounds
438	5.028	385.083	Methyl 2-hydroxy-6-(4-hydroxy-2-methoxy-6-methoxycarbonylphenoxy)-4-methylbenzoate	[M+Na] <sup>+</sup>	Benzenoids
439	5.061	447.0937	Kaempferol-3-O-glucoside	[M-H] <sup>-</sup>	Undefined
440	5.062	463.0869	Hyperoside	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides

441	5.064	519.2398	[(2R,3S,4S,5R,6S)-3,4,5-Trihydroxy-6-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl)methyl 8-methylnonanoate	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
442	5.069	325.1628	Citalopram	[M+H] <sup>+</sup>	Benzenoids
443	5.07	535.2133	Aerucyclamide A	[M+H] <sup>+</sup>	Organic acids and derivatives
444	5.076	415.1949	Hexose + C <sub>13</sub> H <sub>19</sub> O	[M+HCOO] <sup>-</sup>	Lipids and lipid-like molecules
445	5.079	222.0224	5-Ammonio-2-naphthalenesulfonate	[M-H] <sup>-</sup>	Benzenoids
446	5.103	321.1291	[2-[(E)-3,4-Dihydroxypent-1-enyl]-6-oxooxan-3-yl] (E)-2-methylbut-2-enoate	[M+Na] <sup>+</sup>	Organoheterocyclic compounds
447	5.116	89.0587	Isobutyric acid	[M+H] <sup>+</sup>	Organic acids and derivatives
448	5.116	187.0982	Hydron;nonanedioate	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
449	5.134	489.2258	Cytidine 5'-diphosphocholine	[M+H] <sup>+</sup>	Nucleosides, nucleotides, and analogues
450	5.138	275.1386	N-[1H-Indol-3-yl-acetyl]valine acid	[M+H] <sup>+</sup>	Organic acids and derivatives
451	5.142	385.2152	Corynoxine B	[M+H] <sup>+</sup>	Undefined
452	5.145	207.0633	Sinapoyl malate	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
453	5.147	158.0619	Indole-3-acetaldehyde	[M-H] <sup>-</sup>	Organoheterocyclic compounds
454	5.147	172.0416	Quinoline-4-carboxylic acid	[M-H] <sup>-</sup>	Organoheterocyclic compounds
455	5.153	188.0707	3-Indolepropionic acid	[M-H] <sup>-</sup>	Organoheterocyclic compounds
456	5.162	269.1727	3-[4-Methyl-1-(2-methylpropanoyl)-3-oxocyclohexyl]butanoic acid	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
457	5.171	327.1764	4-{Methyl[3-phenyl-3-(pyridin-2-yl)propyl]amino}-4-oxobutanoic acid	[M+H] <sup>+</sup>	Organoheterocyclic compounds
458	5.171	457.2367	Vindoline	[M+H] <sup>+</sup>	Undefined
459	5.172	209.1174	Pilocarpine	[M+H] <sup>+</sup>	Alkaloids and derivatives
460	5.183	343.1166	Kanakugiol	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
461	5.23	191.1033	Ligustilide	[M+H] <sup>+</sup>	Organoheterocyclic compounds
462	5.235	271.152	Quinolactacin A	[M+H] <sup>+</sup>	Organoheterocyclic compounds
463	5.245	325.1605	(2E)-4-{Methyl[3-phenyl-3-(pyridin-2-yl)propyl]amino}-4-oxobut-2-enoic acid	[M+H] <sup>+</sup>	Organoheterocyclic compounds
464	5.248	341.1335	8-Prenylnaringenin	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
465	5.258	243.0863	Lumichrome	[M+H] <sup>+</sup>	Organoheterocyclic compounds
466	5.263	385.2178	Corynoxine	[M+H] <sup>+</sup>	Undefined
467	5.264	362.1485	9-Fluoro-3-methyl-10-(4-methylpiperazin-4-ium-1-yl)-7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylate	[M+H] <sup>+</sup>	Organoheterocyclic compounds
468	5.272	174.0562	1-Methoxyindole-3-carbaldehyde	[M-H] <sup>-</sup>	Organoheterocyclic compounds
469	5.277	176.0703	4-Methoxy-1H-indole-3-carbaldehyde	[M+H] <sup>+</sup>	Organoheterocyclic compounds
470	5.282	547.1782	[4a,7-Dihydroxy-7-methyl-1-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-1,5,6,7a-tetrahydrocyclopenta[c]pyran-5-yl] (E)-3-(4-methoxyphenyl)prop-2-enoate	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
471	5.289	529.2615	Chaetoglobosin C	[M+H] <sup>+</sup>	Alkaloids and derivatives
472	5.294	253.1054	(2S)-2-[(1S,2R)-1,2-Dihydroxypentyl]-4-methoxy-2,3-dihdropyran-6-one	[M+Na] <sup>+</sup>	Organoheterocyclic compounds

473	5.324	266.0891	Adenosine	[M-H]-	Nucleosides, nucleotides, and analogues
474	5.334	483.1787	(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	[M+Na]+	Lipids and lipid-like molecules
475	5.334	248.1828	5-(Hydroxymethyl)-3-(1-hydroxy-4-methylhexyl)oxolan-2-one	[M+NH4]+	Lipids and lipid-like molecules
476	5.334	227.1236	12-Hydroxyjasmonic acid	[M+H]+	Lipids and lipid-like molecules
477	5.336	172.1319	1-(Aminomethyl)cyclohexaneacetate	[M+H]+	Organic acids and derivatives
478	5.34	275.1227	Heteropeucenin, methyl ether	[M+H]+	Organoheterocyclic compounds
479	5.347	349.1256	(+)-Camptothecin	[M+H]+	Alkaloids and derivatives
480	5.357	609.23	(1S,2S,3R,4S,7R,10S,12R,15S)-4,12-bis(acetyloxy)-1,9,15-trihydroxy-10,14,17,17-tetramethyl-11-oxo-6-oxatetracyclo[11.3.1.0 <sup>3,10</sup> .0 <sup>4,7</sup> ]heptadec-13-en-2-yl benzoate	[M+Na]+	Lipids and lipid-like molecules
481	5.413	173.1194	3-Hydroxynonanoic acid	[M-H]-	Organic acids and derivatives
482	5.415	225.1483	Methyl jasmonate	[M+H]+	Lipids and lipid-like molecules
483	5.424	263.1299	Dormin	[M-H]-	Lipids and lipid-like molecules
484	5.429	229.1222	Bisphenol A	[M+H]+	Benzenoids
485	5.429	247.1311	Ambrosic acid	[M-H2O+H]+	Organoheterocyclic compounds
486	5.441	285.1673	[5-Hydroxy-3-(hydroxymethyl)-2-oxo-6-propan-2-ylcyclohex-3-en-1-yl] 3-methylbutanoate	[M+H]+	Lipids and lipid-like molecules
487	5.441	193.1209	Senkyunolide A	[M+H]+	Undefined
488	5.455	149.0597	L(+)-Tartaric acid	[M-H]-	Organic oxygen compounds
489	5.485	429.2069	Majdine	[M+H]+	Organoheterocyclic compounds
490	5.494	379.1355	xi-3-Hydroxy-5-phenylpentanoic acid O-beta-D-Glucopyranoside	[M+Na]+	Lipids and lipid-like molecules
491	5.519	197.1531	Neryl acetate	[M+H]+	Lipids and lipid-like molecules
492	5.524	271.0895	(+)-Dihydrokawain-5-ol	[M+Na]+	Phenylpropanoids and polyketides
493	5.554	202.1101	N-(3-Methylbut-2-EN-1-YL)-9H-purin-6-amine	[M-H]-	Organoheterocyclic compounds
494	5.584	441.2451	N-Methyl-N-[(2E,4E,6E)-2,4,6-octatrienoyl]valylalanylprolinamide	[M+Na]+	Organic acids and derivatives
495	5.59	401.2051	Reserpine acid	[M+H]+	Alkaloids and derivatives
496	5.594	353.1546	(2,6,6-Trimethyl-4-oxo-2-cyclohexen-1-yl)methyl beta-D-glucopyranoside	[M+Na]+	Organic oxygen compounds
497	5.641	408.2719	Isotalatizidine	[M+H]+	Lipids and lipid-like molecules
498	5.659	397.2181	3,5,5-Trimethyl-4-[3-[(beta-D-glucopyranosyl)oxy]butyl]-3-cyclohexen-1-ol	[M+Na]+	Lipids and lipid-like molecules
499	5.689	289.1545	Indole-3-acetyl-L-leucine	[M+H]+	Organic acids and derivatives
500	5.696	295.1504	11-(Phenylcarbonyl)-7,11-diazatricyclo[7.3.1.0<2,7>]trideca-2,4-dien-6-one	[M+H]+	Organoheterocyclic compounds
501	5.698	148.074	3-Methyloxindole	[M+H]+	Organoheterocyclic compounds
502	5.832	343.2119	FA 18:2;4O	[M-H]-	Lipids and lipid-like molecules
503	5.832	201.112	Sebacic acid	[M-H]-	Lipids and lipid-like molecules
504	5.851	117.0542	3-Methyl-2-oxobutanoic acid	[M+H]+	Organic acids and derivatives
505	5.903	233.1529	Atractylenolide II	[M+H]+	Undefined

506	5.913	423.2342	Bonactin	[M+Na] <sup>+</sup>	Organic acids and derivatives
507	6.003	353.1383	3-(4-Hydroxyphenyl)propanoic acid 3-(4-hydroxy-3-methoxyphenyl)propyl ester	[M+Na] <sup>+</sup>	Benzenoids
508	6.015	590.3046	Benzoylmesaconine	[M+H] <sup>+</sup>	Undefined
509	6.028	403.1387	Methyl 2-(4,5-dihydroxy-6-methoxy-3,6-dimethyl-2-oxocyclohex-3-en-1-yl)oxy-4-hydroxy-3,6-dimethylbenzoate	[M+Na] <sup>+</sup>	Benzenoids
510	6.053	399.2364	Mitragynine	[M+H] <sup>+</sup>	Alkaloids and derivatives
511	6.078	229.1439	Dodecanedioic acid	[M-C <sub>6</sub> H <sub>8</sub> O <sub>6</sub> -H] <sup>-</sup>	Lipids and lipid-like molecules
512	6.111	327.2161	9,12,13-Trihydroxyoctadeca-10,15-dienoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
513	6.141	267.1549	Sambucinol	[M+H] <sup>+</sup>	Organoheterocyclic compounds
514	6.152	471.2184	(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	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
515	6.159	273.0416	2-Phenyl-3H-benzimidazol-1-ium-5-sulfonate	[M-H] <sup>-</sup>	Organoheterocyclic compounds
516	6.164	285.0405	Kaempferol	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
517	6.166	255.0278	Purpurin	[M-H] <sup>-</sup>	Benzenoids
518	6.196	341.1945	Pentamidine	[M+H] <sup>+</sup>	Benzenoids
519	6.198	281.1736	Brefeldin A	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
520	6.207	421.2183	2-[5-[2-[2-[5-(2-Oxopropyl)oxolan-2-yl]propanoyloxy]butyl]oxolan-2-yl]propanoic acid	[M+Na] <sup>+</sup>	Organic acids and derivatives
521	6.222	249.194	Matrine	[M+H] <sup>+</sup>	Alkaloids and derivatives
522	6.222	249.1496	Pterosin A	[M+H] <sup>+</sup>	Benzenoids
523	6.237	269.0472	Apigenin	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
524	6.259	427.1711	Fragransin B2	[M+Na] <sup>+</sup>	Lignans, neolignans and related compounds
525	6.26	299.18	Roquefortine A	[M+H] <sup>+</sup>	Alkaloids and derivatives
526	6.273	409.1809	4-[4-(beta-D-Glucopyranosyloxy)-2-hydroxy-2,6,6-trimethylcyclohexylidene]-3-buten-2-one	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
527	6.325	113.0594	1,4-Cyclohexanedione	[M+H] <sup>+</sup>	Organic oxygen compounds
528	6.328	305.1722	Zeranol	[M-H <sub>2</sub> O+H] <sup>+</sup>	Phenylpropanoids and polyketides
529	6.395	214.1789	N-(9-Oxodecyl)acetamide	[M+H] <sup>+</sup>	Organic acids and derivatives
530	6.397	399.1773	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	[M+Na] <sup>+</sup>	Organoheterocyclic compounds
531	6.404	367.2453	Isomuronic acid	[M+H] <sup>+</sup>	Organoheterocyclic compounds
532	6.408	209.1192	Jasmonic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
533	6.412	339.1752	(+)-18-Hydroxygardnutine	[M+H] <sup>+</sup>	Alkaloids and derivatives
534	6.452	439.0963	Daidzin	[M+Na] <sup>+</sup>	Phenylpropanoids and polyketides
535	6.453	329.2317	9,12,13-Trihydroxyoctadec-10-enoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules

536	6.475	352.2443	Jacobine	[M+H] <sup>+</sup>	Alkaloids and derivatives
537	6.503	192.1376	Diethyltoluamide	[M+H] <sup>+</sup>	Benzenoids
538	6.542	309.1667	Vincanidine	[M+H] <sup>+</sup>	Alkaloids and derivatives
539	6.543	435.2126	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	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
540	6.561	337.196	Tabersonine	[M+H] <sup>+</sup>	Alkaloids and derivatives
541	6.596	315.1104	Pyraclonil	[M+H] <sup>+</sup>	Organic nitrogen compounds
542	6.596	207.1355	Dexibuprofen	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
543	6.643	289.1786	12-Hydroxy-13-(hydroxymethyl)-3,5,7-trimethyl-2,4-tetradecadienedioic acid	[M-3H <sub>2</sub> O+H] <sup>+</sup>	Lipids and lipid-like molecules
544	6.7	163.1096	Valerophenone	[M+H] <sup>+</sup>	Organic oxygen compounds
545	6.736	323.1812	Gelsemine	[M+H] <sup>+</sup>	Alkaloids and derivatives
546	6.741	428.078	SMZ-PtO	[M-H] <sup>-</sup>	Benzenoids
547	6.749	341.1921	Yohimbic Acid	[M+H] <sup>+</sup>	Alkaloids and derivatives
548	6.755	327.2181	Corchorifatty acid F	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
549	6.796	325.202	FA 18:3;3O	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
550	6.815	623.3127	Tetrandrine	[M+H] <sup>+</sup>	Lignans, neolignans and related compounds
551	6.823	395.1982	Brucine	[M+H] <sup>+</sup>	Alkaloids and derivatives
552	6.83	266.1715	Mirtazapine	[M+H] <sup>+</sup>	Organoheterocyclic compounds
553	6.842	350.1569	Erucifoline	[M+H] <sup>+</sup>	Alkaloids and derivatives
554	6.845	367.2068	Hirsuteine	[M+H] <sup>+</sup>	Alkaloids and derivatives
555	6.848	209.1499	5-(6-Methyl-6-hydroxyoctyl)furan-2(5H)-one	[M-H <sub>2</sub> O+H] <sup>+</sup>	Organoheterocyclic compounds
556	6.852	343.2116	9-Hydroxy-11-[3-hydroxy-5-(1-hydroxypropyl)oxolan-2-yl]undec-10-enoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
557	6.868	335.1802	Strychnine sulfate	[M+H] <sup>+</sup>	Undefined
558	6.876	322.1997	Toxin HT 2	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
559	6.898	369.1617	(2S)-8-[(E)-3-Hydroxy-3-methylbut-1-enyl]-5,7-dimethoxy-2-phenyl-2,3-dihydrochromen-4-one	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
560	6.907	193.0877	Butylparaben	[M-H] <sup>-</sup>	Benzenoids
561	6.907	313.0347	Wedelolactone	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
562	6.912	585.3193	Lappaconitine hydrobromide	[M+H] <sup>+</sup>	Undefined
563	6.952	213.1493	12-Hydroxydodec-3-enoic acid	[M-H] <sup>-</sup>	Organic acids and derivatives
564	7.011	161.1303	Trinoranastreptene	[M+H] <sup>+</sup>	Undefined
565	7.017	279.092	Triphenylphosphine oxide	[M+H] <sup>+</sup>	Benzenoids
566	7.048	361.1972	Cortisone	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
567	7.079	223.1353	13-Oxotrideca-9,11-dienoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
568	7.092	189.1254	2-(1-Phenylethyl)-3,6-Dihydro-2H-Pyran	[M+H] <sup>+</sup>	Undefined

569	7.099	409.2201	2-[5-[2-[2-[5-(2-Hydroxypropyl)oxolan-2-yl]propanoyloxy]propyl]oxolan-2-yl]propanoic acid	[M+Na] <sup>+</sup>	Organic acids and derivatives
570	7.12	363.2142	Hydrocortisone	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
571	7.131	376.2551	7''-ethyl-6-methyl-4'',7''-dihydro-3''H-dispiro[oxane-2,6'-[7,9,12]triazatricyclo[6.3.1.04,12]dodecane-10',2''-oxepin]-8'-en-3-ol	[M+H] <sup>+</sup>	Undefined
572	7.149	373.1679	1,7-Bis(3,4-dihydroxyphenyl)heptan-3-yl acetate	[M-H] <sup>-</sup>	Phenylpropanoids and polyketides
573	7.158	202.2152	1-Decanamine, N,N-dimethyl-, N-oxide	[M+H] <sup>+</sup>	Organic nitrogen compounds
574	7.179	381.2038	4-Hydroxy-3-[(2E,6E)-4-hydroxy-3,7,11-trimethyldodeca-2,6,10-trienyl]benzoic acid	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
575	7.188	316.1872	(E)-Piperolein A	[M+H] <sup>+</sup>	Organoheterocyclic compounds
576	7.204	275.1978	9s,13r-12-Oxophytodienoic Acid	[M-H <sub>2</sub> O+H] <sup>+</sup>	Lipids and lipid-like molecules
577	7.223	121.0637	Phenylacetaldehyde	[M+H] <sup>+</sup>	Benzenoids
578	7.223	195.1363	5-(6-Methyl-6-hydroxyheptyl)furan-2(5H)-one	[M-H <sub>2</sub> O+H] <sup>+</sup>	Organoheterocyclic compounds
579	7.224	127.0375	Phloroglucinol	[M+H] <sup>+</sup>	Benzenoids
580	7.225	425.1321	8-(2,3-Dihydroxy-3-methylbutyl)-5,7-dimethoxy-2-phenyl-2,3-dihydrochromen-4-one	[M+K] <sup>+</sup>	Phenylpropanoids and polyketides
581	7.229	373.1931	3,4-Dihydro-6,8-dihydroxy-3-(10-hydroxyundecyl)isocoumarin	[M+Na] <sup>+</sup>	Benzenoids
582	7.23	311.2178	(5S,6E,8S,9Z,13S,14R)-5-Hydroxy-8-methoxy-5,9,13,14-tetramethyl-1-oxacyclotetradeca-6,9-dien-2-one	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
583	7.235	351.2134	Vinpocetine	[M+H] <sup>+</sup>	Alkaloids and derivatives
584	7.24	183.078	Atractylodin	[M+H] <sup>+</sup>	Undefined
585	7.249	249.1432	Parthenolide	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
586	7.257	297.3147	Phytol	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
587	7.259	264.1931	Dendrobine	[M+H] <sup>+</sup>	Undefined
588	7.274	181.121	Jasmolone	[M+H] <sup>+</sup>	Undefined
589	7.276	383.1822	2-[1-(1H-Benzimidazol-2-yl)-3-(2-methoxyphenyl)propan-2-yl]-1H-benzimidazole	[M+H] <sup>+</sup>	Organoheterocyclic compounds
590	7.295	329.2323	(Z)-5,8,11-Trihydroxyoctadec-9-enoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
591	7.297	353.2287	(15Z)-9,12,13-Trihydroxy-15-octadecenoic acid	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
592	7.318	637.3721	Decahydrogamibogic acid	[M-H] <sup>-</sup>	Organoheterocyclic compounds
593	7.319	130.0629	Indole-3-carbinol	[M+H-H <sub>2</sub> O] <sup>+</sup>	Organoheterocyclic compounds
594	7.342	403.133	Hexamethylquercetaetin	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
595	7.353	271.1682	Trenbolone	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
596	7.355	229.1414	9-(Methoxycarbonyl)dec-9-enoic acid	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
597	7.367	327.0069	Tris(1-chloro-2-propyl)phosphate	[M+H] <sup>+</sup>	Organic acids and derivatives

598	7.429	427.2088	1'(2'H)-Naphthalene]-7-carboxaldehyde, 3',4',4'a,5',6',7',8',8'a-octahydro-4,6',7'-trihydroxy-6-(hydroxymethyl)-2',5',5',8'a-tetramethyl-spiro[benzofuran-2(3H)	[M+Na]+	Organoheterocyclic compounds
599	7.438	271.0973	(2r)-1-(2,4-Dihydroxyphenyl)-2-(4-methoxyphenyl)propan-1-one	[M-H]-	Phenylpropanoids and polyketides
600	7.466	291.1954	FA 18:4;O	[M-H]-	Lipids and lipid-like molecules
601	7.48	307.1925	16-Hydroxy-9-oxooctadeca-10,12,14-trienoic acid	[M-H]-	Lipids and lipid-like molecules
602	7.529	437.091	(5-Benzoyloxy-4,6-dihydroxy-3-methoxycyclohexen-1-yl)methyl benzoate	[M+K]+	Benzenoids
603	7.535	265.1791	Koninginin E	[M-H <sub>2</sub> O+H]+	Organoheterocyclic compounds
604	7.536	925.5025	Saikosaponin C	[M-H]-	Undefined
605	7.539	293.1752	Gingerol	[M-H]-	Benzenoids
606	7.539	609.3427	Kaempferol 3,7-diglucoside	[M-H]-	Phenylpropanoids and polyketides
607	7.565	376.2437	Tuberostemonine	[M+H]+	Undefined
608	7.565	329.2328	FA 18:1;3O	[M-H]-	Lipids and lipid-like molecules
609	7.584	239.0669	Dinoterb	[M-H]-	Benzenoids
610	7.627	153.1257	(1S,4R)-(+)-Fenchone	[M+H]+	Lipids and lipid-like molecules
611	7.628	291.1953	8-(2-Oxo-5-pent-2-enylcyclopent-3-en-1-yl)octanoic acid	[M-H]-	Lipids and lipid-like molecules
612	7.663	235.1675	2-(8-Hydroxy-4a,8-dimethyldecahydro-2-naphthalenyl)acrylic acid	[M-H <sub>2</sub> O+H]+	Lipids and lipid-like molecules
613	7.683	415.2107	(1S,2R,4aR,8aR)-1-Acetoxy-7-isopropylidene-1,4a-dimethyl-6-oxodecahydro-2-naphthalenyl 2,3-dimethyl-2-oxiranecarboxylate	[M+Na]+	Lipids and lipid-like molecules
614	7.722	353.1888	Ajmalicine	[M+H]+	Alkaloids and derivatives
615	7.722	411.1814	Isoapetalic acid	[M+Na]+	Organoheterocyclic compounds
616	7.723	378.2587	Karakoline	[M+H]+	Lipids and lipid-like molecules
617	7.73	353.17	Candidone	[M+H]+	Phenylpropanoids and polyketides
618	7.735	291.1941	h_92_Oxabolone	[M+H]+	Lipids and lipid-like molecules
619	7.777	387.2096	Sufentanil	[M+H]+	Benzenoids
620	7.79	153.1259	p-Menth-4(8)-en-3-one	[M+H]+	Lipids and lipid-like molecules
621	7.87	174.0543	Deisopropylatrazine	[M+H]+	Organoheterocyclic compounds
622	7.876	309.207	9-Hydroperoxy-, (Z,Z,Z)-10,12,15-octadecatrienoic acid	[M-H]-	Lipids and lipid-like molecules
623	7.877	423.2098	Fludrocortisone acetate	[M+H]+	Lipids and lipid-like molecules
624	7.893	373.1285	Tangeretin	[M+H]+	Phenylpropanoids and polyketides
625	7.914	194.0824	L-beta-Homotyrosine	[M-H]-	Organic acids and derivatives
626	7.929	251.1697	2-[(1S,2S,4aR,8aS)-1-Hydroxy-4a-methyl-8-methylenedeca-2-hydro-2-naphthalenyl]acrylic acid	[M+H]+	Lipids and lipid-like molecules
627	7.982	285.1155	Loureirin A	[M-H]-	Undefined
628	8.03	432.2353	[1,14-Dihydroxy-8-(hydroxymethyl)-4,12,12,15-tetramethyl-5-oxo-13-tetracyclo[8.5.0.0.2,6.0.11,13]pentadeca-3,8-dienyl] acetate	[M+ACN+H]+	Lipids and lipid-like molecules

629	8.031	437.1903	Methyl 3-[(1E,3E)-3,5-dimethyl-1,3-heptadien-1-yl]-8-hydroxy-6a,8-dimethyl-6-oxo-6a,8,9,9a-tetrahydro-6H-furo[2,3-h]isochromene-9-carboxylate	[M+Na] <sup>+</sup>	Organic oxygen compounds
630	8.032	133.0641	Cinnamaldehyde	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
631	8.035	293.2129	8-hydroxyoctadeca-9,12,15-trienoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
632	8.037	253.1761	Wallemine	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
633	8.047	151.1124	Perillene	[M+H] <sup>+</sup>	Undefined
634	8.049	175.1447	4-(2,3,6-trimethylphenyl)butan-2-ol	[M+H-H <sub>2</sub> O] <sup>+</sup>	Undefined
635	8.09	311.22	9-HPODE	[M-H] <sup>-</sup>	Undefined
636	8.12	353.229	Anileridine	[M+H] <sup>+</sup>	Organoheterocyclic compounds
637	8.179	278.2077	Venlafaxine	[M+H] <sup>+</sup>	Benzenoids
638	8.224	535.2888	Tenuigenin	[M-H] <sup>-</sup>	Undefined
639	8.236	321.1681	8-(3-((2-Carboxypropan-2-yl)oxy)phenyl)octanoic acid	[M-H] <sup>-</sup>	Benzenoids
640	8.254	237.182	Curcumol	[M+H] <sup>+</sup>	Undefined
641	8.257	407.222	Lincomycine	[M+H] <sup>+</sup>	Organic acids and derivatives
642	8.259	357.267	Dinoprost	[M-H] <sup>1-</sup>	Lipids and lipid-like molecules
643	8.29	219.1742	5-hydroxyculmorin	[M-2H <sub>2</sub> O+H] <sup>+</sup>	Lipids and lipid-like molecules
644	8.305	349.1758	Enalaprilat	[M+H] <sup>+</sup>	Organic acids and derivatives
645	8.313	293.2099	8-[3-Oxo-2-[(E)-pent-2-enyl]cyclopenten-1-yl]octanoic acid	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
646	8.323	448.1982	Oxaline	[M+H] <sup>+</sup>	Organoheterocyclic compounds
647	8.326	318.299	2-Aminooctadecane-1,3,4-triol	[M+H] <sup>+</sup>	Organic nitrogen compounds
648	8.332	415.2124	6-[3-[(3,4-Dimethoxyphenyl)methyl]-4-methoxy-2-(methoxymethyl)butyl]-4-methoxy-1,3-benzodioxole	[M-H <sub>2</sub> O+H] <sup>+</sup>	Lignans, neolignans and related compounds
649	8.35	553.296	(all-E)-beta-Cryptoxanthin	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
650	8.404	303.1366	4-[Formyl(6-methoxyquinolin-8-yl)amino]pentanoic acid	[M+H] <sup>+</sup>	Organoheterocyclic compounds
651	8.409	313.2351	(9Z,12E)-15,16-Dihydroxyoctadeca-9,12-dienoic acid	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
652	8.414	357.2014	Fibleucin	[M+H] <sup>+</sup>	Organoheterocyclic compounds
653	8.416	214.2515	N,N-Dimethyldodecylamine	[M+H] <sup>+</sup>	Organic nitrogen compounds
654	8.431	428.8873	Tris(1,3-dichloro-2-propyl)phosphate	[M+H] <sup>+</sup>	Organic acids and derivatives
655	8.471	313.2379	12,13-Dihydroxyoctadec-9-enoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
656	8.475	358.2336	Songorine	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
657	8.498	200.2363	N-Methyldodecylamine	[M+H] <sup>+</sup>	Organic nitrogen compounds
658	8.524	327.0759	Triphenyl phosphate	[M+H] <sup>+</sup>	Organic acids and derivatives
659	8.528	309.2044	Albocycline	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
660	8.556	465.28	4-[3-Methyl-5-(5,6,7-trihydroxy-1,2,4a,5-tetramethyl-3,4,6,7,8,8a-hexahydro-2H-naphthalen-1-yl)pentoxy]-4-oxobutanoic acid	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
661	8.575	277.1791	Tetradecane-7-sulfonic acid	[M-H] <sup>-</sup>	Organic acids and derivatives

662	8.578	237.0776	5,6,7-Trimethoxycoumarin	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
663	8.586	309.2082	FA 18:3;2O	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
664	8.607	347.2174	Corticosterone	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
665	8.616	277.1812	1,8-dimethyl-6-oxo-7-(propan-2-ylidene)-2,3,4,8-tetrahydro-1H-naphthalen-2-ylacetate	[M+H] <sup>+</sup>	Undefined
666	8.643	311.2218	9-Hydroperoxyoctadeca-10,12-dienoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
667	8.686	251.1995	Clareolide	[M+H] <sup>+</sup>	Undefined
668	8.703	349.2369	(5beta,8alpha,9beta,10alpha,13alpha)-18-Methoxy-18-oxokauran-17-oic acid	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
669	8.707	487.34	Asiatic acid	[M-H] <sup>-</sup>	Undefined
670	8.759	481.2563	Decaethylene glycol	[M+Na] <sup>+</sup>	Organic oxygen compounds
671	8.775	359.2147	(2E,6E,10Z)-12-Hydroxy-10-(hydroxymethyl)-6-methyl-2-(4-methylpent-3-enyl)dodeca-2,6,10-trienoic acid	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
672	8.778	343.2921	Lauramidopropylbetaine	[M] <sup>+</sup>	Organic acids and derivatives
673	8.779	311.2552	Avocadoene 2-acetate	[M-H <sub>2</sub> O+H] <sup>+</sup>	Lipids and lipid-like molecules
674	8.802	360.248	Napelline	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
675	8.807	369.2193	Hirsutine	[M+H] <sup>+</sup>	Undefined
676	8.819	316.2831	2-Aminooctadec-8-ene-1,3,4-triol	[M+H] <sup>+</sup>	Organic nitrogen compounds
677	8.82	407.2783	Cholic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
678	8.842	230.2463	N,N-Dimethyldodecylamine N-oxide	[M+H] <sup>+</sup>	Organic nitrogen compounds
679	8.85	304.2999	Benzododecinium	[M] <sup>+</sup>	Benzenoids
680	8.878	318.24	Drofenine	[M+H] <sup>+</sup>	Benzenoids
681	8.926	263.1989	(1R,2R,4aS,8aS)-2-[(2R)-2-Hydroxybutyl]-1,3-dimethyl-1,2,4a,5,6,7,8,8a-octahydro-1-naphthalenecarboxylic acid	[M-H <sub>2</sub> O+H] <sup>+</sup>	Organic oxygen compounds
682	8.984	269.0455	Emodin	[M-H] <sup>-</sup>	Benzenoids
683	9.002	223.0946	Diethyl phthalate	[M+H] <sup>+</sup>	Benzenoids
684	9.005	313.237	FA 18:1;2O	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
685	9.023	351.2513	Avocadoene 4-acetate	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
686	9.026	327.2103	Ajmaline	[M+H] <sup>+</sup>	Alkaloids and derivatives
687	9.039	293.212	14-(3-Ethylloxiran-2-yl)tetradeca-9,12-dienoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
688	9.047	272.2568	N-(2-Hydroxyethyl)tetradecanamide	[M+H] <sup>+</sup>	Organic nitrogen compounds
689	9.075	267.172	Triisobutyl phosphate	[M+H] <sup>+</sup>	Organic acids and derivatives
690	9.097	305.1747	9,16-Dioxooctadec-10,12,14-trienoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
691	9.1	345.1673	(1R,9R)-3,4,9-Trihydroxy-11,11-dimethyl-5-propan-2-yl-16-oxatetracyclo[6.6.2.0.1,10.0.2,7]hexadeca-2,4,6-trien-15-one	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
692	9.103	277.1426	Dibutyl phthalate	[M-H] <sup>-</sup>	Benzenoids
693	9.116	449.2846	Maritimein	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides

694	9.117	315.1946	Kahweol	[M+H] <sup>+</sup>	Organoheterocyclic compounds
695	9.141	275.2026	FA 18:4	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
696	9.144	293.2131	9-HOTrE	[M-H]1 <sup>-</sup>	Lipids and lipid-like molecules
697	9.147	289.217	h_61_17_Epioxandrolone	[M-H2O+H] <sup>+</sup>	Lipids and lipid-like molecules
698	9.152	241.1942	19-Norandrosterone	[M-2H2O+H] <sup>+</sup>	Lipids and lipid-like molecules
699	9.154	303.2138	Aleuritic acid	[M-H] <sup>-</sup>	Undefined
700	9.157	309.2055	9-Oxo-11-(3-pentylloxiran-2-YL)undec-10-enoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
701	9.165	437.2498	Nonaethylene glycol	[M+Na] <sup>+</sup>	Organic oxygen compounds
702	9.169	327.2159	Hydroquinidine	[M+H] <sup>+</sup>	Undefined
703	9.182	328.2449	(E)-4-[(1R,2S,3S,4R,8As)-2,3,4-trihydroxy-2,5,5,8a-tetramethyl-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl]but-3-en-2-one	[M+NH4] <sup>+</sup>	Lipids and lipid-like molecules
704	9.183	331.1885	5-[2-(Furan-3-yl)ethyl]-8-hydroxy-5,6,8a-trimethyl-3,4,4a,6,7,8-hexahydronaphthalene-1-carboxylic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
705	9.215	285.2061	Hexadecanedioic acid	[M-H2O-H] <sup>-</sup>	Lipids and lipid-like molecules
706	9.222	349.232	Avocadyne 4-acetate	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
707	9.225	371.2386	Aspidocarpine	[M+H] <sup>+</sup>	Alkaloids and derivatives
708	9.229	301.1405	Enterodiol	[M-H] <sup>-</sup>	Undefined
709	9.383	402.1562	Droperidol	[M+Na] <sup>+</sup>	Organic oxygen compounds
710	9.391	235.1687	Dihydroartemisinic acid	[M-H] <sup>-</sup>	Undefined
711	9.414	419.1795	(E)-3-(4-Methoxyphenyl)-1-[2,4,6-trimethoxy-3-(3-methylbut-2-enyl)phenyl]prop-2-en-1-one	[M+Na] <sup>+</sup>	Phenylpropanoids and polyketides
712	9.431	295.2278	9-Hydroxy-10E,12Z-octadecadienoic acid	[M-H]1 <sup>-</sup>	Lipids and lipid-like molecules
713	9.483	242.2828	Dioctylamine	[M+H] <sup>+</sup>	Organic nitrogen compounds
714	9.485	258.2776	1-Tetradecanamine, N,N-dimethyl-, N-oxide	[M+H] <sup>+</sup>	Organic nitrogen compounds
715	9.521	293.2132	13-HoTrE	[M-H]1 <sup>-</sup>	Lipids and lipid-like molecules
716	9.524	277.2169	3-(2,5-Octadienyl)-oxiraneoctanoic acid	[M+H-H2O] <sup>+</sup>	Lipids and lipid-like molecules
717	9.536	431.2768	hyocholic acid	[M+Na] <sup>+</sup>	Undefined
718	9.57	353.1861	Humantenine	[M-H] <sup>-</sup>	Undefined
719	9.574	341.2054	(Ent-7α)-7-Hydroxy-8(14),15-pimaradien-19-oic acid	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
720	9.587	319.2248	Steviol	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
721	9.587	137.13	(-)-α-Terpineol	[M+H-H2O] <sup>+</sup>	Lipids and lipid-like molecules
722	9.595	375.2873	[5-(2-Hydroxy-2,5,5,8a-tetramethyl-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl)-3-methylpentyl] acetate	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
723	9.6	419.2723	Radiclonic acid	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
724	9.613	89.05787	Acetoin	[M+NH4] <sup>+</sup>	Organic oxygen compounds
725	9.627	298.2744	Palmitoleoyl Ethanolamide	[M+H] <sup>+</sup>	Organic nitrogen compounds

726	9.628	163.0373	Umbelliferone	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
727	9.629	219.1747	Germacrone	[M+H] <sup>+</sup>	Undefined
728	9.65	417.2582	Alfentanil	[M+H] <sup>+</sup>	Benzenoids
729	9.671	325.235	(2S,3S)-4-Methylidene-5-oxo-2-tridecyloxolane-3-carboxylic acid	[M+H] <sup>+</sup>	Organoheterocyclic compounds
730	9.738	721.3671	[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	[M+HCOO] <sup>-</sup>	Lipids and lipid-like molecules
731	9.783	300.2891	Sphingosine	[M+H] <sup>+</sup>	Organic nitrogen compounds
732	9.808	443.2052	Trichoverrol A	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
733	9.808	459.1773	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	[M+Na] <sup>+</sup>	Phenylpropanoids and polyketides
734	9.843	343.223	5-[(8aS)-2,5,5,8a-tetramethyl-3-oxo-4a,6,7,8-tetrahydro-4H-naphthalen-1-yl]-3-methylpentanoic acid	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
735	9.875	363.3102	Tetraethylene glycol monododecyl ether	[M+H] <sup>+</sup>	Organic oxygen compounds
736	9.881	468.2893	Lycottonine	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
737	9.888	562.3143	(2-Hydroxy-3-octadeca-9,12,15-trienoyloxypropyl) 2-(trimethylazaniumyl)ethyl phosphate	[M+HCOO] <sup>-</sup>	Lipids and lipid-like molecules
738	9.888	502.2932	Phosphatidylcholine lyso 18:3	[M-CH <sub>3</sub> ] <sup>-</sup>	Lipids and lipid-like molecules
739	9.92	243.1951	3-Hydroxytetradecanoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
740	9.965	318.3001	Phytosphingosine	[M+H] <sup>+</sup>	Organic nitrogen compounds
741	10.009	346.2689	Himbacine	[M+H] <sup>+</sup>	Organoheterocyclic compounds
742	10.011	313.2375	Octadecanedioic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
743	10.013	325.1832	Dodecylbenzenesulfonic acid	[M-H] <sup>-</sup>	Benzenoids
744	10.02	393.1691	Triamcinolone	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
745	10.021	559.3133	3-(Hexopyranosyloxy)-2-hydroxypropyl ester, (9Z,12Z,15Z)-9,12,15-octadecatrienoic acid	[M+FA-H] <sup>-</sup>	Lipids and lipid-like molecules
746	10.049	438.2814	Neoline/Bullatine B	[M+H] <sup>+</sup>	Undefined
747	10.052	665.2623	Syrosingopine	[M-H] <sup>-</sup>	Alkaloids and derivatives
748	10.084	749.4367	alpha-Hederin	[M-H] <sup>-</sup>	Undefined
749	10.089	476.2769	[1-[2-Aminoethoxy(hydroxy)phosphoryl]oxy-3-hydroxypropan-2-yl] octadeca-6,9,12-trienoate	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
750	10.103	331.2466	2'-Deoxyinosine 5'-monophosphate	[M-H] <sup>-</sup>	Nucleosides, nucleotides, and analogues
751	10.105	252.2305	(2E,4E)-N-(2-Methylpropyl)dodeca-2,4-dienamide	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
752	10.107	413.2638	2-Acetoxy-4-pentadecylbenzoic acid	[M+Na] <sup>+</sup>	Benzenoids
753	10.121	249.1856	FA 16:3	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
754	10.131	273.1815	Galaxolidone	[M+H] <sup>+</sup>	Organoheterocyclic compounds
755	10.152	319.2273	Ginkgolic acid (C13:0)	[M-H] <sup>-</sup>	Undefined

756	10.162	343.2226	2-[(2'R,8R,8aS)-2',4,4,7,8a-Pentamethylspiro[2,3,4a,5-tetrahydro-1H-naphthalene-8,5'-oxolane]-2'-yl]acetic acid	[M+Na]+	Lipids and lipid-like molecules
757	10.162	321.2415	5-(1,2,4a,5-Tetramethyl-7-oxo-3,4,8,8a-tetrahydro-2H-naphthalen-1-yl)-3-methylpentanoic acid	[M+H]+	Lipids and lipid-like molecules
758	10.173	413.1769	Erysubin F	[M+Na]+	Phenylpropanoids and polyketides
759	10.187	305.2464	13-Hydroxy-7,14-labdadien-6-one	[M+H]+	Lipids and lipid-like molecules
760	10.189	323.2583	(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	[M-H]-	Lipids and lipid-like molecules
761	10.22	330.338	Cyclic AMP	[M+H]+	Nucleosides, nucleotides, and analogues
762	10.225	313.2359	(12Z)-9,10-Dihydroxyoctadec-12-enoic acid	[M-C6H10O4-H]-	Lipids and lipid-like molecules
763	10.244	344.2555	Bullatine A	[M+H]+	Undefined
764	10.257	299.2578	Vernolic acid	[M-H]1-	Lipids and lipid-like molecules
765	10.273	302.306	2-Aminooctadecane-1,3-diol	[M+H]+	Organic nitrogen compounds
766	10.274	493.3098	Primulin	[M]+	Phenylpropanoids and polyketides
767	10.294	504.3082	Phosphatidylcholine lyso 18:2	[M-CH3]-	Lipids and lipid-like molecules
768	10.321	476.277	[3-[2-Aminoethoxy(hydroxy)phosphoryl]oxy-2-hydroxypropyl] octadeca-9,12-dienoate	[M-H]-	Lipids and lipid-like molecules
769	10.326	478.2888	4-[5-[[4-[5-[Acetyl(hydroxy)amino]pentylamino]-4-oxobutanoyl]-hydroxyamino]pentylamino]-4-oxobutanoic acid	[M+NH4]+	Lipids and lipid-like molecules
770	10.328	555.2839	Dronedarone	[M-H]-	Organic oxygen compounds
771	10.344	297.2433	12-Hydroxyoctadec-9-enoic acid	[M-H]-	Lipids and lipid-like molecules
772	10.348	339.1984	Canrenone	[M-H]-	Lipids and lipid-like molecules
773	10.399	375.2508	2-Hydroxy-4-methoxy-3,5-bis(3-methylbut-2-enyl)-6-pentylbenzoic acid	[M+H]+	Benzenoids
774	10.405	482.3207	1-Pentadecanoyl-sn-glycero-3-phosphocholine	[M+H]+	Lipids and lipid-like molecules
775	10.407	356.3508	N-(2-Hydroxyethyl)icosanamide	[M+H]+	Organic nitrogen compounds
776	10.409	261.2192	8-Hydroxy-9,10-epoxystearic acid	[M-3H2O+H]+	Lipids and lipid-like molecules
777	10.412	277.2169	Linolenic acid	[M-H]-	Lipids and lipid-like molecules
778	10.438	300.2284	Dehydroabietamide	[M+H]+	Lipids and lipid-like molecules
779	10.45	345.2378	2-[2-[(1S,8aR)-1,4,4a,5,6,7,8,8a-Octahydro-2-(hydroxymethyl)-5,5,8a-trimethyl-1-naphthalenyl]ethyl]-, (2Z)-2-butene-1,4-diol	[M+Na]+	Lipids and lipid-like molecules
780	10.455	564.3295	(2-Hydroxy-3-octadeca-9,12-dienoyloxypropyl) 2-(trimethylazaniumyl)ethyl phosphate	[M+HCOO]-	Lipids and lipid-like molecules
781	10.463	427.2087	3-[5-Hydroxy-7-methoxy-2,3-dimethyl-6-(3-methylbut-2-enyl)-4-oxo-2,3-dihydrochromen-8-yl]hexanoic acid	[M+Na]+	Organoheterocyclic compounds
782	10.467	299.2	Dehydroabietic acid	[M-H]-	Lipids and lipid-like molecules
783	10.521	271.2291	FA 16:0;2O	[M-H]-	Lipids and lipid-like molecules

784	10.529	311.2189	(9Z,15Z)-12,13-Dihydroxyoctadeca-9,15-dienoate	[M-H]-	Lipids and lipid-like molecules
785	10.545	585.3526	Dehydroxynocardamine	[M+H]+	Phenylpropanoids and polyketides
786	10.551	415.2809	Deoxycholic acid	[M+Na]+	Lipids and lipid-like molecules
787	10.554	279.2328	Linoleic acid	[M-H]-	Lipids and lipid-like molecules
788	10.579	467.294	Cephaeline	[M+H]+	Alkaloids and derivatives
789	10.579	745.4093	Naadp	[M]+	Nucleosides, nucleotides, and analogues
790	10.579	540.3308	1-Palmitoylphosphatidylcholine	[M+HCOO]-	Lipids and lipid-like molecules
791	10.582	295.2617	Methyl linoleate	[M+H]+	Undefined
792	10.587	496.3401	1-Hexadecanoyl-sn-glycero-3-phosphocholine	[M+H]+	Lipids and lipid-like molecules
793	10.682	297.2418	9,10-Epoxy stearic acid	[M-H]-	Lipids and lipid-like molecules
794	10.735	478.2918	2-Azaniumylethyl (2-hydroxy-3-octadec-9-enoyloxypropyl) phosphate	[M-H]-	Lipids and lipid-like molecules
795	10.736	285.2434	Luteolin	[M-H]-	Phenylpropanoids and polyketides
796	10.737	480.31	Phosphatidylcholine lyso 16:0	[M-CH3]-	Lipids and lipid-like molecules
797	10.745	518.3213	(2-Hydroxy-3-octadeca-6,9,12-trienoyloxypropyl) 2-(trimethylazaniumyl)ethyl phosphate	[M+H]+	Lipids and lipid-like molecules
798	10.754	452.2802	2-Azaniumylethyl (3-hexadecanoyloxy-2-hydroxypropyl) phosphate	[M-H]-	Lipids and lipid-like molecules
799	10.761	454.2915	1-Hexadecanoyl-sn-glycero-3-phosphoethanolamine	[M+H]+	Lipids and lipid-like molecules
800	10.772	293.1774	Hydron;tetradecyl sulfate	[M-H]-	Organic acids and derivatives
801	10.774	355.2837	[4,6-diethyl-6-(4-ethyl-2-methyloctyl)-3H-1,2-dioxin-3-yl]acetic acid	[M+H]+	Undefined
802	10.781	297.1506	4-(Decan-4-yl)benzenesulfonic acid	[M-H]-	Benzenoids
803	10.789	432.2075	Guan-fu base Y	[M+FA-H]-	Undefined
804	10.794	519.2573	Genistein 7-O-beta-d-glucoside-6"-O-malonate	[M+H]+	Phenylpropanoids and polyketides
805	10.797	227.2017	Myristic acid	[M-H]-	Lipids and lipid-like molecules
806	10.855	522.3554	(2-Hydroxy-3-octadec-9-enoyloxypropyl) 2-(trimethylazaniumyl)ethyl phosphate	[M+H]+	Lipids and lipid-like molecules
807	10.855	506.3263	Phosphatidylcholine lyso 18:1	[M-CH3]-	Lipids and lipid-like molecules
808	10.87	381.2999	Persin	[M+H]+	Undefined
809	10.879	907.5356	Chlorophyll b from Chlorella	[M]+	Organoheterocyclic compounds
810	10.905	271.2054	h_193_Quinolone_m	[M-H2O+H]+	Lipids and lipid-like molecules
811	10.915	349.2752	8-[5-(Acetyloxy)-3-methylpentyl]octahydro-4,4,8a-trimethyl-7-methylene-2(1H)-naphthalenone	[M+H]+	Lipids and lipid-like molecules
812	10.916	400.3398	(+)-Palmitoylcarnitine	[M+H]+	Lipids and lipid-like molecules
813	10.925	281.2484	Vaccenic acid	[M-H]-	Lipids and lipid-like molecules
814	10.95	510.3518	1-Heptadecanoyl-sn-glycero-3-phosphocholine	[M+H]+	Lipids and lipid-like molecules
815	10.95	349.2383	5-(5-Methoxycarbonyl-5,8a-dimethyl-2-methylidene-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl)-3-methylpentanoic acid	[M-H]-	Lipids and lipid-like molecules

816	10.963	256.2661	Palmitic amide	[M+H] <sup>+</sup>	Undefined
817	10.964	301.2157	Abietic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
818	10.995	609.2681	Tulipanin	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
819	11.008	241.216	Pentadecanoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
820	11.013	838.6406	Isobutyryl CoA	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
821	11.019	313.2709	2,4-Dihydroxyheptadecyl acetate	[M-H <sub>2</sub> O+H] <sup>+</sup>	Lipids and lipid-like molecules
822	11.02	427.3005	Acetyl-Leu-Leu-Arg-al	[M+H] <sup>+</sup>	Organic acids and derivatives
823	11.027	331.2808	2-Palmitoylglycerol	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
824	11.038	275.1978	Nandrolone	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
825	11.066	345.2034	1,3,4,9,10,10a-Hexahydro-5,6-dihydroxy-1,1-dimethyl-7-(1-methylethyl)-, methyl ester, (4aR)-4a(2H)-phenanthrenecarboxylic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
826	11.067	345.2429	Ginkgolic Acid C15:1	[M-H] <sup>-</sup>	Undefined
827	11.075	845.4692	Ginsenoside-Rg1	[M+FA-H] <sup>-</sup>	Undefined
828	11.091	304.2611	Fenpropimorph	[M+H] <sup>+</sup>	Benzenoids
829	11.092	404.3119	2-(14-Methylpentadecanoylamino)-3-phenylpropanoic acid	[M+H] <sup>+</sup>	Organic acids and derivatives
830	11.093	311.1486	beta-D-Glucopyranoside, 5-methyl-2-(1-methylethyl)phenyl	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
831	11.098	579.5297	Procyanidin B2	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
832	11.101	223.2047	cis-Nerolidol	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
833	11.109	283.2642	Methyl heptadecanoate	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
834	11.119	315.251	Methyl hexadecanoate	[M-H] <sup>-</sup>	Undefined
835	11.123	309.1724	2-Dodecoxyethyl hydrogen sulfate	[M-H] <sup>-</sup>	Organic acids and derivatives
836	11.123	265.1464	Lauryl sulfate	[M-H] <sup>-</sup>	Organic acids and derivatives
837	11.124	311.1681	5-(4-Sulfophenyl)undecane	[M-H] <sup>-</sup>	Benzenoids
838	11.128	529.3046	Kukoamine B	[M-H] <sup>-</sup>	Undefined
839	11.139	609.2679	Reserpine	[M+H] <sup>+</sup>	Alkaloids and derivatives
840	11.151	255.2323	Palmitic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
841	11.182	777.4218	Heterophyllin B	[M-H] <sup>-</sup>	Undefined
842	11.187	463.2813	Pristimerin	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
843	11.193	611.4613	(S)-7-(((2-O-6-Deoxy-alpha-L-mannopyranosyl)-beta-D-glucopyranosyl)oxy)-2,3-dihydro-5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-4H-1-benzopyran-4-one	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides
844	11.196	551.2595	Chaetoglobosin A	[M+Na] <sup>+</sup>	Alkaloids and derivatives
845	11.212	705.3981	Atazanavir	[M+H] <sup>+</sup>	Organic acids and derivatives
846	11.213	513.3505	Alisol A	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
847	11.217	232.168	alpha-Pyrrolidinovalerophenone	[M+H] <sup>+</sup>	Organic oxygen compounds
848	11.234	357.2967	Glyceryl monooleate	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
849	11.246	295.2229	9-Oxoctadeca-10,12-dienoic acid	[M+H] <sup>+</sup>	Lipids and lipid-like molecules

850	11.246	73.06405	Butyraldehyde	[M+Li]+	Organic oxygen compounds
851	11.256	394.3309	N-Oleoyl leucine	[M-H]-	Organic acids and derivatives
852	11.289	184.0722	Phosphocholine	[M]+	Organic nitrogen compounds
853	11.3	250.1771	N-Desmethyltramadol	[M+H]+	Benzenoids
854	11.3	264.1543	(2E,4E)-N-(1,3-Dihydroxy-3-methylpentan-2-yl)-2-methylhexa-2,4-dienamide	[M+Na]+	Lipids and lipid-like molecules
855	11.314	524.3715	1-Stearoyl-sn-glycero-3-phosphocholine	[M+H]+	Lipids and lipid-like molecules
856	11.345	305.2469	FA 20:3	[M-H]-	Lipids and lipid-like molecules
857	11.407	253.2158	Palmitoleic acid	[M-H]-	Lipids and lipid-like molecules
858	11.413	295.2257	FA 18:2;O	[M-H]-	Lipids and lipid-like molecules
859	11.418	311.2355	3-(10-Phenyldecyl)Phenol	[M+H]+	Undefined
860	11.424	293.2462	14-(Hydroxymethyl)-5,9-dimethyltetracyclo[11.2.1.0~1,10~.0~4,9~]hexadecan-5-ol	[M+H]+	Lipids and lipid-like molecules
861	11.465	541.3862	18-Deoxyeucopaxillone A	[M+H-H <sub>2</sub> O]+	Undefined
862	11.498	563.5032	2-Oahsa	[M-H]-	Lipids and lipid-like molecules
863	11.499	281.2506	trans-Vaccenic acid	[M-H]-	Lipids and lipid-like molecules
864	11.528	789.4617	Ginsenoside Rk1	[M+H]+	Undefined
865	11.533	284.296	Octadecanamide	[M+H]+	Organic acids and derivatives
866	11.576	269.2492	Heptadecanoic acid	[M-H]-	Lipids and lipid-like molecules
867	11.597	313.2688	Glyceryl palmitate	[M-H <sub>2</sub> O+H]+	Lipids and lipid-like molecules
868	11.601	332.2918	5-[(1S,4aS,8aS)-Decahydro-5,5,8a-trimethyl-2-methylene-1-naphthalenyl]-3-methyl-, (2E)-2-penten-1-ol	[M+ACN+H]+	Lipids and lipid-like molecules
869	11.605	293.2825	(2R)-1-(5-Hydroxy-3-methylpentyl)-2,5,5,8a-tetramethyldecahydro-2-naphthalenol	[M-H <sub>2</sub> O+H]+	Lipids and lipid-like molecules
870	11.619	803.5429	(22E)-3alpha,12alpha-Dihydroxy-5beta-chol-22-en-24-oic Acid	[2M+Na]+	Lipids and lipid-like molecules
871	11.629	307.2608	Linolenic acid ethyl ester	[M+H]+	Undefined
872	11.629	327.2884	FA 20:0;2O	[M-H]-	Lipids and lipid-like molecules
873	11.64	715.3841	[(2R,3R,4S,5S,6R)-3-Acetyloxy-2-(acetyloxymethyl)-5-hexanoyloxy-6-[(2S,3R)-2,3,4-trihydroxybutoxy]oxan-4-yl] 14-hydroxytetradecanoate	[M+Na]+	Lipids and lipid-like molecules
874	11.644	307.2632	FA 20:2	[M-H]-	Lipids and lipid-like molecules
875	11.658	283.2644	Stearic acid	[M-H]-	Lipids and lipid-like molecules
876	11.662	359.3142	Glyceryl monostearate	[M+H]+	Lipids and lipid-like molecules
877	11.671	295.2641	FA 19:1	[M-H]-	Lipids and lipid-like molecules
878	11.675	529.382	16-hydroxy-2,2,4a,6a,6b,11,11,14b-octamethyl-4H,4bH,5H,6H,7H,8H,9H,10H,12H,12aH,14H,14aH,15H,16H,16aH-piceno[3,4-d][1,3]dioxine-8a-carboxylic acid	[M+H]+	Undefined
879	11.678	501.3167	Medicagenic acid	[M-H]-	Lipids and lipid-like molecules

880	11.692	583.3944	Diacetylpyxinol	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
881	11.794	551.4219	Echinenone	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
882	11.799	326.233	3-Hydroxy-N-(2-oxoxolan-3-yl)tetradecanamide	[M-H] <sup>-</sup>	Organic acids and derivatives
883	11.865	779.4506	Saikosaponin a	[M-H] <sup>-</sup>	Undefined
884	11.892	683.4287	Ginsenoside Rh1	[M+FA-H] <sup>-</sup>	Undefined
885	11.912	107.0471	Benzaldehyde	[M+H] <sup>+</sup>	Benzenoids
886	11.92	613.4742	L-Glutathione (oxidized form)	[M+H] <sup>+</sup>	Organic acids and derivatives
887	11.921	299.2585	(R)-2-Hydroxystearic acid	[M-H] <sup>-</sup>	Undefined
888	11.922	783.4782	Ginsenoside Rg2	[M-H] <sup>-</sup>	Undefined
889	11.945	679.5057	Avocadene 1-acetate	[2M+Na] <sup>+</sup>	Lipids and lipid-like molecules
890	11.961	573.4817	3-{7-[5-(1-hydroxyhenicosa-4,8-dien-1-yl)oxolan-2-yl]heptyl}-5-methyl-5H-furan-2-one	[M+H] <sup>+</sup>	Undefined
891	11.979	734.4785	Erythromycin	[M-H] <sup>-</sup>	Organic oxygen compounds
892	11.985	309.28	trans-11-Eicosenoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
893	11.997	401.3371	7-Ketocholesterol	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
894	11.999	835.5231	PI 34:1	[M-H] <sup>-</sup>	Undefined
895	12.026	457.3674	alpha-Boswellic acid	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
896	12.03	535.2726	3-Deoxo-3-beta-Acetoxydeoxydihydrogedunin	[M+Na] <sup>+</sup>	Organoheterocyclic compounds
897	12.032	533.2481	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	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
898	12.036	497.3585	Bryodulcosigenin	[M+Na] <sup>+</sup>	Lipids and lipid-like molecules
899	12.065	409.4026	FA 27:0	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
900	12.07	297.2786	FA 19:0	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
901	12.078	355.3202	2-Hydroxydocosanoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
902	12.079	391.2794	Diocetyl phthalate	[M+H] <sup>+</sup>	Benzenoids
903	12.079	360.3236	N-(2-Phenylethyl)hexadecanamide	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
904	12.085	589.4777	3-[12-hydroxy-12-[5'-(1-hydroxydodecyl)-[2,2'-bioxolan]-5-yl]dodecyl]-5-methyl-5H-furan-2-one	[M+H-H <sub>2</sub> O] <sup>+</sup>	Undefined
905	12.089	263.2337	5-dodecyl-4-hydroxy-4-methylcyclopent-2-en-1-one	[M+H-H <sub>2</sub> O] <sup>+</sup>	Undefined
906	12.212	471.3417	Enoxolone	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
907	12.237	431.1773	Bidwillon A	[M+Na] <sup>+</sup>	Phenylpropanoids and polyketides
908	12.276	485.3582	Glycyrrhetic acid, Me ester	[M+H] <sup>+</sup>	Undefined
909	12.279	445.3647	Topsentisterol A2	[M+H] <sup>+</sup>	Undefined
910	12.285	415.3558	2,3-dimethyl-5-(3,7,11,15-tetramethylhexadec-2-en-1-yl)cyclohexa-2,5-diene-1,4-dione	[M+H] <sup>+</sup>	Undefined

911	12.307	369.3357	FA 23:0;2O	[M-H]-	Lipids and lipid-like molecules
912	12.4	195.121	Hexylresorcinol	[M+H]+	Benzenoids
913	12.409	405.2603	6,7-Diketolithocholic acid	[M+H]+	Lipids and lipid-like molecules
914	12.434	306.2764	Cyclic cmp	[M+H]+	Organic oxygen compounds
915	12.46	333.2387	(3R,4R,5R)-3-[(11E)-11,15-Hexadecadien-9-yn-1-yl]-4-hydroxy-5-methyldihydro-2(3H)-furanone	[M+H]+	Organoheterocyclic compounds
916	12.464	855.4994	PI 36:5	[M-H]-	Undefined
917	12.482	959.5378	Soyasaponin Ba	[M+H]+	Lipids and lipid-like molecules
918	12.485	738.5043	PE 36:4	[M-H]-	Undefined
919	12.552	383.3518	FA 24:0;2O	[M-H]-	Lipids and lipid-like molecules
920	12.569	165.089	Phenethyl acetate	[M+H]+	Benzenoids
921	12.57	429.3727	13'-Hydroxy-alpha-tocopherol	[M+H-H2O]+	Undefined
922	12.628	815.4758	Ginsenoside F3	[M+FA-H]-	Undefined
923	12.67	325.3107	Heneicosanoic acid	[M-H]-	Lipids and lipid-like molecules
924	12.675	383.3666	Campesterol	[M+H-H2O]+	Lipids and lipid-like molecules
925	12.73	945.5363	Ginsenoside Re	[M-H]-	Undefined
926	12.731	363.2165	CORTISOL	[M+H]+	Undefined
927	12.755	559.3099	[2-Hydroxy-3-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxypropyl]octadeca-9,12,15-trienoate	[M+HCOO]-	Lipids and lipid-like molecules
928	12.835	769.5025	PG 36:4	[M-H]-	Undefined
929	12.906	893.5522	Chlorophyll a from Chlorella	[M]+	Organoheterocyclic compounds
930	12.919	415.2211	7-Hydroxymitragynine	[M+H]+	Alkaloids and derivatives
931	12.921	863.4926	{6-[2-(hexadecanoyloxy)-3-(icosa-5,8,11,14,17-pentaenoyloxy)propoxy]-3,4,5-trihydroxyoxan-2-yl}methanesulfonic acid	[M+Na]+	Undefined
932	12.936	551.5006	Methyl 18-(hexadecanoyloxy)octadec-9-enoate	[M+H]+	Undefined
933	12.936	339.327	Docosanoic acid	[M-H]-	Lipids and lipid-like molecules
934	12.956	467.4098	2-Mahpda	[M-H]-	Lipids and lipid-like molecules
935	12.983	365.3415	Nervonic acid	[M-H]-	Lipids and lipid-like molecules
936	13.007	833.5208	PI 34:2	[M-H]-	Undefined
937	13.034	423.4206	Octacosanoic acid	[M-H]-	Lipids and lipid-like molecules
938	13.049	723.5169	[(2R)-2,3-Di(hexadecanoyloxy)propyl] 2,3-dihydroxypropyl phosphate	[M+H]+	Lipids and lipid-like molecules
939	13.059	411.3829	FA 26:0;2O	[M-H]-	Lipids and lipid-like molecules
940	13.075	612.5556	1-Palmitoyl-2-oleoyl-rac-glycerol	[M+NH4]+	Lipids and lipid-like molecules
941	13.086	745.5049	PG 34:2	[M-H]-	Undefined
942	13.133	395.3645	Fucosterol	[M+H-H2O]+	Lipids and lipid-like molecules

943	13.155	683.5244	3-{1,10-dihydroxy-10-methyl-3-[2-methyl-4-(2,5,6,6-tetramethylcyclohex-1-en-1-yl)buta-1,3-dien-1-yl]-7-(1-oxopropan-2-ylidene)-2-oxaspiro[4.5]decan-6-yl}propyl dodecanoate	[M+H] <sup>+</sup>	Undefined
944	13.16	847.5347	PI 35:2	[M-H] <sup>-</sup>	Undefined
945	13.185	719.4848	PG 32:1	[M-H] <sup>-</sup>	Undefined
946	13.191	1019.502	Madecassoside	[M+FA-H] <sup>-</sup>	Undefined
947	13.205	259.2029	Octadeca-2,4,9-trien-6-yne-1,18-diol	[M+H-H <sub>2</sub> O] <sup>+</sup>	Undefined
948	13.242	712.4929	PE 34:3	[M-H] <sup>-</sup>	Undefined
949	13.243	740.523	PE 36:3	[M-H] <sup>-</sup>	Undefined
950	13.283	765.4642	Ginsenoside Rg5	[M-H] <sup>-</sup>	Undefined
951	13.33	285.2411	2,3-Dihydroxypropyl tetradecanoate	[M-H <sub>2</sub> O+H] <sup>+</sup>	Lipids and lipid-like molecules
952	13.364	277.2149	gamma-Linolenic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
953	13.384	338.3393	Erucamide	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
954	13.393	399.3623	Fecosterol	[M+H] <sup>+</sup>	Undefined
955	13.409	721.502	Dipalmitoylphosphatidylglycerol	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
956	13.465	747.5156	PG 34:1	[M-H] <sup>-</sup>	Undefined
957	13.507	367.3564	Tetracosanoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
958	13.542	861.5491	gamma-Aminobutyrate	[M-H <sub>2</sub> O-H] <sup>-</sup>	Organic acids and derivatives
959	13.549	545.4189	12-Desoxydiacetylpyxinol	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
960	13.55	337.2721	12,19,20-Trihydroxy-14-methylenegeranylnol	[M+H-H <sub>2</sub> O] <sup>+</sup>	Undefined
961	13.554	393.3732	FA 26:1	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
962	13.584	742.5376	PE 36:2	[M-H] <sup>-</sup>	Undefined
963	13.586	430.3789	Vitamin E	[M] <sup>+</sup>	Lipids and lipid-like molecules
964	13.587	647.4634	1,2-Dipalmitoyl-sn-glycerol 3-phosphate	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
965	13.59	714.5087	PE 34:2	[M-H] <sup>-</sup>	Undefined
966	13.659	413.3749	Stigmasterol	[M+H] <sup>+</sup>	Lipids and lipid-like molecules
967	13.662	395.3625	alpha-Spinasterol	[M+H-H <sub>2</sub> O] <sup>+</sup>	Lipids and lipid-like molecules
968	13.688	403.2465	Telocinobufagin	[M+H] <sup>+</sup>	Undefined
969	13.716	363.2888	2-Methoxy-4-pentadecylbenzoic acid	[M+H] <sup>+</sup>	Benzenoids
970	13.734	381.3702	Pentacosanoic acid	[M-H] <sup>-</sup>	Lipids and lipid-like molecules
971	13.756	547.4684	3-{7-[5-(1-hydroxynonadec-4-en-1-yl)oxolan-2-yl]heptyl}-5-methyl-5H-furan-2-one	[M+H] <sup>+</sup>	Undefined
972	13.783	728.5223	PE 35:2	[M-H] <sup>-</sup>	Undefined
973	13.803	184.0708	Phosphorylcholine	[M+H] <sup>+</sup>	Organic nitrogen compounds
974	13.88	933.574	Petunidin-3-O-(6''-O-(4'''-O-E-coum)-alpha-rhamnopyranosyl-beta-glucopyranosyl)-5-O-beta-glucopyranoside	[M+H] <sup>+</sup>	Phenylpropanoids and polyketides

975	13.919	581.5256	FA 40:5	[M-H]-	Lipids and lipid-like molecules
976	13.96	397.3806	6-{9a,11a-dimethyl-1H,2H,3H,3aH,3bH,4H,8H,9H,9bH,10H,11H-cyclopenta[a]phenanthren-1-yl}-3-ethyl-2-methylheptane	[M+H]+	Undefined
977	14.059	150.1116	Triethanolamine	[M+H]+	Organic nitrogen compounds