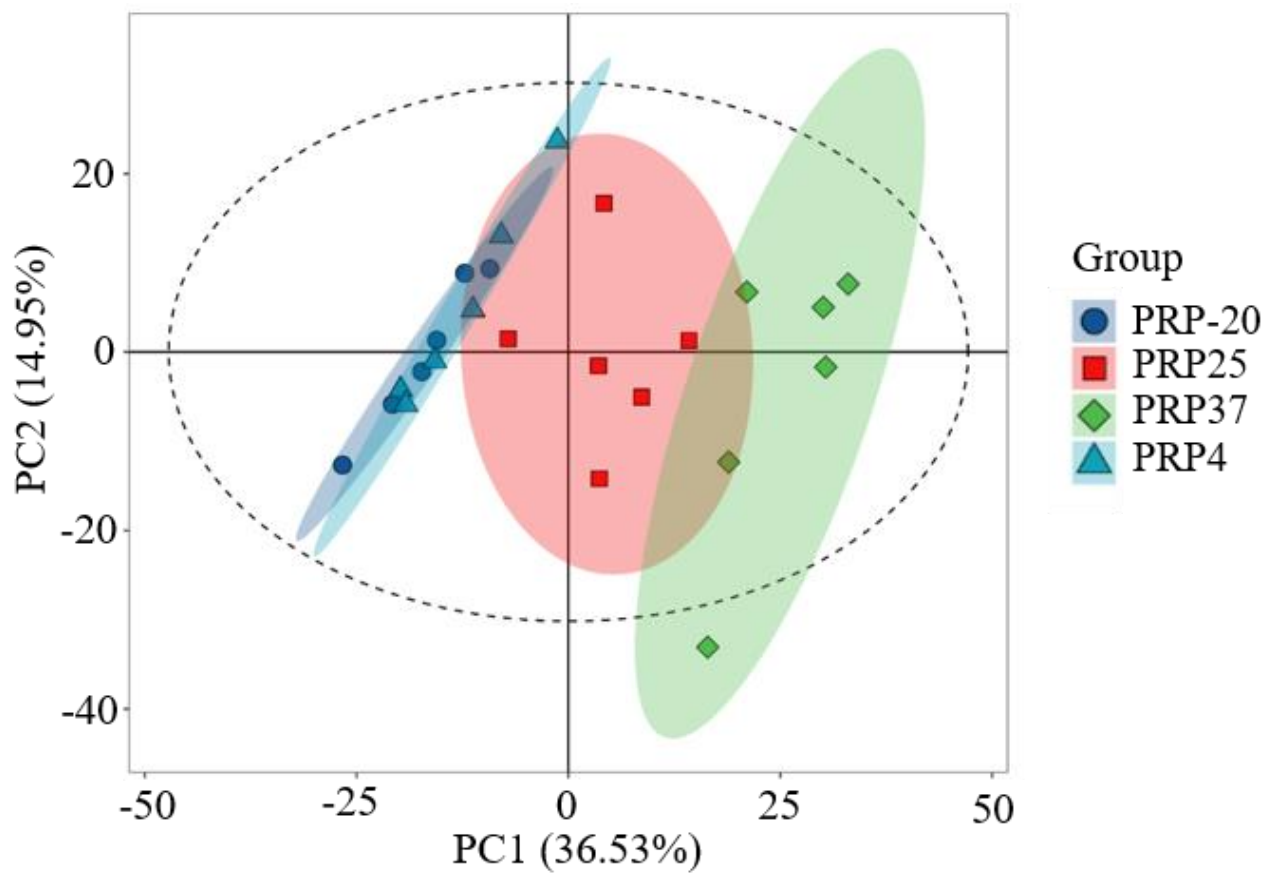
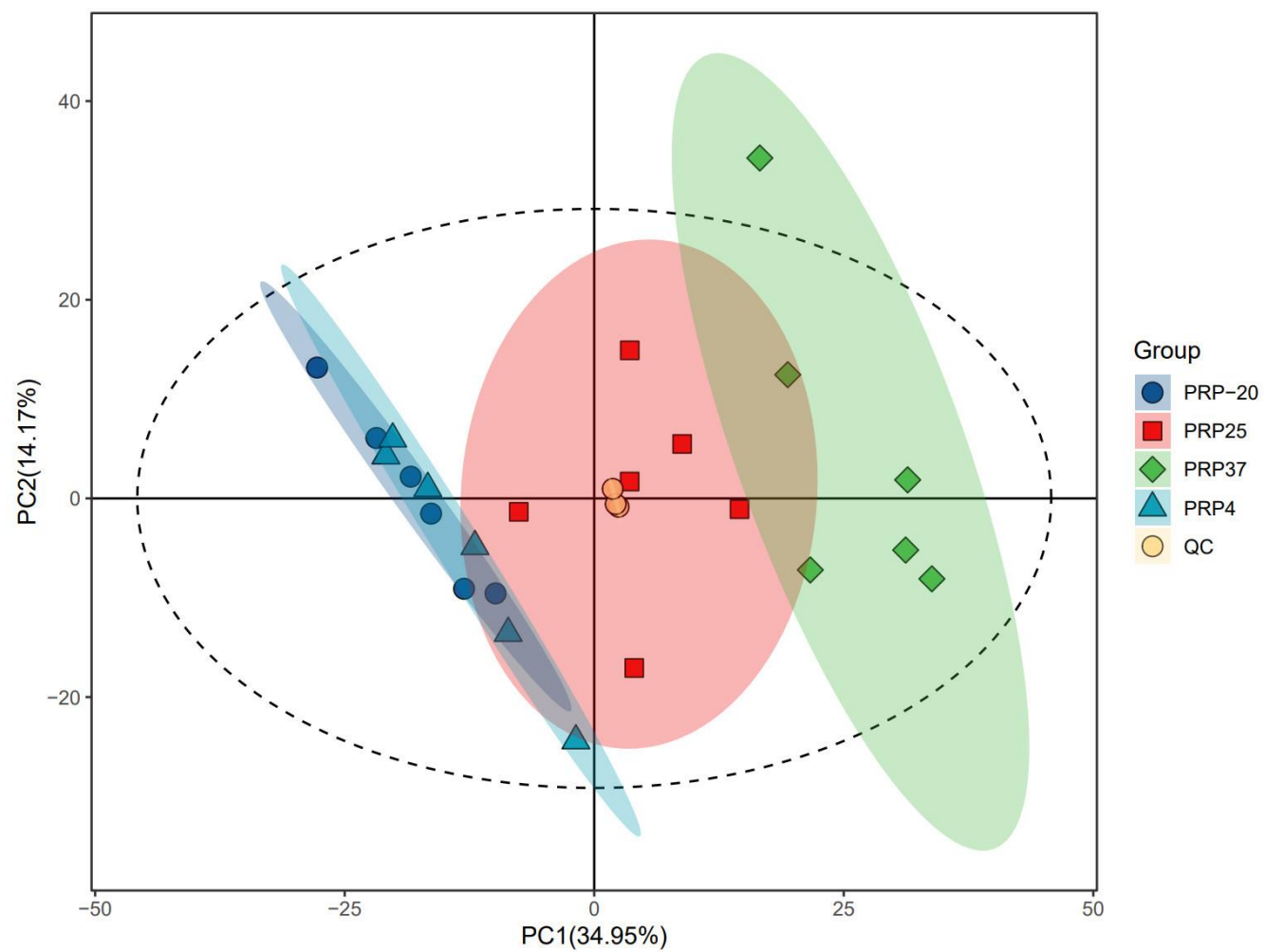
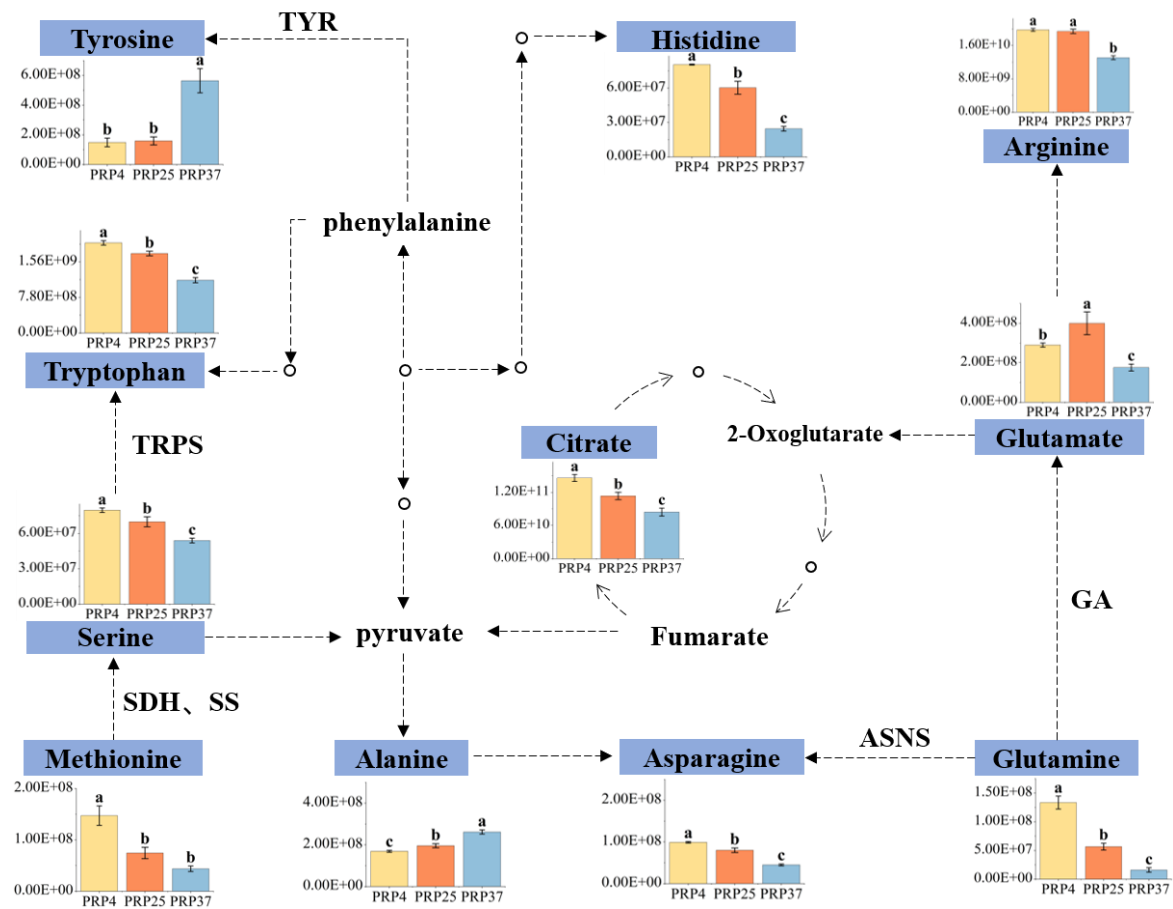


Supplementary Information



Supplementary Figure S1





Supplementary Figure S3

Table S1 Information on all metabolites detected by UHPLC

	Metabolite name	Rt(min)	Expreiment Mz	Adduct type	Formula	Ontology	KEGGID
1	1,6-Anhydro-beta-glucopyranose	1.192	145.04672	[M+H-H ₂ O] ⁺	C6H10O5	Oxepanes	C22350
2	8-Geranyloxypsoralen	6.918	361.14545	[M+Na] ⁺	C21H22O4	Terpene lactones	C22152
3	Fumiquinazoline A	0.924	490.17386	[M-H] ⁻	C24H23N5O4	Quinazolines	C22147
4	Fumiquinazoline A	7.488	490.16916	[M-H ₂ O-H] ⁻	C24H23N5O4	Quinazolines	C22147
5	3-Hydroxymyristic Acid	12.238	243.19438	[M-H] ⁻	C14H28O3	Fatty Acyls	C22001
6	Aprepitant	6.32	535.15253	[M+Na] ⁺	C23H21F7N4O3	Phenylmorpholines	C21555
7	Indole-3-acrylic acid	6.696	170.05911	[M+H-H ₂ O] ⁺	C11H9NO2	Indoles	C21283
8	Mevinolinic acid	12.359	405.2594	[M+NH ₄] ⁺	C24H38O6	Medium-chain hydroxy acids and derivatives	C21130
9	Alanylglutamic acid	1.991	219.09633	[M+H] ⁺	C8H14N2O5	Carboxylic acids and derivatives	C20958
10	Liriodendrin	7.426	787.26288	[M-H] ⁻	C34H46O18	Lignan glycosides	C20786
11	Disogluside	11.251	599.35071	[M+Na] ⁺	C33H52O8	Steroidal saponins	C20709
12	2-Furanmethanol	5.414	99.04414	[M+H] ⁺	C5H6O2	Heteroaromatic compounds	C20441
13	Fumigaclavine C	9.444	367.23929	[M+H] ⁺	C23H30N2O2	Clavines and derivatives	C20438
14	beta-carboline	7.513	169.0753	[M+H] ⁺	C11H8N2	Beta carbolines	C20157
15	Acridine	7.74	180.08029	[M+H] ⁺	C13H9N	Acridines	C20141
16	alpha-Methyltryptamine	6.546	175.12224	[M+H-H ₂ O] ⁺	C11H14N2	Indoles and derivatives	C20127
17	2-hydroxy-dAMP	2.153	346.05383	[M-H] ⁻	C10H14N5O7P	Purine nucleotides	C19970
18	Iminodiacetic acid	0.894	132.02806	[M-H] ⁻	C4H7NO4	Carboxylic acids and derivatives	C19911
19	Colneleic acid	9.951	295.2254	[M+H-H ₂ O] ⁺	C18H30O3	Fatty Acyls	C19827
20	Colneleic acid	10.624	295.22531	[M+H] ⁺	C18H30O3	Fatty Acyls	C19827
21	Apocarotenal	11.832	417.31778	[M+H-H ₂ O] ⁺	C30H40O	Triterpenoids	C19728
22	Apocarotenal	12.75	439.30096	[M+H] ⁺	C30H40O	Triterpenoids	C19728
23	Apocarotenal	12.599	439.30096	[M+CH ₃ OH+H] ⁺	C30H40O	Triterpenoids	C19728
24	Oleamide	13.144	282.27731	[M+H] ⁺	C18H35NO	Fatty Acyls	C19670
25	Oleamide	11.619	282.27838	[M+NH ₄] ⁺	C18H35NO	Fatty Acyls	C19670
26	Floionolic acid	10.479	331.24643	[M-H] ⁻	C18H36O5	Fatty Acyls	C19621
27	Succinic anhydride	2.604	99.00665	[M-H ₂ O-H] ⁻	C4H4O3	Carboxylic acids and derivatives	C19524
28	Succinic anhydride	7.933	99.00664	[M-H] ⁻	C4H4O3	Carboxylic acids and derivatives	C19524
29	1,5-Naphthalenediamine	6.695	159.09117	[M+H] ⁺	C10H10N2	Naphthalenes	C19463
30	9,10-Epoxyoctadecanoic acid	11.488	313.23685	[M-H] ⁻	C18H34O4	Fatty Acyls	C19418
31	4-Vinylcyclohexene	10.854	109.10101	[M+H-H ₂ O] ⁺	C8H12	Unsaturated hydrocarbons	C19310
32	4-Methylimidazole	13.538	83.06068	[M+H] ⁺	C4H6N2	Azoles	C19262
33	Buturon	8.481	235.06281	[M-H] ⁻	C12H13ClN2O	N-phenylureas	C19074
34	Iprovalicarb	6.522	343.19653	[M+H] ⁺	C18H28N2O3	Toluenes	C18866
35	Imazapyr	6.854	262.11798	[M+H] ⁺	C13H15N3O3	Amino acids and derivatives	C18864
36	Halofenozide	4.073	331.12265	[M+H] ⁺	C18H19ClN2O2	Halobenzoic acids and derivatives	C18791
37	Dodemorph	12.15	282.27725	[M+H] ⁺	C18H35NO	Morpholines	C18786
38	Propetamphos	7.462	280.08078	[M-H ₂ O-H] ⁻	C10H20NO4PS	Fatty acid esters	C18669
39	Formetanate HCl	2.597	258.09671	[M+H-H ₂ O] ⁺	C11H16ClN3O2	Phenyl methylcarbamates	C18668
40	DNOC	0.979	197.01967	[M-H] ⁻	C7H6N2O5	Dinitrophenols	C18653

41	Forchlorfenuron	7.148	246.04202	[M-H ₂ O-H]-	C ₁₂ H ₁₀ ClN ₃ O	2-halopyridines	C18604
42	Forchlorfenuron	6.401	246.04195	[M-H]-	C ₁₂ H ₁₀ ClN ₃ O	2-halopyridines	C18604
43	Dicamba	1.111	220.97992	[2M+H] ⁺	C ₈ H ₆ Cl ₂ O ₃	Methoxybenzoic acids and derivatives	C18597
44	MCPB	7.361	227.04713	[M-H]-	C ₁₁ H ₁₃ ClO ₃	Phenol ethers	C18529
45	Dinotefuran	1.948	203.1132	[M+H] ⁺	C ₇ H ₁₄ N ₄ O ₃	Nitroguanidines	C18509
46	Cymoxanil	6.714	221.06493	[2M+H] ⁺	C ₇ H ₁₀ N ₄ O ₃	Oxime ethers	C18498
47	Myclobutanil	6.99	289.12469	[M+H] ⁺	C ₁₅ H ₁₇ ClN ₄	Chlorobenzenes	C18477
48	Tricaine	3.334	166.08553	[M+H] ⁺	C ₉ H ₁₁ NO ₂	Benzoic acid esters	C18090
49	Corynanthine	8.004	355.2178	[M+2H] ²⁺	C ₂₁ H ₂₆ N ₂ O ₃	Yohimbine alkaloids	C17872
50	Kukoamine A	8.597	531.3183	[M+H] ⁺	C ₂₈ H ₄₂ N ₄ O ₆	Catechols	C17615
51	Furanone A	14.863	85.02877	[M+H] ⁺	C ₄ H ₄ O ₂	Dihydrofurans	C17602
52	Furanone A	14.719	85.02879	[2M+H] ⁺	C ₄ H ₄ O ₂	Dihydrofurans	C17602
53	Furanone A	1.697	85.02859	[M+Na] ⁺	C ₄ H ₄ O ₂	Dihydrofurans	C17602
54	Lotusine	1.878	337.15848	[M+H] ⁺	C ₁₉ H ₂₄ NO ₃ ⁺	Benzylisoquinolines	C17567
55	Lotusine	1.687	337.15845	[M+CH ₃ OH+H] ⁺	C ₁₉ H ₂₄ NO ₃ ⁺	Benzylisoquinolines	C17567
56	Icariin	1.453	711.20569	[M-H]-	C ₃₃ H ₄₀ O ₁₅	Flavonoid O-glycosides	C17555
57	Cauloside C	10.6	765.43604	[M-H]-	C ₄₁ H ₆₆ O ₁₃	Triterpenoids	C17547
58	Isofraxidin	8.299	221.04369	[M-H]-	C ₁₁ H ₁₀ O ₅	7-hydroxycoumarins	C17480
59	Ophiopogonin A	8.594	765.44556	[M+2H] ²⁺	C ₄₁ H ₆₄ O ₁₃	Steroidal saponins	C17041
60	Liquiritin	8.129	417.1228	[M-H]-	C ₂₁ H ₂₂ O ₉	Flavonoid O-glycosides	C16989
61	Liquiritin	1.019	417.1228	[2M-H]-	C ₂₁ H ₂₂ O ₉	Flavonoid O-glycosides	C16989
62	Ligustilide	6.951	229.0634	[M+H] ⁺	C ₁₂ H ₁₄ O ₂	Isobenzofurans	C16987
63	Ligustilide	7.361	229.06343	[M+NH ₄] ⁺	C ₁₂ H ₁₄ O ₂	Isobenzofurans	C16987
64	Genipin 1-gentiobioside	3.58	568.21979	[M+CH ₃ OH+H] ⁺	C ₂₃ H ₃₄ O ₁₅	Iridoid O-glycosides	C16965
65	Gastrodin	6.289	304.13828	[M+H] ⁺	C ₁₃ H ₁₈ O ₇	Glycosyl compounds	C16964
66	Patulin	7.348	153.01698	[M-H]-	C ₇ H ₆ O ₄	Pyrans	C16748
67	5-Hydroxylysine	4.604	185.09126	[M+Na] ⁺	C ₆ H ₁₄ N ₂ O ₃	Amino acids and derivatives	C16741
68	6-Methylthiopurine	1.111	189.02354	[2M+H] ⁺	C ₆ H ₆ N ₄ S	6-thiopurines	C16614
69	Palmidrol	13.034	300.28799	[M+H] ⁺	C ₁₈ H ₃₇ NO ₂	Carboximide acids	C16512
70	Fructosyl-lysine	9.305	309.16614	[M+H] ⁺	C ₁₂ H ₂₄ N ₂ O ₇	Amino acids and derivatives	C16488
71	N ⁶ -Isopentenyladenosine	6.54	336.16406	[M+H] ⁺	C ₁₅ H ₂₁ N ₅ O ₄	Purine nucleosides	C16427
72	N ⁶ -Isopentenyladenosine	6.507	334.14856	[M-H]-	C ₁₅ H ₂₁ N ₅ O ₄	Purine nucleosides	C16427
73	Trinitrotoluene	10.805	227.01706	[M-H]-	C ₇ H ₅ N ₃ O ₆	Nitrobenzenes	C16391
74	9-HOTrE	9.953	277.21436	[M+H-H ₂ O] ⁺	C ₁₈ H ₃₀ O ₃	Lineolic acids and derivatives	C16326
75	9-HOTrE	12.35	317.20654	[2M+H] ⁺	C ₁₈ H ₃₀ O ₃	Lineolic acids and derivatives	C16326
76	13-HOTrE	11.163	277.21448	[M+H-H ₂ O] ⁺	C ₁₈ H ₃₀ O ₃	Lineolic acids and derivatives	C16316
77	Traumatin	9.956	211.1322	[M-H]-	C ₁₂ H ₂₀ O ₃	Fatty Acyls	C16309
78	Lipoic acid	0.987	207.04898	[M-H]-	C ₈ H ₁₄ O ₂ S ₂	Lipoic acids and derivatives	C16241
79	Medicarpin 3-O-glucoside-6'-malonate	2.271	517.1366	[M-H]-	C ₂₅ H ₂₆ O ₁₂	Pterocarpan	C16224
80	Malonylgenistin	2.133	517.10059	[M-H]-	C ₂₄ H ₂₂ O ₁₃	Isoflavonoid O-glycosides	C16192
81	Benzeneacetonitrile	6.696	118.06499	[M+H] ⁺	C ₈ H ₇ N	Benzene and substituted derivatives	C16074
82	Hyodeoxycholic acid	11.886	391.28323	[M-H]-	C ₂₄ H ₄₀ O ₄	Steroids and steroid derivatives	C15517

83	Asiaticoside	10.52	941.50964	[M+H] ⁺	C48H78O19	Triterpene glycosides	C15428
84	9,10,13-TriHOME	9.96	329.23157	[M-H] ⁻	C18H34O5	Fatty Acyls	C14835
85	9,12,13-TriHOME	11.026	329.23145	[M-H] ⁻	C18H34O5	Fatty Acyls	C14833
86	N-Hydroxy-1-aminonaphthalene	6.697	160.07486	[M+H-H2O] ⁺	C10H9NO	Naphthalenes	C14789
87	13-OxoODE	12.15	317.20529	[M+Na] ⁺	C18H30O3	Lineolic acids and derivatives Gluc/mineralocorticoids, progestogens and derivatives	C14765
88	Medrysone	11.176	379.20789	[M-H] ⁻	C22H32O3	Anilides	C14643
89	Pretilachlor	11.301	312.17288	[M+H] ⁺	C17H26ClNO2	Pyranones and derivatives	C14517
90	Kojic acid	4.083	143.03333	[M+H] ⁺	C6H6O4	Morpholines	C14516
91	Morpholine	12.4	88.07582	[M+H] ⁺	C4H9NO	Pyridines and derivatives	C14452
92	2-Methylpyridine	5.67	94.06523	[M+NH4] ⁺	C6H7N	Alkyl phosphates	C14447
93	Tri(butoxyethyl)phosphate	12.352	421.23016	[M+Na] ⁺	C18H39O7P	Pyrethroids	C14446
94	Phenothrin	8.147	351.19833	[M+2H] ²⁺	C23H26O3	Flavones	C14387
95	4',6-Dihydroxyflavone	9.337	255.06412	[M+H] ⁺	C15H10O4	Dithiophosphate O-esters	C14344
96	Dimethoate	0.464	251.99179	[M+H] ⁺	C5H12NO3PS2	Dithiophosphate O-esters	C14326
97	Dimethoate	0.614	251.99184	[M+H-H2O] ⁺	C5H12NO3PS2	Phenyl naphthalenes	C14326
98	Nafoxidine	8.321	426.24301	[M+2H] ²⁺	C29H31NO2	Isoflavanols	C14212
99	Equol	8.783	241.09038	[M-H] ⁻	C15H14O3	Aminoglycosides	C14131
100	Kitasamycin	12.542	786.46045	[M+2H] ²⁺	C40H67NO14	Resorcinols	C14064
101	Joro spider toxin	8.695	588.34662	[M+NH4] ⁺	C27H47N7O6	Diacylglycerophosphates	C13931
102	PA(16:0/18:1)	12.927	697.48199	[M+H] ⁺	C37H71O8P	Diacylglycerophosphates	C13889
103	PA(16:0/18:1)	13.46	697.48212	[M+Na] ⁺	C37H71O8P	Phosphatidylglycerols	C13889
104	PG(16:0/18:1)	11.429	747.51508	[M-H] ⁻	C40H77O10P	Carboximide acids	C13883
105	Stearic acid amide	13.013	284.29303	[M+H] ⁺	C18H37NO	Fatty Acyls	C13846
106	Dodecanamide	12.234	200.19977	[M+H] ⁺	C12H25NO	Hydropyridines	C13831
107	Isoguvacine	0.884	128.07018	[M+H] ⁺	C6H9NO2	Tetrahydroisoquinolines	C13694
108	Hydrocotarnine	6.338	222.11197	[M+H] ⁺	C12H15NO3	Phenylpyrazoles	C13534
109	Antipyrine	6.573	189.10179	[M+H] ⁺	C11H12N2O	Amino acids and derivatives	C13244
110	Kainic acid	6.364	236.09056	[M+Na] ⁺	C10H15NO4	Angucyclines	C12819
111	Rabelomycin	6.288	337.0759	[M-H] ⁻	C19H14O6	Phenanthridines and derivatives	C12402
112	Ungeremine	1.104	267.09088	[M+H] ⁺	C16H12NO3+	Alkanolamines	C12189
113	Phytosphingosine	10.867	318.29865	[M+H] ⁺	C18H39NO3	Alkanolamines	C12144
114	Phytosphingosine	10.865	300.28815	[M+H-H2O] ⁺	C18H39NO3	Alkanolamines	C12144
115	Phytosphingosine	10.318	340.28036	[M+Na] ⁺	C18H39NO3	Carboxylic acids and derivatives	C12144
116	Dihydroceramide	11.32	330.29843	[M+H] ⁺	C19H39NO3	Phenanthrols	C12126
117	Resistomycin	6.861	375.08337	[M-H] ⁻	C22H16O6	Oxirane carboxylic acids and derivatives	C12080
118	Cerulenin	6.599	246.11191	[M+Na] ⁺	C12H17NO3	Amino acids and derivatives	C12058
119	Actinonin	11.222	403.29181	[M+H] ⁺	C19H35N3O5	Pyranones and derivatives	C12056
120	Maltol	0.261	125.02293	[M+H] ⁺	C6H6O3	Pyranones and derivatives	C11918
121	Maltol	13.562	125.0229	[M+H-H2O] ⁺	C6H6O3	7-O-methylated flavonoids	C11918
122	Tectochrysin	13.813	269.07962	[M+H] ⁺	C16H12O4		C11621

123	Phenylglucoside	10.27	274.12482	[M+CH ₃ OH+H] ⁺	C ₁₂ H ₁₆ O ₆	Glycosyl compounds	C11611
124	Raltitrexed	4.243	457.11966	[M-H] ⁻	C ₂₁ H ₂₂ N ₄ O ₆ S	Amino acids and derivatives	C11372
125	Triadimefon	2.616	294.09909	[M+H] ⁺	C ₁₄ H ₁₆ ClN ₃ O ₂	Phenol ethers	C11156
126	Dimethyl sulfoxide	2.161	79.02161	[M+H] ⁺	C ₂ H ₆ O _S	Sulfoxides	C11143
127	Dimethyl sulfone	1.111	95.01917	[M+H] ⁺	C ₂ H ₆ O ₂ S	Sulfones	C11142
128	7-Ethoxycoumarin	10.514	191.06969	[M+Na] ⁺	C ₁₁ H ₁₀ O ₃	Coumarins and derivatives	C11052
129	Aspartame	6.513	295.12796	[M+H] ⁺	C ₁₄ H ₁₈ N ₂ O ₅	Peptides	C11045
130	Aspartame	7.926	277.11685	[M+Na] ⁺	C ₁₄ H ₁₈ N ₂ O ₅	Peptides	C11045
131	Cycloxydim	7.979	324.1647	[M-H] ⁻	C ₁₇ H ₂₇ N ₃ O ₃ S	Ketones	C10913
132	Bromacil	0.9	259.0108	[M-H] ⁻	C ₉ H ₁₃ BrN ₂ O ₂	Halopyrimidines	C10911
133	2-Benzimidazolylguanidine	1.035	174.07489	[M-H] ⁻	C ₈ H ₉ N ₅	Benzimidazoles	C10898
134	Steganacin	11.58	495.12317	[M+Na] ⁺	C ₂₄ H ₂₄ O ₉	Lignan lactones	C10886
135	Steganacin	11.167	495.12299	[M+H] ⁺	C ₂₄ H ₂₄ O ₉	Lignan lactones	C10886
136	Sesamol	7.367	137.02202	[M-H] ⁻	C ₇ H ₆ O ₃	Benzodioxoles	C10832
137	Zygadenine	13.418	494.31152	[M+2H] ²⁺	C ₂₇ H ₄₃ N ₇ O	Cerveratrum-type alkaloids	C10831
138	Protoveratrine A	13.235	816.47876	[M+2H] ²⁺	C ₄₁ H ₆₃ N ₁₁ O ₁₄	Cerveratrum-type alkaloids	C10815
139	Thermopsine	6.694	267.14346	[M+Na] ⁺	C ₁₅ H ₂₀ N ₂ O	Anagyrine-type alkaloids	C10789
140	Cytisine	7.801	213.10138	[M+Na] ⁺	C ₁₁ H ₁₄ N ₂ O	Cytisine and derivatives	C10763
141	Skimmianine	9.793	262.10571	[M+H] ⁺	C ₁₄ H ₁₅ N ₃ O ₄	Dihydrofuranoquinolines	C10740
142	Picein	6.214	316.13785	[M+Na] ⁺	C ₁₄ H ₁₈ O ₇	Glycosyl compounds	C10720
143	Dictamnine	6.344	200.06958	[M+H] ⁺	C ₁₂ H ₉ N ₃ O ₂	Furanoquinolines	C10660
144	3-Deoxyvasicine	6.548	173.10672	[M+H] ⁺	C ₁₁ H ₁₂ N ₂	Quinazolines	C10656
145	cephalotaxine	6.817	338.13361	[M+H] ⁺	C ₁₈ H ₂₁ N ₃ O ₄	Cephalotaxus alkaloids	C10580
146	Eudesmin	10.696	409.16016	[M+Na] ⁺	C ₂₂ H ₂₆ O ₆	Furanoid lignans	C10561
147	Ononin	1.093	475.12613	[2M-H] ⁻	C ₂₂ H ₂₂ O ₉	Isoflavonoid O-glycosides	C10509
148	Ononin	1.244	475.12616	[M-H] ⁻	C ₂₂ H ₂₂ O ₉	Isoflavonoid O-glycosides	C10509
149	Ononin	5.442	429.12122	[M-H ₂ O-H] ⁻	C ₂₂ H ₂₂ O ₉	Isoflavonoid O-glycosides	C10509
150	6-Shogaol	8.115	315.13907	[M+H] ⁺	C ₁₇ H ₂₄ O ₃	Shogaols	C10494
151	Isoferulic acid	3.357	212.09087	[M+H] ⁺	C ₁₀ H ₁₀ O ₄	Hydroxycinnamic acids	C10470
152	Isoferulic acid	3.902	212.09077	[M+H-H ₂ O] ⁺	C ₁₀ H ₁₀ O ₄	Hydroxycinnamic acids	C10470
153	Cinnamic acid	6.308	131.04868	[M+H-H ₂ O] ⁺	C ₉ H ₈ O ₂	Cinnamic acids	C10438
154	Caffeic acid 3-glucoside	1.232	365.08325	[M+H] ⁺	C ₁₅ H ₁₈ O ₉	Glycosyl compounds	C10431
155	Piceid	5.259	389.12643	[M-H] ⁻	C ₂₀ H ₂₂ O ₈	Stilbene glycosides	C10275
156	Vicenin 2	7.139	593.14825	[M-H] ⁻	C ₂₇ H ₃₀ O ₁₅	Flavonoid C-glycosides	C10195
157	Nevadensin	10.637	343.07999	[M-H] ⁻	C ₁₈ H ₁₆ O ₇	8-O-methylated flavonoids	C10111
158	Myricetin	8.734	319.04068	[M-H] ⁻	C ₁₅ H ₁₀ O ₈	Flavonols	C10107
159	Gambogic acid	7.418	627.30914	[M-H] ⁻	C ₃₈ H ₄₄ O ₈	Dibenzopyrans	C10062
160	Gambogic acid	7.949	629.30994	[M+H] ⁺	C ₃₈ H ₄₄ O ₈	Dibenzopyrans	C10062
161	Galangin	1.217	292.9783	[M+H] ⁺	C ₁₅ H ₁₀ O ₅	Flavonols	C10044
162	Peoniflorin	7.635	525.15918	[M-H] ⁻	C ₂₃ H ₂₈ O ₁₁	Terpene glycosides	C09959
163	(S)-Actinidine	6.488	148.11171	[M+H] ⁺	C ₁₀ H ₁₃ N	Pyridines and derivatives	C09910

164	Sakuranetin	8.993	287.09009	[M+H] ⁺	C16H14O5	7-O-methylated flavonoids	C09833
165	Sakuranetin	10.252	285.07443	[M-H] ⁻	C16H14O5	7-O-methylated flavonoids	C09833
166	Fellavine	6.655	563.17822	[M-H] ⁻	C26H30O11	Flavonoid O-glycosides	C09808
167	Neohesperidin	8.4	609.17749	[M-H] ⁻	C28H34O15	Flavonoid O-glycosides	C09806
168	Neohesperidin	1.044	609.18469	[2M-H] ⁻	C28H34O15	Flavonoid O-glycosides	C09806
169	Neerioicitrin	7.817	595.16418	[M-H] ⁻	C27H32O15	Flavonoid O-glycosides	C09805
170	Neerioicitrin	7.813	597.17963	[M+H] ⁺	C27H32O15	Flavonoid O-glycosides	C09805
171	Naringin	8.33	579.16907	[M-H] ⁻	C27H32O14	Flavonoid O-glycosides	C09789
172	Aucubin	7.406	345.11716	[M-H] ⁻	C15H22O9	Iridoid O-glycosides	C09771
173	Aucubin	8.345	345.11575	[M-H2O-H] ⁻	C15H22O9	Iridoid O-glycosides	C09771
174	Diacetoxyscirpenol	8.227	384.2027	[M+H] ²⁺	C19H26O7	Trichothecenes	C09662
175	Noscapine	8.8	412.13785	[M-H] ⁻	C22H23NO7	Phthalide isoquinolines	C09592
176	Liriodenine	7.262	276.06769	[M+H] ⁺	C17H9NO3	Aporphines	C09567
177	Liriodenine	14.865	276.06549	[M+2H] ²⁺	C17H9NO3	Aporphines	C09567
178	Artemisinin	11.515	283.15085	[M-H] ⁻	C15H22O5	Terpene lactones	C09538
179	Hymenoxon	10.439	281.13724	[M-H2O-H] ⁻	C15H22O5	Oxanes	C09482
180	Furanoheliangolide	11.016	359.11179	[M-H] ⁻	C19H20O7	Terpene lactones	C09467
181	Emetine	12.969	481.31018	[M+H] ⁺	C29H40N2O4	Emetine alkaloids	C09421
182	Marmesin	9.714	247.09518	[M+H] ⁺	C14H14O4	Psoralens	C09276
183	Aesculetin	1.249	201.01508	[M+Na] ⁺	C9H6O4	6,7-dihydroxycoumarins	C09263
184	Vincamine	6.669	353.04199	[M-H] ⁻	C21H26N2O3	Eburnan-type alkaloids	C09251
185	Tabernamine	12.109	617.38446	[M+2H] ²⁺	C40H48N4O2	Ibogan-type alkaloids	C09242
186	Perlolyrine	8.381	265.09607	[M+H] ⁺	C16H12N2O2	Harmala alkaloids	C09231
187	Harman	7.801	183.09076	[M+H] ⁺	C12H10N2	Harmala alkaloids	C09209
188	Byakangelicin	9.64	357.09229	[M+Na] ⁺	C17H18O7	5-methoxypsoralens	C09141
189	Prunin	10.793	435.12854	[M+CH3OH+H] ⁺	C21H22O10	Flavonoid O-glycosides	C09099
190	Khelloside	7.019	409.10886	[M+H] ⁺	C19H20O10	Chromones	C09011
191	Cimifugin	13.801	329.10049	[M+Na] ⁺	C16H18O6	Chromones	C09000
192	Soyasaponin I	10.184	965.50128	[M+Na] ⁺	C48H78O18	Triterpene glycosides	C08983
193	Soyasaponin I	10.182	943.51984	[M+H] ⁺	C48H78O18	Triterpene glycosides	C08983
194	Soyasaponin I	10.186	941.50757	[M-H] ⁻	C48H78O18	Triterpene glycosides	C08983
195	Soyasaponin I	10.187	987.50903	[M+HCOO] ⁻	C48H78O18	Triterpene glycosides	C08983
196	Saikosaponin C	13.512	927.52869	[M-H] ⁻	C48H78O17	Triterpene glycosides	C08975
197	Calenduloside E	8.46	655.3772	[M+2H] ²⁺	C36H56O9	Triterpene glycosides	C08964
198	alpha-Hederin	10.459	795.44904	[M-H] ⁻	C41H66O12	Triterpenoids	C08954
199	Diosgenin	9.123	415.31781	[M+H] ⁺	C27H42O3	Triterpenoids	C08898
200	Cyasterone	7.655	521.25391	[M+Na] ⁺	C29H44O8	Triterpenoids	C08816
201	Cyasterone	13.383	538.33887	[M+2H] ²⁺	C29H44O8	Triterpenoids	C08816
202	Songorine	6.843	380.21701	[M+H] ⁺	C22H31NO3	Napelline-type diterpenoid alkaloids	C08707
203	Indaconitine	8.39	630.32489	[M+H] ⁺	C34H47NO10	Aconitane-type diterpenoid alkaloids	C08691
204	Pristimerin	9.409	463.2879	[M-H] ⁻	C30H40O4	Triterpenoids	C08633
205	Canthaxanthin	8.703	603.35535	[M+2H] ²⁺	C40H52O2	Carotenoids	C08583

206	Astaxanthin	12.786	619.37848	[2M+H] ⁺	C40H52O4	Carotenoids	C08580
207	Galanthamine hydrobromide	3.022	368.0834	[M+H] ⁺	C17H22BrNO3	Galanthamine-type amaryllidaceae alkaloids	C08526
208	Indole-3-carboxyaldehyde	6.696	146.0596	[M+H] ⁺	C9H7NO	Indoles	C08493
209	Jasmonic acid	10.799	211.13177	[M+H-H2O] ⁺	C12H18O3	Jasmonic acids	C08491
210	Chelidonic acid	2.499	185.00719	[M+H] ⁺	C7H4O6	Pyranones and derivatives	C08476
211	Vaccenic acid	13.445	281.24677	[M-H] ⁻	C18H34O2	Long-chain fatty acids	C08367
212	Ricinoleic acid	11.858	299.25671	[M+NH4] ⁺	C18H34O3	Long-chain fatty acids	C08365
213	Palmitoleic acid	12.343	253.21555	[M-H] ⁻	C16H30O2	Long-chain fatty acids	C08362
214	12-Hydroxydodecanoic acid	11.966	239.16238	[M+H] ⁺	C12H24O3	Medium-chain hydroxy acids and derivatives	C08317
215	alpha-Eleostearic acid	10.472	279.23022	[M+H] ⁺	C18H30O2	Fatty Acyls	C08315
216	alpha-Eleostearic acid	10.952	279.23019	[M+NH4] ⁺	C18H30O2	Fatty Acyls	C08315
217	9,10-Dihydroxystearic acid (S)-10,16-	11.861	315.2511	[M-H] ⁻	C18H36O4	Fatty Acyls	C08314
218	Dihydroxyhexadecanoic acid	10.262	287.22076	[M-H] ⁻	C16H32O4	Fatty Acyls	C08285
219	Suberic acid	8.586	175.09554	[M-H] ⁻	C8H14O4	Medium-chain fatty acids	C08278
220	Azelaic acid	8.831	187.09544	[M-H] ⁻	C9H16O4	Medium-chain fatty acids	C08261
221	Verbascose	1.094	827.2627	[M-H] ⁻	C30H52O26	Oligosaccharides	C08252
222	Melezitose	2.375	527.1557	[M+Na] ⁺	C18H32O16	Oligosaccharides	C08243
223	Melezitose	1.497	543.13013	[M+K] ⁺	C18H32O16	Oligosaccharides	C08243
224	Melezitose	6.522	505.17407	[M-H] ⁻	C18H32O16	Oligosaccharides	C08243
225	Gentiobiose	1.49	381.07758	[M+H] ⁺	C12H22O11	Glycosyl compounds	C08240
226	Dexamethasone acetate	9.35	433.20367	[M-H] ⁻	C24H31FO6	Glucocorticoids, progestogens and derivatives	C08174
227	Nafcillin Sodium	11.854	437.11542	[M+H] ⁺	C21H23N2NaO6S	Penams	C08124
228	Amprenavir	6.677	506.23395	[M+NH4] ⁺	C25H35N3O6S	Aminobenzenesulfonamides	C08086
229	DL-Cycloserine	6.309	103.05439	[M+H] ⁺	C3H6N2O2	Amino acids and derivatives	C08057
230	Tolcapone	8.558	272.05225	[M-H] ⁻	C14H11NO5	Benzophenones	C07949
231	Butyl 4-aminobenzoate	9.267	194.11662	[M+H] ⁺	C11H15NO2	Benzene and substituted derivatives	C07875
232	Docusate hydrogen	12.385	421.22299	[M-H] ⁻	C20H38O7S	Fatty acid esters	C07874
233	Diphenhydramine hydrochloride	4.771	292.1488	[M+H] ⁺	C17H22ClNO	Diphenylmethanes	C07784
234	Diphenhydramine hydrochloride	3.022	292.14883	[M+Na] ⁺	C17H22ClNO	Diphenylmethanes	C07784
235	1,4-Dihydro-3H-2-benzopyran-3-one	8.343	147.04292	[M-H] ⁻	C9H8O2	2-benzopyrans	C07728
236	Telmisartan	7.475	537.22717	[M+Na] ⁺	C33H30N4O2	Biphenyls and derivatives	C07710
237	Candesartan cilexetil	10.676	609.24207	[M-H] ⁻	C33H34N6O6	Biphenyls and derivatives	C07709
238	Miglitol	1.4	208.11671	[2M+H] ⁺	C8H17NO5	Piperidines	C07708
239	Repaglinide	11.164	453.27972	[M+H] ⁺	C27H36N2O4	Phenylpiperidines	C07670
240	Sparfloxacin	7.2	391.151	[M-H] ⁻	C19H22F2N4O3	Quinoline carboxylic acids	C07662
241	Colchicine	8.095	444.16278	[M-H] ⁻	C22H25NO6	Tropones	C07592

242	Phenacetin	8.546	180.10088	[M+H] ⁺	C10H13NO2	Acetanilides	C07591
243	Amphetamine	7.343	158.09579	[M+Na] ⁺	C9H13N	Amphetamines and derivatives	C07514
244	Methoxamine	4.245	212.12746	[M+H] ⁺	C11H17NO3	Dimethoxybenzenes	C07513
245	Ethosuximide	6.511	142.08572	[M+H] ⁺	C7H11NO2	Pyrrolidine-2-ones	C07505
246	Zonisamide	8.677	211.02237	[M-H] ⁻	C8H8N2O3S	Benzisoxazoles 1,4-	C07504
247	Nordazepam	1.107	271.06531	[M+H] ⁺	C15H11ClN2O	benzodiazepinesInCh IKey	C07486
248	Zaleplon	6.901	306.13254	[M+H] ⁺	C17H15N5O	Phenylpyrimidines	C07484
249	Caffeine	7.334	195.08672	[M+H] ⁺	C8H10N4O2	Xanthines	C07481
250	Theobromine	1.294	219.0255	[M+H] ⁺	C7H8N4O2	Xanthines	C07480
251	Pilocarpine nitrate	6.615	310.12726	[M+H- H2O] ⁺	C11H17N3O5	Gamma butyrolactones	C07474
252	Pilocarpine	6.234	209.12766	[M+H] ⁺	C11H16N2O2	Alkaloids and derivatives	C07474
253	Pentoxifylline	6.579	279.14404	[M+H] ⁺	C13H18N4O3	Xanthines	C07424
254	Penbutolol	9.358	292.22583	[M+CH3OH +H] ⁺	C18H29NO2	Phenol ethers	C07416
255	Paroxetine	7.232	330.15042	[M+H] ⁺	C19H20FNO3	Phenylpiperidines	C07415
256	Paramethadione	6.437	156.06425	[M-H] ⁻	C7H11NO3	Azolidines	C07411
257	Promethazine	6.655	285.14267	[M+NH4] ⁺	C17H20N2S	Phenothiazines	C07404
258	Paclitaxel	5.998	892.29126	[M+2H] ²⁺	C47H51NO14	Taxanes and derivatives	C07394
259	3- Pyridinecarboxaldehyde	1.99	108.04422	[M+Na] ⁺	C6H5NO	Pyridines and derivatives	C07327
260	3- Pyridinecarboxaldehyde	7.584	108.04418	[M+H- H2O] ⁺	C6H5NO	Pyridines and derivatives	C07327
261	Nefazodone	1.553	506.20697	[M+CH3OH +H] ⁺	C25H33Cl2N5O 2	Phenylpiperazines	C07256
262	Salmeterol	7.183	416.28268	[M+H] ⁺	C25H37NO4	Benzyl alcohols Benzene and	C07241
263	2-Methylbenzaldehyde	8.343	119.048	[M-H] ⁻	C8H8O	substituted derivatives	C07214
264	Zafirlukast	6.159	598.19513	[M+H- H2O] ⁺	C31H33N3O6S	Benzenesulfonamide s	C07206
265	Metronidazole	6.367	172.07503	[M+H] ⁺	C6H9N3O3	Substituted imidazoles	C07203
266	Verapamil	12.041	455.29501	[M+H] ⁺	C27H38N2O4	Phenylbutylamines	C07188
267	Venlafaxine	11.769	278.20755	[M+H] ⁺	C17H27NO2	Anisoles	C07187
268	Protoanemonin	6.131	97.02859	[M+H] ⁺	C5H4O2	Dihydrofurans Benzene and	C07090
269	Phenylacetic acid	6.817	135.04286	[M-H] ⁻	C8H8O2	substituted derivatives	C07086
270	Loperamide	7.484	477.22818	[M+H] ⁺	C29H33ClN2O2	Diphenylmethanes	C07080
271	Lidocaine	7.72	235.17969	[M+H] ⁺	C14H22N2O	m-Xylenes	C07073
272	Labetalol	8.053	329.18521	[M+NH4] ²⁺	C19H24N2O3	Salicylamides	C07063
273	Ketorolac	9.38	256.09589	[M+H] ⁺	C15H13NO3	Aryl-phenylketones	C07062
274	Gabapentin	6.541	172.1328	[M+H] ⁺	C9H17NO2	Amino acids and derivatives	C07018
275	Enalapril	11.624	375.18829	[M-H] ⁻	C20H28N2O5	Peptides	C06977
276	Diphenidol Hydrochloride	7.109	346.19617	[M+NH4] ⁺	C21H28ClNO	Diphenylmethanes	C06961
277	Digitoxin	8.596	787.42383	[M+Na] ⁺	C41H64O13	Cardenolides and derivatives	C06955
278	Deferoxamine	12.718	583.3418	[M+H] ⁺	C25H48N6O8	Carboxylic acid amides	C06940
279	Clozapine	9.158	327.14014	[M+H] ⁺	C18H19ClN4	Dibenzodiazepines	C06924
280	Ceftazidime	2.124	545.09583	[M-H] ⁻	C22H22N6O7S2	Cephems	C06889
281	Azithromycin	13.306	749.51593	[M+H] ⁺	C38H72N2O12	Aminosaccharides	C06838
282	Azithromycin	12.852	787.47107	[M+2H] ²⁺	C38H72N2O12	Aminosaccharides	C06838

283	1,8,9-Trihydroxyanthracene	11.063	225.05902	[M-H]-	C14H10O3	Anthracenes	C06831
284	Lincomycin	9.023	405.20789	[M-H]-	C18H34N2O6S	Amino acids and derivatives	C06812
285	Acyclovir	0.861	224.07613	[M-H]-	C8H11N5O3	Purinones	C06810
286	Acetaminophen	7.632	152.07008	[M+H]+	C8H9NO2	1-hydroxy-2-unsubstituted benzenoids	C06804
287	Acarbose	6.182	668.23743	[M+H]+	C25H43NO18	Aminosaccharides	C06802
288	Fusidic acid	6.694	555.31165	[M+H]+	C31H48O6	Steroid esters	C06694
289	Monensin Sodium Salt	9.958	715.40369	[M+H]+	C36H61NaO11	Acetals	C06693
290	Monensin	8.821	693.41254	[M+2H]2+	C36H62O11	Heterocyclic fatty acids	C06693
291	Cycloheximide	8.83	326.15836	[M-H]-	C15H23NO4	Tetrahydropyridines	C06685
292	Mitomycin	6.817	333.11703	[M-H2O-H]-	C15H18N4O5	Mitomycins, mitosane and mitosene derivatives	C06681
293	Tetracycline hydrochloride	12.667	481.27286	[M+H]+	C22H25ClN2O8	Tetracyclines	C06570
294	Genistein	10.016	271.05899	[M+H]+	C15H10O5	Isoflavones	C06563
295	Veratridine	8.458	674.35333	[M+2H]2+	C36H51NO11	Cerveratrum-type alkaloids	C06544
296	Reserpine	7.625	609.30676	[M+H]+	C33H40N2O9	Yohimbine alkaloids	C06539
297	Reserpine	7.772	609.30585	[M+NH4]+	C33H40N2O9	Yohimbine alkaloids	C06539
298	Harmaline	6.139	253.06989	[M+H-H2O]+	C13H14N2O	Harmala alkaloids	C06536
299	Harmaline	7.419	253.06972	[M+H]+	C13H14N2O	Harmala alkaloids	C06536
300	Normicotine	6.788	149.10664	[M+H]+	C9H12N2	Pyrrolidinylpyridines	C06524
301	Muramic acid	1.404	234.09575	[M+Na]+	C9H17NO7	Sugar acids and derivatives	C06470
302	Muramic acid	3.524	234.09569	[M+H]+	C9H17NO7	Sugar acids and derivatives	C06470
303	Psicose	1.294	203.05141	[M+Na]+	C6H12O6	Monosaccharides	C06468
304	Linolenic acid	11.485	279.23019	[M+H]+	C18H30O2	Lineolic acids and derivatives	C06427
305	Myristic acid	12.231	227.19981	[M-H]-	C14H28O2	Long-chain fatty acids	C06424
306	Caprylic acid	8.83	125.09489	[M-H]-	C8H16O2	Medium-chain fatty acids	C06423
307	4-Hydroxyquinoline	7.093	146.05956	[M+H]+	C9H7NO	Hydroquinolones	C06343
308	2,8-Dihydroxyquinoline	6.33	162.05424	[M+H]+	C9H7NO2	Quinolones and derivatives	C06342
309	Quinolinol	9.09	144.04308	[M-H]-	C9H7NO	Hydroquinolones	C06338
310	Maltopentaose	1.925	829.2782	[M+H]+	C30H52O26	Oligosaccharides	C06218
311	Salicylaldehyde	3.576	123.04376	[M+H]+	C7H6O2	Aldehydes	C06202
312	3'-GMP	2.38	362.04828	[M-H]-	C10H14N5O8P	Ribonucleoside 3'-phosphates	C06193
313	Arbutin	3.349	290.12207	[M+H]+	C12H16O7	Glycosyl compounds	C06186
314	Myoinositol	0.992	179.0537	[M-H]-	C6H12O6	Organooxygen compounds	C06153
315	Myoinositol	1.258	179.05365	[2M-H]-	C6H12O6	Organooxygen compounds	C06153
316	Rhodioloside	7.419	323.108	[M+Na]+	C14H20O7	Glycosyl compounds	C06046
317	2-Hydroxybutyric acid	3.176	103.03781	[M-H]-	C4H8O3	Alpha hydroxy acids and derivatives	C05984
318	3-Methyldioxyindole	4.436	164.06998	[M+H]+	C9H9NO2	Indoles and derivatives	C05834
319	5-Methoxyindoleacetic acid	6.875	206.08015	[M+H]+	C11H11NO3	Indole-3-acetic acid derivatives	C05660
320	6-Hydroxymelatonin	6.25	249.1228	[M+H-H2O]+	C13H16N2O3	Hydroxyindoles	C05643

321	6-Hydroxymelatonin	6.808	249.12273	[M+CH3OH+H] ⁺	C13H16N2O3	Hydroxyindoles	C05643
322	6-Hydroxymelatonin	6.784	247.10686	[M-H] ⁻	C13H16N2O3	Hydroxyindoles	C05643
323	5-Hydroxyindoleacetate	2.877	192.06483	[M+H] ⁺	C10H9NO3	Indole-3-acetic acid derivatives	C05635
324	Eriodictyol	7.809	289.069	[M+H] ⁺	C15H12O6	Flavanones	C05631
325	Rutin	7.887	609.14172	[M-H] ⁻	C27H30O16	Flavonoid O-glycosides	C05625
326	Sinapaldehyde	8.832	209.07704	[M-H] ⁻	C11H12O4	Methoxyphenols	C05610
327	3-Phenyllactic acid	7.38	165.05354	[M-H] ⁻	C9H10O3	Phenylpropanoic acids	C05607
328	Phenylacetylglutamine	9.831	194.08003	[M-H] ⁻	C10H11NO3	Amino acids and derivatives	C05598
329	Benzylpenicillin	3.435	333.0925	[M-H] ⁻	C16H18N2O4S	Peptides	C05551
330	Deoxyinosine	3.163	251.07571	[M-H] ⁻	C10H12N4O4	Purine 2'-deoxyribonucleosides	C05512
331	5b-Cyprinol sulfate	11.814	531.29901	[2M-H] ⁻	C27H48O8S	Steroids and steroid derivatives	C05468
332	Taurodeoxycholic acid	7.3	500.30386	[M+H] ⁺	C26H45NO6S	Taurinated bile acids and derivatives	C05463
333	Taurodeoxycholic acid	7.764	482.29584	[M+NH4] ⁺	C26H45NO6S	Taurinated bile acids and derivatives	C05463
334	Melibiose	13.482	365.10333	[M+Na] ⁺	C12H22O11	Glycosyl compounds	C05402
335	Melibiose	7.66	377.08273	[M-H] ⁻	C12H22O11	Glycosyl compounds	C05402
336	Nicotianamine	6.546	302.13403	[M-H] ⁻	C12H21N3O6	Amino acids and derivatives	C05324
337	Taurocholic acid	7.593	516.29785	[M+Na] ⁺	C26H45NO7S	Hydroxy bile acids, alcohols and derivatives	C05122
338	Imazaquin	9.207	312.13254	[M+H] ⁺	C17H17N3O3	Quinoline carboxylic acids	C05076
339	3-Hydroxy-2-methylpyridine-4,5-dicarboxylate	7.398	196.02298	[M-H] ⁻	C8H7NO5	Pyridines and derivatives	C04604
340	Pyrroline hydroxycarboxylate	2.328	128.03319	[M-H] ⁻	C5H7NO3	Carboxylic acids and derivatives	C04281
341	N,N-Dimethylhistidine	2.981	184.10706	[M+H] ⁺	C8H13N3O2	Amino acids and derivatives	C04259
342	Octopine	2.726	247.13863	[M+H] ⁺	C9H18N4O4	Amino acids and derivatives	C04137
343	LPC(16:0)	9.78	518.32074	[M+Na] ⁺	C24H50NO7P	Lysophosphatidylcholines	C04102
344	LPC(16:0)	13.588	496.33755	[M+H] ⁺	C24H50NO7P	Lysophosphatidylcholines	C04102
345	1-Piperidine-2-carboxylic acid	1.422	128.07018	[M+NH4] ⁺	C6H9NO2	Pyridines and derivatives	C04092
346	1-Piperidine-2-carboxylic acid	10.071	128.07014	[M+H] ⁺	C6H9NO2	Pyridines and derivatives	C04092
347	Rumenic acid	12.512	279.23126	[M-H] ⁻	C18H32O2	Lineolic acids and derivatives	C04056
348	9,11-Linoleic Acid	12.351	279.2312	[M-H] ⁻	C18H32O2	Lineolic acids and derivatives	C04056
349	Flavanone 7-O-Glucoside	10.572	447.12985	[M-H] ⁻	C21H22O8	Flavonoid O-glycosides	C04007
350	Flavanone 7-O-Glucoside	1.029	447.13202	[2M-H] ⁻	C21H22O8	Flavonoid O-glycosides	C04007
351	Thyroliberin	11.088	361.16	[M-H] ⁻	C16H22N6O4	Peptides	C03958
352	LPC(18:1)	10.535	544.33527	[M+Na] ⁺	C26H52NO7P	Lysophosphatidylcholines	C03916

353	LPC(18:1)	10.592	522.35339	[M+H] ⁺	C26H52NO7P	Lysophosphatidylcholines	C03916
354	LPC(18:1)	10.668	566.34143	[M+HCOO] ⁻	C26H52NO7P	Lysophosphatidylcholines	C03916
355	Oxidized Cypridina luciferin	7.202	392.21719	[M-H] ⁻	C21H27N7O	Indoles	C03887
356	Oxidized Cypridina luciferin	7.17	394.23154	[M+H] ⁺	C21H27N7O	Indoles	C03887
357	Targinine	1.363	189.13344	[M+NH4] ⁺	C7H16N4O2	Carboxylic acids and derivatives	C03884
358	3,4-Dehydro-6-hydroxymellein	1.11	191.03912	[M+CH3OH+H] ⁺	C10H8O4	Isocoumarins and derivatives	C03830
359	alpha-Keto-delta-guanidinovaleric acid	1.531	174.0867	[M+H] ⁺	C6H11N3O3	Short-chain keto acids and derivatives	C03771
360	Carbocysteine	9.076	180.03439	[M+2H] ²⁺	C5H9NO4S	Amino acids and derivatives	C03727
361	Carbocysteine	13.975	180.03447	[M+H] ⁺	C5H9NO4S	Amino acids and derivatives	C03727
362	Carbocysteine	10.911	180.03447	[M+H-H2O] ²⁺	C5H9NO4S	Amino acids and derivatives	C03727
363	Carbocysteine	0.202	180.03448	[M+H-H2O] ⁺	C5H9NO4S	Amino acids and derivatives	C03727
364	Carbocysteine	13.529	180.0345	[M+NH4] ²⁺	C5H9NO4S	Amino acids and derivatives	C03727
365	N-Benzyloxycarbonyl-glycine	6.836	208.0593	[M-H] ⁻	C10H11NO4	Benzyloxycarbonyls	C03710
366	1-Kestose	1.496	527.15576	[M+Na] ⁺	C18H32O16	Oligosaccharides	C03661
367	N,N-Dimethylarginine	6.574	225.13368	[M+NH4] ⁺	C8H18N4O2	Amino acids and derivatives	C03626
368	Mannosamine	1.284	162.07571	[M+H-H2O] ⁺	C6H13NO5	Monosaccharides	C03570
369	trans-Zeatin-O-glucoside	9.803	382.17194	[M+NH4] ²⁺	C16H23N5O6	Fatty acyl glycosides	C03423
370	Argininosuccinic acid	2.445	291.12869	[M+H] ⁺	C10H18N4O6	Amino acids and derivatives	C03406
371	3-Hydroxybenzyl alcohol	10.918	107.0491	[M+H-H2O] ⁺	C7H8O2	Benzyl alcohols	C03351
372	L-2,3-Dihydrodipicolinic acid	9.656	168.028	[M-H] ⁻	C7H7NO4	Carboxylic acids and derivatives	C03340
373	Glycerophosphoglycerol	0.9	245.04161	[M-H] ⁻	C6H15O8P	Organic phosphoric acids and derivatives	C03274
374	Leucinic acid (E)-3-(2,3-Dihydroxyphenyl)-2-propenoic acid	7.837	131.06914	[M-H] ⁻	C6H12O3	Fatty Acyls	C03264
375		8.343	179.03259	[M-H] ⁻	C9H8O4	Cinnamic acids and derivatives	C03246
376	2-Hydroxystearic acid	13.285	299.25705	[M-H] ⁻	C18H36O3	Long-chain fatty acids	C03045
377	N-Methylantranilic acid	6.481	150.0537	[M-H] ⁻	C8H9NO2	Aminobenzoic acids and derivatives	C03005
378	N-Caffeoylputrescine	6.381	251.13847	[M+CH3OH+H] ⁺	C13H18N2O3	Catechols	C03002
379	L-3-Aminodihydro-2(3H)-furanone	1.305	102.05488	[M+CH3OH+H] ⁺	C4H7NO2	Carboxylic acids and derivatives	C02926
380	L-3-Aminodihydro-2(3H)-furanone	4.916	102.0549	[M+NH4] ⁺	C4H7NO2	Carboxylic acids and derivatives	C02926
381	Lecanoric acid	7.832	317.06659	[M-H] ⁻	C16H14O7	Depsidic acids and depsidones	C02868
382	Butyrylcarnitine	6.513	232.15305	[M+H] ⁺	C11H21NO4	Acyl carnitines	C02862
383	2,5-Piperazinedione	6.696	115.05417	[M+H] ⁺	C4H6N2O2	Amino acids and derivatives	C02777
384	Feruloyltyramine	9.17	314.13739	[M+H] ⁺	C18H19NO4	Methoxyphenols	C02717
385	Feruloyltyramine	9.177	312.12268	[M-H] ⁻	C18H19NO4	Methoxyphenols	C02717

386	Feruloyltyramine	7.475	312.15421	[M-H ₂ O-H]-	C18H19NO ₄	Methoxyphenols	C02717
387	N-Acetylmethionine	6.972	190.05177	[M-H]-	C7H13NO ₃ S	Amino acids and derivatives	C02712
388	Acetyl-leucine	6.449	196.09584	[M+Na] ⁺	C8H15NO ₃	Amino acids and derivatives	C02710
389	Dodecanedioic acid	10.317	229.14232	[M-H]-	C12H22O ₄	Medium-chain fatty acids	C02678
390	Acetone cyanohydrin	4.357	86.06033	[M+H] ⁺	C4H7NO	Organooxygen compounds	C02659
391	Acetone cyanohydrin	5.443	86.06033	[M+Na] ⁺	C4H7NO	Organooxygen compounds	C02659
392	Pimelic acid	7.367	143.07227	[M+H] ⁺	C7H12O ₄	Medium-chain fatty acids	C02656
393	Pimelic acid	6.696	143.07237	[M+CH ₃ OH+H] ⁺	C7H12O ₄	Medium-chain fatty acids	C02656
394	3-Ureidopropionic acid	1.113	177.02342	[M+CH ₃ OH+H] ⁺	C4H8N ₂ O ₃	Ureas	C02642
395	Crustecdysone	12.576	463.30209	[M+H] ⁺	C27H44O ₇	Hydroxy bile acids, alcohols and derivatives	C02633
396	2-Methylpropanoic acid	6.758	111.04392	[M+Na] ⁺	C4H8O ₂	Carboxylic acids	C02632
397	3-Acetyl-4-hydroxy-6-methyl-2H-pyran-2-one	8.052	167.03261	[M-H]-	C8H8O ₄	Organooxygen compounds	C02543
398	Chenodeoxycholic acid	11.874	357.27618	[M-2H ₂ O+H] ⁺	C24H40O ₄	Hydroxy bile acids, alcohols and derivatives	C02528
399	2-Isopropylmalic acid	7.026	175.05927	[M-H]-	C7H12O ₅	Hydroxy fatty acids	C02504
400	2-Isopropylmalic acid	2.359	177.07483	[M+H] ⁺	C7H12O ₅	Fatty Acyls	C02504
401	2-Phenylphenol	2.529	171.0759	[M+H] ⁺	C12H10O	Biphenyls and derivatives	C02499
402	1-Methyladenosine	2.07	280.10184	[M+CH ₃ OH+H] ⁺	C11H15N ₅ O ₄	Purine nucleosides	C02494
403	cis,cis-Muconic acid	6.503	143.03261	[M-H ₂ O-H]-	C6H6O ₄	Medium-chain fatty acids	C02480
404	cis,cis-Muconic acid	1.207	143.03259	[M-H]-	C6H6O ₄	Medium-chain fatty acids	C02480
405	Liothyronine	7.442	651.79987	[M+2H] ₂ ⁺	C15H12I ₃ NO ₄	Amino acids and derivatives	C02465
406	3-Oxododecanoic acid	11.171	213.14761	[M-H]-	C12H22O ₃	Keto acids and derivatives	C02367
407	2',3'-Cyclic AMP	4.415	330.05814	[M+H] ⁺	C10H12N ₅ O ₆ P	2',3'-cyclic purine nucleotides	C02353
408	2',3'-Cyclic AMP	14.85	329.05078	[2M+H] ⁺	C10H11N ₅ O ₆ P-	2',3'-cyclic purine nucleotides	C02353
409	1,2-Benzoquinone	1.92	109.02843	[M+Na] ⁺	C6H4O ₂	Organooxygen compounds	C02351
410	trans-Aconitic acid	2.367	173.00691	[M-H]-	C6H6O ₆	Tricarboxylic acids and derivatives	C02341
411	Prostaglandin F2b	10.479	353.22928	[M-H]-	C20H34O ₅	Fatty Acyls	C02314
412	Galactosamine	1.284	180.08595	[M+H] ⁺	C6H13NO ₅	Monosaccharides	C02262
413	Galactosamine	1.27	202.06763	[M+Na] ⁺	C6H13NO ₅	Monosaccharides	C02262
414	Castanospermine	7.196	190.10649	[M+H-H ₂ O] ⁺	C8H15NO ₄	Indolizidines	C02256
415	Castanospermine	3.993	190.10648	[M+H] ⁺	C8H15NO ₄	Indolizidines	C02256
416	4-Nitrocatechol	8.543	154.0123	[M-H]-	C6H5NO ₄	Nitrophenols	C02235
417	Methylmalonic acid	2.429	136.06111	[M+NH ₄] ⁺	C4H6O ₄	Dicarboxylic acids and derivatives	C02170
418	Leucylglycine	6.937	171.11197	[M+H-H ₂ O] ⁺	C8H16N ₂ O ₃	Peptides	C02155
419	Glycylleucine	6.372	187.10638	[M-H]-	C8H16N ₂ O ₃	Peptides	C02155
420	beta-D-Fucose	13.613	163.05869	[M-H]-	C6H12O ₅	Organooxygen compounds	C02095
421	Sedoheptulose	1.026	209.06487	[M-H]-	C7H14O ₇	Organooxygen compounds	C02076

422	Vitamin K1	12.759	473.34158	[M+Na]+	C31H46O2	Vitamin K compounds	C02059
423	Vitamin K1	10.061	226.17934	[M+H-H2O]+	C31H46O2	Vitamin K compounds	C02059
424	Vitamin K1	12.421	226.17929	[M+CH3OH+H]+	C31H46O2	Vitamin K compounds	C02059
425	Maltotetraose	2.035	649.21515	[M+H-H2O]+	C24H42O21	Oligosaccharides	C02052
426	Maltotetraose	2.029	667.22693	[M+H]+	C24H42O21	Oligosaccharides	C02052
427	Maltotetraose	9.644	667.23132	[2M+H]+	C24H42O21	Oligosaccharides	C02052
428	Indole-3-Lactic Acid	6.696	188.0696	[M+H-H2O]+	C11H11NO3	Indolyl carboxylic acids and derivatives	C02043
429	Indole-3-Lactic Acid	8.558	204.06461	[M-H]-	C11H11NO3	Indolyl carboxylic acids and derivatives	C02043
430	Indole-3-Lactic Acid	8.553	206.08018	[M+H]+	C11H11NO3	Indolyl carboxylic acids and derivatives	C02043
431	3-Aminobenzene-1,2-diol	1.98	126.05476	[M+H]+	C6H7NO2	Phenols	C02012
432	Acetylcholine	6.121	146.11702	[M]+	C7H16NO2+	Cholines	C01996
433	Pregnenolone	10.074	299.23587	[M+H-H2O]+	C21H32O2	Gluc/mineralocorticoids, progestogens and derivatives	C01953
434	Norleucine	3.192	132.10147	[M+H]+	C6H13NO2	Amino acids and derivatives	C01933
435	Glycocholate	11.483	488.29861	[M+CH3OH+H]+	C26H43NO6	Glycinated bile acids and derivatives	C01921
436	Glycocholate	11.707	488.29868	[M+H]+	C26H43NO6	Glycinated bile acids and derivatives	C01921
437	Desthiobiotin	6.309	237.12254	[M+Na]+	C10H18N2O3	Medium-chain fatty acids	C01909
438	Pyroglutamic acid	4.568	188.0542	[M-H]-	C5H7NO3	Amino acids and derivatives	C01879
439	4-Oxo-L-proline	2.41	130.04958	[M+H-H2O]+	C5H7NO3	Carboxylic acids and derivatives	C01877
440	4-Oxo-L-proline	2.719	130.04955	[M+H]+	C5H7NO3	Carboxylic acids and derivatives	C01877
441	Maltotriose	2.349	487.16443	[M+H-H2O]+	C18H32O16	Oligosaccharides	C01835
442	Norvaline	6.905	116.06954	[M-H]-	C5H11NO2	Amino acids and derivatives	C01826
443	2-Deoxyribose	3.468	135.06459	[M+H]+	C5H10O4	Beta-hydroxy aldehydes	C01801
444	Pyocyanine	11.005	211.08527	[M+H]+	C13H10N2O	Quinoxalines	C01748
445	Neomycin	12.865	637.30188	[M+Na]+	C23H46N6O13	Aminosaccharides	C01737
446	Neomycin	12.869	659.28143	[M-H+2Na]+	C23H46N6O13	Aminosaccharides	C01737
447	Mesaconic acid	1.754	129.01714	[M-H]-	C5H6O4	Branched fatty acids	C01732
448	Lumichrome	8.777	243.08641	[M+H]+	C12H10N4O2	Flavins	C01727
449	Threonic acid	0.967	135.02762	[M-H]-	C4H8O5	Sugar acids and derivatives	C01620
450	Stachyose	2.805	665.21045	[M-H]-	C24H42O21	Oligosaccharides	C01613
451	Stachyose	1.504	689.20593	[M+Na]+	C24H42O21	Oligosaccharides	C01613
452	Stachyose	2.037	684.25183	[M+NH4]+	C24H42O21	Oligosaccharides	C01613
453	Phlorhizin	8.641	435.1279	[M-H]-	C21H24O10	Flavonoid O-glycosides	C01604
454	Melatonin	7.931	231.1116	[M-H]-	C13H16N2O2	3-alkylindoles	C01598
455	Linoleic acid	13.06	279.23114	[M-H]-	C18H32O2	Lineolic acids and derivatives	C01595
456	Leupeptin	12.06	427.30106	[M+H]+	C20H38N6O4	Peptides	C01591
457	Leupeptin	11.735	427.30322	[M+H-H2O]+	C20H38N6O4	Peptides	C01591

458	Etoposide	1.792	606.21912	[M+H] ⁺	C29H32O13	Tetrahydroisoquinolines	C01576
459	D-Leucine	6.514	130.08487	[M-H2O-H] ⁻	C6H13NO2	Carboxylic acids and derivatives	C01570
460	Warfarin	13.568	307.10181	[M-H] ⁻	C19H16O4	4-hydroxycoumarins	C01541
461	Luteolin	9.478	285.03796	[M-H] ⁻	C15H10O6	Flavones	C01514
462	Iditol	1.218	181.06966	[M-H] ⁻	C6H14O6	Sugar alcohols	C01507
463	Guaiacol	6.307	107.04913	[M+H-H2O] ⁺	C7H8O2	Methoxyphenols	C01502
464	3-Hydroxyflavone	9.863	237.10887	[M-H] ⁻	C15H10O3	Flavonols	C01495
465	Ferulic acid	8.456	177.05342	[M-H2O+H] ⁺	C10H10O4	Hydroxycinnamic acids	C01494
466	p-Cresol	6.309	91.05438	[M+CH3OH+H] ⁺	C7H8O	Para cresols	C01468
467	p-Cresol	9.951	91.05439	[M+H] ⁺	C7H8O	Para cresols	C01468
468	Vitexin	8.018	431.09464	[M-H] ⁻	C21H20O10	Flavonoid C-glycosides	C01460
469	Tropic acid	8.343	165.05312	[M-H] ⁻	C9H10O3	Beta hydroxy acids and derivatives	C01456
470	Salicin	8.008	331.1011	[M-H] ⁻	C13H18O7	Glycosyl compounds	C01451
471	Loganin	6.461	389.14301	[M-H] ⁻	C17H26O10	Iridoid O-glycosides	C01433
472	Xylose 6-	1.194	173.04153	[M+H] ⁺	C5H10O5	Monosaccharides	C01394
473	Hydroxypseudooxynicotine 6-	6.248	195.11194	[M+H] ⁺	C10H14N2O2	Ketones	C01297
474	Hydroxypseudooxynicotine	6.748	195.11185	[M+H-H2O] ⁺	C10H14N2O2	Ketones	C01297
475	1-Aminocyclopropane-1-carboxylic acid	4.456	100.03817	[M-H] ⁻	C4H7NO2	Amino acids and derivatives	C01234
476	1-Aminocyclopropane-1-carboxylic acid	4.527	102.0549	[M+H] ⁺	C4H7NO2	Amino acids and derivatives	C01234
477	sn-Glycerol-3-phosphoethanolamine	0.883	214.04678	[M-H] ⁻	C5H14NO6P	Glycerophospholipids	C01233
478	D-myo-Inositol 1,4-bisphosphate	0.769	338.98691	[M-H] ⁻	C6H14O12P2	Organooxygen compounds	C01220
479	Caffeic acid	0.183	181.04855	[M+H] ⁺	C9H8O4	Hydroxycinnamic acids	C01197
480	Deoxycarnitine	1.495	146.11703	[M+H] ⁺	C7H15NO2	Straight chain fatty acids	C01181
481	Pseudouridine 5'-phosphate	1.097	323.02582	[M-H] ⁻	C9H13N2O9P	Organooxygen compounds	C01168
482	O-Succinylhomoserine	1.302	220.0806	[M+Na] ⁺	C8H13NO6	Amino acids and derivatives	C01118
483	O-Succinylhomoserine	4.017	218.06468	[M-H] ⁻	C8H13NO6	Amino acids and derivatives	C01118
484	8-Amino-7-oxononanoic acid	7.904	186.11151	[M-H] ⁻	C9H17NO3	Fatty Acyls	C01092
485	Trehalose	14.131	341.10718	[M-H] ⁻	C12H22O11	Glycosyl compounds	C01083
486	Trehalose	1.722	325.11121	[M+H-H2O] ⁺	C12H22O11	Glycosyl compounds	C01083
487	Trehalose	2.197	365.10431	[M+Na] ⁺	C12H22O11	Glycosyl compounds	C01083
488	N-Methylglutamic acid	13.579	144.06511	[M+H] ⁺	C6H11NO4	Amino acids and derivatives	C01046
489	gamma-Guanidinobutyric acid	2.221	146.09186	[M+H] ⁺	C5H11N3O2	Amino acids and derivatives	C01035
490	Trigonelline	1.479	138.05424	[M+H] ⁺	C7H7NO2	Alkaloids and derivatives	C01004
491	Alanylalanine	1.004	159.07495	[M-H] ⁻	C6H12N2O3	Peptides	C00993
492	Indole-3-ethanol	8.546	162.09038	[M+H] ⁺	C10H11NO	3-alkylindoles	C00955
493	Porphobilinogen	2.805	210.07515	[M+2H-NH4] ⁺	C10H14N2O4	Aralkylamines	C00931

494	3-Methyladenine	4.744	150.07658	[M+H] ⁺	C6H7N5	6-aminopurines	C00913
495	2-Acetolactate	6.059	131.03284	[M-H] ⁻	C5H8O4	Keto acids and derivatives	C00900
496	Arabinonic acid	0.912	165.03799	[M-H] ⁻	C5H10O6	Organooxygen compounds	C00878
497	4-Nitrophenol	9.406	138.01729	[M-H] ⁻	C6H5NO3	Nitrophenols	C00870
498	Pantothenic acid	6.4	218.10139	[M-H] ⁻	C9H17NO5	Amino acids and derivatives	C00864
499	Pantothenic acid	1.398	220.11711	[M+H] ⁺	C9H17NO5	Amino acids and derivatives	C00864
500	Pantothenic acid	1.511	242.10143	[M+Na] ⁺	C9H17NO5	Secondary alcohols	C00864
501	Formononetin	10.539	267.06384	[M-H] ⁻	C16H12O4	4'-O-methylated isoflavonoids	C00858
502	4-Pyridoxate	2.589	184.05968	[M+H] ⁺	C8H9NO4	Pyridinecarboxylic acids	C00847
503	3-Oxoadipic acid	6.035	161.04395	[M+H] ⁺	C6H8O5	Medium-chain keto acids and derivatives	C00846
504	Mandelonitrile glucoside	7.922	294.09607	[M-H] ⁻	C14H17NO6	Glycosyl compounds	C00844
505	Dihydrosphingosine	10.941	324.28577	[M+Na] ⁺	C18H39NO2	Alkanolamines	C00836
506	Vitamin K2	12.322	445.311	[M+Na] ⁺	C31H40O2	Vitamin K compounds	C00828
507	p-Coumaric acid	3.577	165.05406	[M+H] ⁺	C9H8O3	Cinnamic acids and derivatives	C00811
508	D-Sorbitol	1.303	205.06738	[M+Na] ⁺	C6H14O6	Sugar alcohols	C00794
509	D-Sorbitol	0.604	181.06963	[M-H] ⁻	C6H14O6	Sugar alcohols	C00794
510	Westcort	12.709	491.26407	[M-H] ⁻	C26H38O6	21-hydroxysteroids	C00762
511	Berberine	9.314	336.11877	[M] ⁺	C20H18NO4	Protoberberine alkaloids and derivatives	C00757
512	Pyridine	13.556	80.04987	[M+H] ⁺	C5H5N	Pyridines and derivatives	C00747
513	Hydrocortisone butyrate	12.5	477.25012	[M-H] ⁻	C25H36O6	21-hydroxysteroids	C00735
514	Betaine	1.406	118.086	[M+H] ⁺	C5H11NO2	Amino acids and derivatives	C00719
515	Oleic acid	12.747	281.2468	[M-H] ⁻	C18H34O2	Long-chain fatty acids	C00712
516	Trehalose 6-phosphate	0.953	421.07504	[M-H] ⁻	C12H23O14P	Disaccharides	C00689
517	LPA(18:1)	8.378	459.24799	[M+NH4] ²⁺	C21H41O7P	Monoacylglycerophosphates	C00681
518	Glycerophosphocholine	1.307	280.09048	[M-H+Na] ⁺	C8H21NO6P ⁺	Glycerophosphocholines	C00670
519	Glycerophosphocholine	1.342	258.1087	[M+H] ⁺	C8H20NO6P	Glycerophosphocholines	C00670
520	Diaminopimelic acid	2.05	191.10246	[M-H] ⁻	C7H14N2O4	Amino acids and derivatives	C00666
521	Pyridoxamine phosphate	4.111	249.05934	[M+H-H2O] ⁺	C8H13N2O5P	Pyridoxamine 5'-phosphates	C00647
522	Pyridoxamine phosphate	3.552	249.0593	[M+H] ⁺	C8H13N2O5P	Pyridoxamine 5'-phosphates	C00647
523	Indole-3-acetaldehyde	8.557	158.05899	[M-H] ⁻	C10H9NO	3-alkylindoles	C00637
524	4-Hydroxybenzaldehyde	3.361	123.04373	[M+H] ⁺	C7H6O2	Aldehydes	C00633
525	N-Acetylglutamic acid	2.82	188.05418	[M-H] ⁻	C7H11NO5	Amino acids and derivatives	C00624
526	Phosphocholine	1.557	91.02637	[M-H] ⁻	C5H15NO4P	Cholines	C00588
527	Prostaglandin E2	9.953	375.20944	[M+Na] ⁺	C20H32O5	Prostaglandins and related compounds	C00584
528	p-Aminobenzoic acid	7.337	138.05457	[M+H] ⁺	C7H7NO2	Aminobenzoic acids and derivatives	C00568
529	Cyclopentanone	6.81	102.09155	[M+NH4] ⁺	C5H8O	Ketones	C00557
530	Arabitol	0.904	151.05904	[M-H] ⁻	C5H12O5	Sugar alcohols	C00532
531	Rhamnose	1.871	223.08047	[M-H] ⁻	C6H12O5	Monosaccharides	C00507
532	Gentamicin	12.226	478.32034	[2M+H] ⁺	C21H43N5O7	Aminosaccharides	C00505

533	Allantoic acid	1.316	177.06079	[M+H] ⁺	C4H8N4O4	Amino acids and derivatives	C00499
534	Shikimic acid	12.158	192.08311	[M+H] ⁺	C7H10O5	Cyclic alcohols and derivatives	C00493
535	Raffinose	1.542	503.15845	[M-H] ⁻	C18H32O16	Oligosaccharides	C00492
536	Glutaric acid	1.656	115.03896	[2M+H] ⁺	C5H8O4	Dicarboxylic acids and derivatives	C00489
537	Glutaric acid	6.047	115.03894	[M+H] ⁺	C5H8O4	Dicarboxylic acids and derivatives	C00489
538	Glutaric acid	13.644	115.03871	[M+Na] ⁺	C5H8O4	Dicarboxylic acids and derivatives	C00489
539	Sinapic acid	7.022	223.05917	[M-H] ⁻	C11H12O5	Hydroxycinnamic acids	C00482
540	Sinapic acid	7.012	207.06432	[M+H-H2O] ⁺	C11H12O5	Hydroxycinnamic acids	C00482
541	Cytidine	2.249	244.09119	[M+H] ⁺	C9H13N3O5	Pyrimidine nucleosides	C00475
542	Ribitol	1.584	153.0751	[M+H] ⁺	C5H12O5	Sugar alcohols	C00474
543	Ribitol	3.363	175.05692	[M+H-H2O] ⁺	C5H12O5	Sugar alcohols	C00474
544	L-Saccharopine	3.556	259.12817	[M+H-H2O] ⁺	C11H20N2O6	Amino acids and derivatives	C00449
545	Galactose 1-phosphate	0.806	259.02112	[M-H] ⁻	C6H13O9P	Monosaccharides	C00446
546	5-Aminolevulinate	1.413	114.05473	[M-H2O+H] ⁺	C5H9NO3	Amino acids and derivatives	C00430
547	Ginsenoside Rf	11.935	845.48767	[M-H] ⁻	C42H72O14	Triterpenoids	C00422
548	cis-Aconitate	6.589	173.00702	[M-H] ⁻	C6H6O6	Tricarboxylic acids and derivatives	C00417
549	Pipecolic acid	1.983	130.08578	[M+H] ⁺	C6H11NO2	Amino acids and derivatives	C00408
550	Mannitol	1.629	183.08554	[M+H] ⁺	C6H14O6	Sugar alcohols	C00392
551	Quercetin	0.813	336.88535	[M-H] ⁻	C15H10O7	Flavonols	C00389
552	Guanosine	6.208	284.09772	[M+H] ⁺	C10H13N5O5	Purine nucleosides	C00387
553	Carnosine	1.756	249.09569	[2M+H] ⁺	C9H14N4O3	Hybrid peptides	C00386
554	Carnosine	6.063	249.09567	[M+NH4] ⁺	C9H14N4O3	Hybrid peptides	C00386
555	Carnosine	4.782	249.0957	[M+H] ⁺	C9H14N4O3	Hybrid peptides	C00386
556	Carnosine	1.642	249.09563	[M+H-H2O] ⁺	C9H14N4O3	Hybrid peptides	C00386
557	Xanthine	3.869	153.04002	[M+H] ⁺	C5H4N4O2	Xanthines	C00385
558	Cytosine	1.435	112.05039	[M+H] ⁺	C4H5N3O	Pyrimidones	C00380
559	Xylitol	1.165	151.05901	[M-H] ⁻	C5H12O5	Sugar alcohols	C00379
560	dTMP	4.064	321.0473	[M-H] ⁻	C10H15N2O8P	Pyrimidine nucleotide sugars	C00364
561	dGMP	2.511	348.06882	[M+H] ⁺	C10H14N5O7P	Purine deoxyribonucleoside monophosphates	C00362
562	DOPA	2.034	198.07497	[M+H] ⁺	C9H11NO4	Amino acids and derivatives	C00355
563	DOPA	7.84	196.05943	[M-H2O-H] ⁻	C9H11NO4	Amino acids and derivatives	C00355
564	2-Methyl-3-oxopropanoic acid	1.178	101.02216	[M-H] ⁻	C4H6O3	Organooxygen compounds	C00349
565	6-Phosphogluconate	0.958	277.03159	[M-H] ⁻	C6H13O10P	Monosaccharides	C00345
566	GABA	0.921	102.05368	[M-H] ⁻	C4H9NO2	Amino acids and derivatives	C00334
567	GABA	1.402	86.06018	[M+H-H2O] ⁺	C4H9NO2	Amino acids and derivatives	C00334
568	Deoxyguanosine	0.9	266.08591	[M-H2O-H] ⁻	C10H15N5O5	Purine 2'-deoxyribonucleoside	C00330
569	Citrulline	9.448	193.13026	[M+Na] ⁺	C6H13N3O3	Amino acids and derivatives	C00327
570	Sphingosine	11.117	300.28802	[M+H] ⁺	C18H37NO2	Alkanolamines	C00319
571	Carnitine	1.404	162.11145	[M+H] ⁺	C7H15NO3	Carnitines	C00318
572	Pyridoxine	3.13	170.08023	[M+H] ⁺	C8H11NO3	Pyridoxines	C00314

573	Quinic acid	2.184	193.06982	[M-H]-	C7H12O6	Cyclic alcohols and derivatives	C00296
574	Quinaldine	8.558	142.06413	[M-H2O-H]-	C10H9N	Quinolines and derivatives	C00296
575	D-Erythrose 4-phosphate	0.949	201.015	[M-H]-	C4H9O7P	Monosaccharide phosphates	C00279
576	N-Acetylneuraminic acid	1.427	310.11185	[M+CH3OH+H]+	C11H19NO9	Sugar acids and derivatives	C00270
577	N-Acetylneuraminic acid	0.984	308.09705	[M-H]-	C11H19NO9	Sugar acids and derivatives	C00270
578	Homoserine	0.897	118.04855	[M-H]-	C4H9NO3	Amino acids and derivatives	C00263
579	Hypoxanthine	3.151	137.04521	[M+H]+	C5H4N4O	Purinones	C00262
580	Hypoxanthine	6.186	119.03489	[M+H-H2O]+	C5H4N4O	Purinones	C00262
581	Arabinose	9.318	151.06038	[M-H]-	C5H10O5	Monosaccharides	C00259
582	Arabinose	13.67	151.05899	[M-H2O-H]-	C5H10O5	Monosaccharides	C00259
583	Glycerate	1.01	105.01711	[M-H]-	C3H6O4	Organooxygen compounds	C00258
584	Glycerate	6.002	105.0171	[M-H2O-H]-	C3H6O4	Organooxygen compounds	C00258
585	Gluconic acid	0.912	195.04857	[M-H]-	C6H12O7	Medium-chain hydroxy acids and derivatives	C00257
586	Riboflavin	7.281	377.14316	[M+H]+	C17H20N4O6	Flavins	C00255
587	Nicotinic acid	2.437	124.03903	[M+H]+	C6H5NO2	Pyridinecarboxylic acids	C00253
588	Pyridoxal	2.585	168.06506	[M+H]+	C8H9NO3	Pyridoxals and derivatives	C00250
589	Pyridoxal	8.185	168.06404	[M-H]-	C8H9NO3	Pyridoxals and derivatives	C00250
590	Palmitic acid	0.445	257.24637	[M+H]+	C16H32O2	Long-chain fatty acids	C00249
591	Guanine	6.204	152.05635	[M+H]+	C5H5N5O	Purines and purine derivatives	C00242
592	Guanine	13.774	152.06015	[M-H]-	C5H5N5O	Purines and purine derivatives	C00242
593	Amide	3.866	160.10759	[M+H]+	C6H13N3O2	Amino acids and derivatives	C00241
594	Malonic semialdehyde	2.05	87.00637	[M-H]-	C3H4O3	Organooxygen compounds	C00222
595	D-Arabinose	1.059	149.04337	[M-H]-	C5H10O5	Organooxygen compounds	C00216
596	Thymidine	6.321	287.08685	[M-H2O-H]-	C10H14N2O5	Pyrimidine 2'-deoxyribonucleosides	C00214
597	Adenosine	6.185	268.10266	[M+H]+	C10H13N5O4	Purine nucleosides	C00212
598	2,3-Dihydroxybenzoate	7.725	153.01689	[M-H]-	C7H6O4	Hydroxybenzoic acid derivatives	C00196
599	Cellobiose	2.029	325.11133	[M+H-H2O]+	C12H22O11	Glycosyl compounds	C00185
600	Valine	1.815	118.08601	[M+H]+	C5H11NO2	Amino acids and derivatives	C00183
601	Agmatine	1.274	131.12865	[M+H]+	C5H14N4	Guanidines	C00179
602	Methylthioadenosine	6.61	298.09549	[M+H]+	C11H15N5O3S	5'-deoxy-5'-thionucleosides	C00170
603	DG(16:0/18:1)	12.484	577.51758	[M+H-H2O]+	C37H70O5	Diacylglycerols	C00165
604	Acetoacetic acid	0.99	103.03899	[M+H]+	C4H6O3	Short-chain keto acids and derivatives	C00164
605	Mannose	0.899	215.03082	[M-H2O-H]-	C6H12O6	Monosaccharides	C00159

606	Citric acid	2.054	191.01715	[M-H]-	C6H8O7	Tricarboxylic acids and derivatives	C00158
607	Citric acid	2.114	230.98907	[2M+H]+	C6H8O7	Tricarboxylic acids and derivatives	C00158
608	Asparagine	0.888	131.0437	[M-H]-	C4H8N2O3	Amino acids and derivatives	C00152
609	Malic acid	1.3	133.01178	[M-H]-	C4H6O5	Beta hydroxy acids and derivatives	C00149
610	Proline	1.275	116.07033	[M+H]+	C5H9NO2	Amino acids and derivatives	C00148
611	Adenine	6.186	136.06152	[M+H]+	C5H5N5	6-aminopurines	C00147
612	Phenol	6.306	95.04931	[M+H]+	C6H6O	Aralkylamines	C00146
613	Phenol	9.263	93.03246	[M-H]-	C6H6O	Aralkylamines	C00146
614	alpha-Ketoisovalerate	1.61	117.05445	[M+H-H2O]+	C5H8O3	Short-chain keto acids and derivatives	C00141
615	alpha-Ketoisovalerate	0.996	117.05443	[M+Na]+	C5H8O3	Short-chain keto acids and derivatives	C00141
616	alpha-Ketoisovalerate	6.696	117.05708	[2M+H]+	C5H8O3	Short-chain keto acids and derivatives	C00141
617	GlcNAc	0.95	280.10178	[M-H]-	C8H15NO6	Aminosaccharides	C00140
618	Histidine	0.875	154.05981	[M-H]-	C6H9N3O2	Amino acids and derivatives	C00135
619	IMP	2.232	347.03723	[M-H]-	C10H13N4O8P	Purine ribonucleoside monophosphates	C00130
620	Glutathione (oxidized)	4.202	611.1394	[M-H]-	C20H32N6O12S ₂	Peptides	C00127
621	Fumaric acid	1.114	115.0013	[M-H]-	C4H4O4	Dicarboxylic acids and derivatives	C00122
622	Fumaric acid	2.507	139.00217	[M+Na]+	C4H4O4	Dicarboxylic acids and derivatives	C00122
623	Biotin	7.559	227.08377	[M+H-H2O]+	C10H16N2O3S	Biotin and derivatives	C00120
624	Choline	1.374	104.10691	[M]+	C5H14NO	Cholines	C00114
625	Uracil	3.864	113.03431	[M+H]+	C4H4N2O2	Pyrimidones	C00106
626	Sucrose	4.819	341.10703	[M-H]-	C12H22O11	Glycosyl compounds	C00089
627	Sucrose	1.49	365.10431	[M+Na]+	C12H22O11	Glycosyl compounds	C00089
628	Tyrosine	5.248	182.08051	[M+H]+	C9H11NO3	Amino acids and derivatives	C00082
629	Phenylalanine	6.293	164.0695	[M-H]-	C9H11NO2	Amino acids and derivatives	C00079
630	Phenylalanine	10.298	166.08513	[M-H2O-H]-	C9H11NO2	Amino acids and derivatives	C00079
631	Tryptophan	6.696	205.09607	[M+H]+	C11H12N2O2	Amino acids and derivatives	C00078
632	Ornithine	0.875	131.08041	[M-H]-	C5H12N2O2	Amino acids and derivatives	C00077
633	Methionine	1.933	150.05785	[M+H]+	C5H11NO2S	Amino acids and derivatives	C00073
634	Serine	0.892	104.03305	[M-H]-	C3H7NO3	Amino acids and derivatives	C00065
635	Glutamine	0.889	145.05939	[M-H]-	C5H10N2O3	Amino acids and derivatives	C00064
636	Arginine	1.296	175.11786	[M+H]+	C6H14N4O2	Amino acids and derivatives	C00062
637	Arginine	0.875	173.10194	[M-H]-	C6H14N4O2	Amino acids and derivatives	C00062
638	Arginine	1.281	197.10031	[M+Na]+	C6H14N4O2	Amino acids and derivatives	C00062
639	FMN	6.837	455.0946	[M-H]-	C17H21N4O9P	Flavin nucleotides	C00061

640	Lysine	1.155	147.1122	[M+NH4] ⁺	C6H14N2O2	D-alpha-amino acids	C00047
641	Succinic acid	2.624	117.017	[M-H] ⁻	C4H6O4	Dicarboxylic acids and derivatives	C00042
642	Alanine	0.909	88.03831	[M-H] ⁻	C3H7NO2	Amino acids and derivatives	C00041
643	Glutamic acid	1.318	148.05954	[M+H] ⁺	C5H9NO4	Amino acids and derivatives	C00025
644	Acetyl-CoA	6.409	808.1156	[M-H] ⁻	C23H38N7O17P 3S	Acyl CoAs	C00024
645	Pyruvate	6.715	111.0076	[M+Na] ⁺	C3H4O3	Alpha-keto acids and derivatives	C00022
646	S-Adenosylmethionine	2.184	399.14743	[M+H] ⁺	C15H23N6O5S	5'-deoxy-5'-thionucleosides	C00019
647	FAD	6.499	784.14563	[M-H] ⁻	C27H33N9O15P 2	Flavin nucleotides	C00016
648	Phosphoric acid	0.957	96.9674	[M-H] ⁻	H3O4P	Non-metal phosphates	C00009
649	Phosphoric acid	11.333	98.98428	[M+H] ⁺	H3O4P	Non-metal phosphates	C00009
650	NADP ⁺	4.105	540.0498	[M-H] ⁻	C21H29N7O17P 3+	(5'->5')-dinucleotides	C00006
651	NAD ⁺	4.45	664.11237	[M] ⁺	C21H28N7O14P 2	(5'->5')-dinucleotides	C00003
652	NAD ⁺	4.47	332.56009	[M+2H] ²⁺	C21H28N7O14P 2+	(5'->5')-dinucleotides	C00003
653	NAD	4.116	662.09692	[M-H] ⁻	C21H27N7O14P 2	(5'->5')-dinucleotides	C00003
654	Ziyuglycoside I	8.301	789.43933	[M+H] ⁺	C41H66O13	Triterpene glycosides	---
655	Zeaxanthin-palmitate	12.836	807.0036	[M+2H] ²⁺	C56H86O3	Carotenoids	---
656	Zaprinast	3.748	272.11179	[M+H] ⁺	C13H13N5O2	Triazolopyrimidines	---
657	YohimbicÃÃÃ AcidÃÃÃ Monohydrate xi-7-	12.143	339.21332	[M-H] ⁻	C20H26N2O4	Corynanthean-type alkaloids	---
658	Hydroxyhexadecanedioic acid	9.285	301.19977	[M-H] ⁻	C16H30O5	Fatty Acyls	---
659	Xanthopterin	13.526	218.01006	[2M+H] ⁺	C6H5N5O2	Pterins and derivatives	---
660	Vinorelbine	8.177	801.38617	[2M+H] ⁺	C45H54N4O8	Vinca alkaloids	---
661	Vindesine	8.572	754.41962	[M+2H] ²⁺	C43H55N5O7	Vinca alkaloids	---
662	Vincadifformine(1+)	8.147	340.20724	[M+H] ²⁺	C21H27N2O2+	Aspidospermatan-type alkaloids	---
663	Viequeamide_A	8.641	826.49457	[2M+H] ²⁺	C42H69N5O10	Cyclic depsipeptides	---
664	ViequeamideB	12.525	830.47437	[M+H] ⁺	C44H65N5O9	Cyclic depsipeptides	---
665	Verbaspinoside	9.007	637.21808	[M+Na] ⁺	C30H38O15	Cinnamic acid esters	---
666	Verbascoside A	9.22	691.21844	[M+Na] ⁺	C31H40O16	Cinnamic acid esters	---
667	Veratrine	7.776	632.38251	[M+H] ⁺	C32H49NO9	Cerveratrum-type alkaloids	---
668	Vardenafil	9.233	489.22818	[M+H] ⁺	C23H32N6O4S	Benzenesulfonamide s	---
669	Vanilloylglycine	7.442	224.05461	[M-H] ⁻	C10H11NO5	Benzene and substituted derivatives	---
670	Val-Leu	8.567	213.15816	[M+H-H2O] ⁺	C11H22N2O3	Peptides	---
671	Valganciclovir	9.858	353.15842	[M-H] ⁻	C14H22N6O5	Amino acids and derivatives	---
672	Uridine (Not validated)	3.444	243.06041	[M-H] ⁻	C9H12N2O6	Pyrimidine nucleosides	---
673	Undecanedioic acid	9.862	215.12694	[M-H] ⁻	C11H20O4	Medium-chain fatty acids	---
674	Tyr-Pro-Leu-Gly-NH2	8.377	448.25739	[M+H] ²⁺	C22H33N5O5	Peptides	---
675	Tyrosylproline	6.416	279.13287	[M+NH4] ⁺	C14H18N2O4	Carboxylic acids and derivatives	---

676	Tyrosine (Not validated)	6.591	180.06451	[M-H]-	C9H11NO3	Tyrosine and derivatives	---
677	Tunicamycin A	7.427	853.40503	[M+2H]2+	C38H62N4O16	Aminosaccharides	---
678	Tubuloside A	5.621	851.25763	[M+Na]+	C37H48O21	Oligosaccharides	---
679	Tubuloside A	2.24	829.27856	[M+H]+	C37H48O21	Oligosaccharides	---
680	Tubuloside A	2.372	829.27893	[M+CH3OH+H]+	C37H48O21	Oligosaccharides	---
681	Tsangane L 3-glucoside	11.116	395.20282	[M-H]-	C19H34O7	Terpene glycosides	---
682	Tryptoquivaline L	5.205	431.13684	[M-H]-	C23H20N4O5	Amino acids and derivatives	---
683	Tryptoquivaline L	7.743	431.13687	[M-H2O-H]-	C23H20N4O5	Amino acids and derivatives	---
684	Troxipide	6.666	295.16394	[M+H]+	C15H22N2O4	Anisoles	---
685	Tryptophenolide	12.291	311.16635	[M-H]-	C20H24O3	Oxosteroids	---
686	Tripterine	9.555	449.27179	[M-H]-	C29H38O4	Triterpenoids	---
687	Tripterine	11.4	449.27383	[2M-H]-	C29H38O4	Triterpenoids	---
688	Triphenylmethylphosphonium	1.507	278.12177	[M+Na]+	C19H18P	Phenylphosphines and derivatives	---
689	Triphenylmethylphosphonium	1.814	278.1217	[M+H-H2O]+	C19H18P	Phenylphosphines and derivatives	---
690	Trinexapac	10.917	225.07442	[M+H]+	C11H12O5	Vinylogous acids	---
691	Trimetozine	3.925	282.13235	[M+H]+	C14H19NO5	Morpholine	---
692	Trimethadione	4.454	142.04872	[M-H]-	C6H9NO3	carboxylic acids and derivatives	---
693	Trifluoroacetic acid	0.839	112.98331	[M-H]-	C2HF3O2	Azolidines	---
694	Triethyl citrate	10.216	299.10831	[M+Na]+	C12H20O7	Alpha-halocarboxylic acids	---
695	Tricaproin	11.1	409.25412	[M+H]+	C21H38O6	Tricarboxylic acids and derivatives	---
696	Triamcinolone	8.358	393.17487	[M-H]-	C21H27FO6	Triacylglycerols	---
697	Triamcinolone	8.2	393.1749	[2M-H]-	C21H27FO6	21-hydroxysteroids	---
698	Triacetyl resveratrol trans-4-[4-(4-Amino-7,8-dimethyl-7H-pyrimido[4,5-b][1,4]oxazin-6-yl)phenyl]cyclohexanecarboxylic acid	6.25	353.10648	[M-H]-	C20H18O6	21-hydroxysteroids	---
699	pyrimido[4,5-b][1,4]oxazin-6-yl)phenyl]cyclohexanecarboxylic acid	8.939	393.19302	[M-H]-	C22H26N4O3	Stilbenes	---
700	trans-2-Hexyl-1-cyclopropaneacetic acid	10.796	183.13695	[M-H]-	C11H20O2	Diazines	---
701	Thuggacin A	8.789	632.36023	[M+2H]2+	C35H53NO7S	Carboxylic acids and derivatives	---
702	Thr-Pro	6.275	217.11757	[M+H]+	C9H16N2O4	Thiazoles	---
703	Thermoactinoamide_D	12.871	765.45569	[M+2H]2+	C41H60N6O8	Peptides	---
704	Theophylline, n-propyl derivative	6.583	223.11514	[M+H]+	C10H14N4O2	Peptides	---
705	Thalifaricine	12.094	669.32031	[M+Na]+	C39H44N2O8	Xanthines	---
706	Tetrahydropyridine	1.564	84.08102	[M+NH4]+	C5H9N	Aporphines	---
707	Tetrahydropyridine	1.154	84.08112	[M+H]+	C5H9N	Pyridines and derivatives	---
708	Tetrahydrocurcumin	11.202	395.1449	[M+Na]+	C21H24O6	Pyridines and derivatives	---
709	Tetradecyldiethanolamine	10.946	302.3031	[M+H]+	C18H39NO2	Curcuminoids	---
710	Terebic acid	2.378	159.06459	[M+H]+	C7H10O4	Alkanolamines	---
711	Terebic acid	2.04	159.06454	[M+NH4]+	C7H10O4	Gamma butyrolactones	---
712	Terasin	2.929	424.17459	[M+H-H2O]+	C19H26ClN5O4	Gamma butyrolactones	---
713	TC1	12.595	523.24335	[M+H]+	C27H34ClF3N4O	N-arylpiperazines	---
714	Syrosingopine	1.403	689.26654	[2M+H]+	C35H42N2O11	Triquinane sesquiterpenoids	---
715	Syrosingopine	1.603	689.26587	[M+H]+	C35H42N2O11	Yohimbine alkaloids	---

716	Swinholide F	12.341	695.46881	[M+H-H ₂ O] ⁺	C ₇₈ H ₁₃₂ O ₂₀	Macrolides and analogues	---
717	Swinholide F	11.659	695.46832	[M+H] ⁺	C ₇₈ H ₁₃₂ O ₂₀	Macrolides and analogues	---
718	Sunitinib malate	6.696	399.22131	[M+H] ⁺	C ₂₆ H ₃₃ FN ₄ O ₇	Indolines	---
719	Sulthiame	6.677	291.04599	[M+H] ⁺	C ₁₀ H ₁₄ N ₂ O ₄ S ₂	Sulfanilides	---
720	Sulisobenzone	4.211	307.0289	[M-H] ⁻	C ₁₄ H ₁₂ O ₆ S	Benzophenones	---
721	Sulfooxyjasmonate	7.293	305.06784	[M-H] ⁻	C ₁₂ H ₁₈ O ₇ S	Sulfate containing metabolites	---
722	Succinoadenosine	6.321	382.09744	[M-H] ⁻	C ₁₄ H ₁₇ N ₅ O ₈	Purine nucleosides	---
723	Subsessiline	8.147	717.36279	[M+H] ⁺	C ₄₃ H ₄₈ N ₄ O ₆	Aspidospermatan-type alkaloids	---
724	STL564777	12.718	862.51447	[M+2H] ²⁺	C ₄₃ H ₇₅ N ₁₀	Aminoglycosides	---
725	Sternbin	9.693	303.08212	[M+H] ⁺	C ₁₆ H ₁₄ O ₆	7-O-methylated flavonoids	---
726	Stearoylethanolamide	11.711	328.31903	[M+H] ⁺	C ₂₀ H ₄₁ NO ₂	Alkanolamines	---
727	stanozolol-16-OH	9.44	367.23264	[M+NH ₄] ⁺	C ₂₁ H ₃₂ N ₂ O ₂	Estrane steroids	---
728	St088588	6.55	267.09692	[M-H ₂ O-H] ⁻	C ₁₁ H ₁₄ N ₂ O ₃	Amino acids and derivatives	---
729	St031318	1.88	270.09558	[M+H] ⁺	C ₁₆ H ₁₅ NOS	Retrochalcones	---
730	Spongiacidin C	6.139	247.0798	[M+H] ⁺	C ₁₁ H ₁₀ N ₄ O ₃	Hydantoins	---
731	Splendoline	8.097	371.19568	[M+NH ₄] ²⁺	C ₂₁ H ₂₆ N ₂ O ₄	Strychnos alkaloids	---
732	Spirobrassinin	1.268	251.02992	[M+H] ⁺	C ₁₁ H ₁₀ N ₂ OS ₂	Indolines	---
733	Spiro[furan-3(2H),1'(4'H)-naphthalene]-4'a,5'(5'H)-dicarboxylic acid, 6'-(acetyloxy)-5-(3-furanyl)-4,5,6',7',8',8'a-hexahydro-5'-hydroxy-2'-methyl-2-oxo-, dimethyl ester	1.011	521.16974	[M-H] ⁻	C ₂₄ H ₂₈ O ₁₀	Diterpene lactones	---
734	Spiculisporic acid	11.445	327.1788	[M-H] ⁻	C ₁₇ H ₂₈ O ₆	Tricarboxylic acids and derivatives	---
735	Spiculisporic acid	9.133	329.19385	[M+H] ⁺	C ₁₇ H ₂₈ O ₆	Tricarboxylic acids and derivatives	---
736	Soyasapogenol B base + O-HexA-HexA-Hex+Me+Acetyl	9.922	1027.50513	[M-H] ⁻	C ₅₁ H ₈₀ O ₂₁	Triterpene saponins-soyasapogenol B	---
737	Soyasapogenol B 3-O-b-D-glucuronide	11.128	633.39594	[M-H] ⁻	C ₃₆ H ₅₈ O ₉	Triterpene glycosides	---
738	Sodium taurocholate monohydrate	7.475	516.30042	[M+NH ₄] ⁺	C ₂₆ H ₄₆ NNaO ₈ S	Taurinated bile acids and derivatives	---
739	Sodium myristyl sulfate	12.438	339.15622	[M+Na] ⁺	C ₁₄ H ₂₉ NaO ₄ S	Sulfuric acid monoesters	---
740	Sodium Danshensu	1.105	243.01895	[M+CH ₃ OH+H] ⁺	C ₉ H ₉ NaO ₅	Phenylpropanoic acids	---
741	Smenamide C or D	7.304	468.27902	[M+NH ₄] ⁺	C ₂₅ H ₄₀ ClN ₂ O ₄	Carboxylic acid imides	---
742	SM(d18:2/24:0)	12.301	835.66266	[M+Na] ⁺	C ₄₇ H ₉₃ N ₂ O ₆ P	Sphingomyelins	---
743	SM(d18:1/24:1)	12.135	813.68201	[2M+H] ²⁺	C ₄₇ H ₉₃ N ₂ O ₆ P	Phosphosphingolipids	---
744	SM(d18:1/24:1)	11.135	813.68182	[M+H] ⁺	C ₄₇ H ₉₃ N ₂ O ₆ P	Phosphosphingolipids	---
745	SM(d18:1/24:1)	10.799	813.6817	[M+NH ₄] ⁺	C ₄₇ H ₉₃ N ₂ O ₆ P	Phosphosphingolipids	---
746	SM(d18:1/23:0)	11.131	859.68378	[M-H] ⁻	C ₄₆ H ₉₃ N ₂ O ₆ P	Phosphosphingolipids	---
747	SM(d18:1/18:1(9Z))	11.192	763.54645	[M-H] ⁻	C ₄₁ H ₈₁ N ₂ O ₆ P	Phosphosphingolipids	---

748	SM(d18:1/16:0)	12.675	687.53778	[2M-H]-	C39H79N2O6P	Phosphosphingolipids	---
749	Skimmin	7.675	323.07858	[M-H]-	C15H16O8	Coumarin glycosides	---
750	SKF-75670 hydrobromide	4.607	270.15445	[M+H]+	C17H20BrNO2	Benzazepines	---
751	Sesquiterpenes	6.226	245.11662	[M-H]-	C15H18O3	Prenol lipids	---
752	Sedanonic acid	10.004	209.11647	[M-H]-	C12H18O3	Keto acids and derivatives	---
753	Sebuthylazine	9.581	230.11667	[M+H]+	C9H16ClN5	1,3,5-triazine-2,4-diamines	---
754	Scytophycin A	12.839	804.52576	[M+2H]2+	C45H75NO12	Diterpene lactones	---
755	Scutellarioside II	8.789	507.14813	[M-H]-	C24H28O12	Hydroxycinnamic acid esters	---
756	Scutellarioside I	9.363	515.15088	[M+Na]+	C24H28O11	Glycosyl compounds	---
757	Scutellarioside I	1.196	491.15814	[2M-H]-	C24H28O11	Glycosyl compounds	---
758	Scutellarioside I	1.062	491.15823	[M-H]-	C24H28O11	Glycosyl compounds	---
759	Scoparin	8.197	461.10654	[M-H]-	C22H22O11	Flavonoid C-glycosides	---
760	Sativic acid	9.531	347.24158	[M-H]-	C18H36O6	Fatty Acyls	---
761	Salsolinol-1-carboxylic acid	7.073	224.09047	[M+H]+	C11H13NO4	Tetrahydroisoquinolines	---
762	S4:19(P3:17/F1:2)	12.865	682.3587	[M+H]+	C31H52O15	Saccharolipids	---
763	S4:17(P3:15/F1:2)	12.861	681.29272	[M-H]-	C29H48O15	Saccharolipids	---
764	S4:17(P3:15/F1:2)	12.865	654.32849	[M+NH4]+	C29H48O15	Saccharolipids	---
765	Rosamicin	13.351	582.3645	[M+2H]2+	C31H51NO9	Aminosaccharides	---
766	Roquefortine E	6.884	456.24307	[M-H]-	C27H31N5O2	Pyroloindoles	---
767	Roccellic Acid	7.612	318.2619	[M+H]+	C17H32O4	Long-chain fatty acids	---
768	Rhodiocyanoside A	1.509	260.11194	[M+H]+	C11H17NO6	Fatty acyl glycosides	---
769	Rhodiocyanoside A	7.166	258.0965	[M-H]-	C11H17NO6	Fatty acyl glycosides	---
770	Rhizocarpic acid	7.13	468.1445	[M-H]-	C28H23NO6	Amino acids and derivatives	---
771	Retusin 7-methyl ether	13.796	299.09003	[M+H]+	C17H14O5	7-O-methylated isoflavonoids	---
772	Reboxetine mesylate hydrate	2.927	428.17365	[M+NH4]+	C20H29NO7S	Phenol ethers	---
773	Reboxetine mesylate hydrate	1.68	428.17404	[M+H]+	C20H29NO7S	Phenol ethers	---
774	Reboxetine mesylate hydrate	3.215	428.17358	[2M+H]+	C20H29NO7S	Phenol ethers	---
775	Radiclonic acid	12.482	397.29309	[M+Na]+	C23H40O5	Acyclic diterpenoids	---
776	Raddeanin A	8.722	919.50433	[M+Na]+	C47H76O16	Triterpenoids	---
777	Raclopride	1.517	347.09293	[M+H]+	C15H20Cl2N2O3	Salicylamides	---
778	Raclopride	13.478	347.09302	[M+H-H2O]+	C15H20Cl2N2O3	Salicylamides	---
779	Raclopride	5.736	347.09302	[2M+H]+	C15H20Cl2N2O3	Salicylamides	---
780	Raclopride	6.164	347.09314	[M+Na]+	C15H20Cl2N2O3	Salicylamides	---
781	Racecadotril	6.258	386.1423	[2M+H]+	C21H23NO4S	N-acyl-alpha amino acids and derivatives	---
782	Quinolacetic acid	6.483	167.03259	[M-H]-	C8H8O4	Organooxygen compounds	---
783	Pyrrhoxanthinol	12.377	571.341	[M+Na]+	C37H46O5	Terpene lactones	---
784	Pyroglutamyl-Isoleucine	7.598	241.11707	[M-H]-	C11H18N2O4	Dipeptides	---
785	PyroGlu-Pro-Arg	6.232	383.20108	[M+H]+	C16H26N6O5	Peptides	---
786	PyroGlu-Ile-Lys	6.405	371.22787	[M+H]+	C17H30N4O5	Peptides	---

787	PyroGlu-Ile-Arg	6.46	399.23428	[M+H] ⁺	C17H30N6O5	Peptides	---
788	Pyrogallin	7.733	205.04865	[M+H] ⁺	C11H8O4	Tropolones	---
789	Pyridoxine-Alpha-Glucoside	4.489	332.13229	[M+CH3OH+H] ⁺	C14H21NO8	Pyridines and derivatives	---
790	Putrebactin	6.553	373.20624	[M+H-H2O] ⁺	C16H28N4O6	Macrolactams	---
791	Pulvinic acid	2.913	307.06473	[M-H] ⁻	C18H12O5	Butenolides	---
792	Pseurotin	0.917	476.15936	[M-H] ⁻	C22H25NO8	Ketones	---
793	PS(17:0/16:1)	12.989	746.50232	[M-H] ⁻	C39H74NO10P	Phosphatidylserines	---
794	Prosapogenin A	8.228	745.41626	[M+Na] ⁺	C39H62O12	Steroidal saponins	---
795	Prosapogenin A	8.229	723.43323	[M+H] ⁺	C39H62O12	Steroidal saponins	---
796	Propylparaben	11.079	179.06895	[M-H] ⁻	C10H12O3	Benzoic acid esters	---
797	Propentofylline	8.871	329.15555	[M+Na] ⁺	C15H22N4O3	Xanthines	---
798	Propanoic acid, 2-methyl-2-(3-pentadecylphenoxv)-	10.075	413.30237	[M+Na] ⁺	C25H42O3	Phenoxyacetic acid derivatives	---
799	Propanoic acid, 2-methyl-2-(3-pentadecylphenoxv)-	8.997	413.30249	[M+H] ⁺	C25H42O3	Phenoxyacetic acid derivatives	---
800	Promethazine sulfoxide	11.973	301.13742	[M+Na] ⁺	C17H20N2OS	Benzothiazines	---
801	Prolylproline	6.513	213.12274	[M+H-H2O] ⁺	C10H16N2O3	Peptides	---
802	Prolylproline	6.339	213.12276	[M+H] ⁺	C10H16N2O3	Peptides	---
803	Prolylphenylalanine	6.91	263.13803	[M+H] ⁺	C14H18N2O3	Peptides	---
804	Prolylhydroxyproline	6.723	229.11688	[M+CH3OH+H] ⁺	C10H16N2O4	Peptides	---
805	Prolylhydroxyproline	6.929	227.10162	[M-H2O-H] ⁻	C10H16N2O4	Peptides	---
806	Pratol	13.838	267.06381	[M-H] ⁻	C16H12O4	4'-O-methylated flavonoids	---
807	Prantscimgin	12.077	329.13715	[M+H] ⁺	C19H20O5	Psoralens	---
808	Posaconazole	6.417	351.17499	[M+Na] ⁺	C37H42F2N8O4	Phenylpiperazines	---
809	Posaconazole	1.482	351.17514	[M+H] ⁺	C37H42F2N8O4	Phenylpiperazines	---
810	Poricoic acid A	8.229	497.33035	[M-H] ⁻	C31H46O5	Triterpenoids	---
811	Ponatinib	9.086	267.11859	[M+H] ⁺	C29H27F3N6O	Aromatic anilides	---
812	Polyethylene, oxidized	8.761	243.1216	[M-H] ⁻	C12H20O5	Keto acids and derivatives	---
813	P-Nitrophenyl Glutamine	9.322	268.09329	[M+H] ⁺	C11H13N3O5	Amino acids and derivatives	---
814	Platyphylloside	10.809	521.20081	[M-H] ⁻	C25H32O9	Curcuminoids	---
815	Piperonylic acid	7.209	165.01688	[M-H] ⁻	C8H6O4	Benzodioxoles	---
816	Piperochromanoic acid	12.601	355.19247	[M-H] ⁻	C22H28O4	Prenol lipids	---
817	piperidyl 2,4,5-trimethoxyphenyl ketone	2.661	302.13361	[M+Na] ⁺	C15H21NO4	1-benzoylpiperidines	---
818	Piperidine, 1-[(2-oxo-2H-1-benzopyran-6-yl)sulfonyl]-	2.149	294.07999	[M+H-H2O] ⁺	C14H15NO4S	Coumarins and derivatives	---
819	Piperidine, 1-[(2-oxo-2H-1-benzopyran-6-yl)sulfonyl]-	2.263	294.07999	[M+H] ⁺	C14H15NO4S	Coumarins and derivatives	---
820	Pimelylcarnitine	6.476	304.17609	[2M+H] ⁺	C14H25NO6	Fatty Acyls	---
821	Piconol	2.69	110.06002	[M+CH3OH+H] ⁺	C6H7NO	Pyridines and derivatives	---
822	Picfeltarraenin IA	8.183	785.41058	[M+Na] ⁺	C41H62O13	Steroidal saponins	---
823	PI(18:0/22:6)	13.495	909.55536	[M-H] ⁻	C49H83O13P	Phosphatidylinositols	---
824	PI(18:0/20:4)	12.25	885.54565	[M-H] ⁻	C47H83O13P	Phosphatidylinositols	---
825	PI(17:0/20:3)	13.414	875.56702	[M+H] ⁺	C46H83O13P	Phosphatidylinositols	---
826	PI(17:0/20:3)	12.583	875.56744	[M+Na] ⁺	C46H83O13P	Phosphatidylinositols	---

827	PI(17:0/18:1)	13.378	873.54993	[M+2H] ²⁺	C44H83O13P	Phosphatidylinositols	---
828	PI(17:0/14:1)	13.435	795.50684	[M+Na] ⁺	C40H75O13P	Phosphatidylinositols	---
829	PI(16:1/13-HODE)	11.829	847.5022	[M-H] ⁻	C43H77O14P	Phosphatidylinositols	---
830	PI(16:0/18:2)	12.325	833.51532	[M-H] ⁻	C43H79O13P	Phosphatidylinositols	---
831	Phthalic anhydride	12.445	149.0229	[M+H] ⁺	C8H4O3	Phthalic anhydrides	---
832	Phe-Pro	8.51	245.12711	[M+H-H2O] ⁺	C14H18N2O3	Peptides	---
833	Phenyl Hexopyranoside	8.124	255.0851	[M-H] ⁻	C12H16O6	Phenolic glycosides	---
834	Phenacylamine Hydrochloride	6.842	172.04877	[M+H-H2O] ⁺	C8H10ClNO	Ketones	---
835	Phenacylamine Hydrochloride	13.524	172.04831	[M+NH4] ²⁺	C8H10ClNO	Ketones	---
836	Phenacylamine Hydrochloride	8.928	172.04829	[M+H] ⁺	C8H10ClNO	Ketones	---
837	Phenacylamine Hydrochloride	10.739	172.04825	[M+CH3OH+H] ⁺	C8H10ClNO	Ketones	---
838	Phenacylamine Hydrochloride	5.89	172.0482	[M+2H] ²⁺	C8H10ClNO	Ketones	---
839	PharmaGSID_47333	12.59	381.2294	[M-H] ⁻	C22H30N4O2	Naphthyridines	---
840	PG(18:1/18:2)	13.332	771.51636	[M-H] ⁻	C42H77O10P	Phosphatidylglycerols	---
841	PG(18:1/18:2)	12.352	771.51154	[2M-H] ⁻	C42H77O10P	Phosphatidylglycerols	---
842	PG(18:1/18:1)	12.686	773.53333	[M-H] ⁻	C42H79O10P	Glycerophospholipids	---
843	PG(18:1/16:0)	12.527	747.5191	[M-H] ⁻	C40H77O10P	Glycerophospholipids	---
844	PG(18:0/18:1)	13.443	775.54797	[M-H] ⁻	C42H81O10P	Phosphatidylglycerols	---
845	PG(18:0/18:0)	12.348	777.55859	[M-H] ⁻	C42H83O10P	Phosphatidylglycerols	---
846	PG(17:0/20:3)	12.513	785.53125	[M-H] ⁻	C43H79O10P	Phosphatidylglycerols	---
847	PG(17:0/18:1)	10.729	761.52936	[M-H] ⁻	C41H79O10P	Phosphatidylglycerols	---
848	PG(17:0/16:1)	12.47	733.5014	[M-H] ⁻	C39H75O10P	Phosphatidylglycerols	---
849	PG(17:0/16:1)	13.245	752.54565	[M+H] ⁺	C39H75O10P	Phosphatidylglycerols	---
850	PG(16:1/16:1)	12.822	717.47559	[M-H] ⁻	C38H71O10P	Phosphatidylglycerols	---
851	PG(16:0/18:2)	12.61	745.50317	[M-H] ⁻	C40H75O10P	Phosphatidylglycerols	---
852	PG(16:0/16:1)	12.365	719.4845	[M-H] ⁻	C38H73O10P	Phosphatidylglycerols	---
853	PG(16:0/16:0)	12.347	721.49829	[M-H] ⁻	C38H75O10P	Phosphatidylglycerols	---
854	PG(16:0/16:0)	12.523	745.49817	[M+Na] ⁺	C38H75O10P	Phosphatidylglycerols	---
855	PG(16:0/16:0)	12.2	723.51337	[M+2H] ²⁺	C38H75O10P	Phosphatidylglycerols	---
856	PG(16:0/16:0)	10.771	723.51196	[M+H] ⁺	C38H75O10P	Phosphatidylglycerols	---
857	PG(14:0/16:1)	13.427	691.45697	[M-H] ⁻	C36H69O10P	Phosphatidylglycerols	---
858	PG(14:0/16:1)	12.446	691.45728	[2M-H] ⁻	C36H69O10P	Phosphatidylglycerols	---
859	PFCA-H	6.331	287.03265	[M-H] ⁻	C8H8F8O2	PFSA	---
860	PFCA-H	2.996	157.01212	[M-H2O-H] ⁻	C4H5F3O3	PFSA	---
861	PFAP-PAP	0.823	164.95511	[M-H] ⁻	CH2F3O4P	PFSA	---
862	PFAP-FT_PAP	0.803	276.98691	[M-H] ⁻	C5H6F7O3P	PFSA	---

863	PFAP-diPAP	0.853	232.94258	[M-H]-	C2HF6O4P	PFSA	---
864	Perospirone	7.232	427.21716	[M+H]+	C23H30N4O2S	N-arylpiperazines	---
865	Peridinin	12.064	631.36249	[2M+H]+	C39H50O7	Terpene lactones	---
866	Peracetic acid	6.006	75.0066	[M-H]-	C2H4O3	Carboxylic acids and derivatives	---
867	Pentasaccharides (Hex-Hex-Hex-Hex-Pentanedioic acid, 3-hydroxy-3-methyl-, [4-	9.082	827.26263	[M-H]-	C30H52O26	Oligosaccharides	---
868	(beta-D-glucopyranosyloxy)phenylmethyl methyl ester	6.201	462.19522	[M+NH4]+	C20H28O11	Saccharolipids	---
869	Pentamethoxyquercetin	12.669	373.29324	[M+Na]+	C20H20O7	7-O-methylated flavonoids	---
870	Pentamethoxyquercetin	12.52	373.29321	[M+NH4]+	C20H20O7	7-O-methylated flavonoids	---
871	-Pentadec-9-enoylcarnitine	10.352	384.30661	[M+NH4]+	C22H41NO4	Fatty Acyls	---
872	PEG-4 diethylhexanoate	12.048	447.32996	[M+NH4]+	C24H46O7	Fatty acid esters	---
873	PE(16:0/18:2)	13.413	738.50073	[M+H]+	C39H74NO8P	Phosphatidylethanolamines	---
874	P-Coumaroyltyramine	9.218	284.1261	[M+H]+	C17H17NO3	Coumaric acids and derivatives	---
875	P-Coumaroyltyramine	9.219	306.10861	[M+Na]+	C17H17NO3	Coumaric acids and derivatives 1-(1Z-alkenyl),2-acyl-	---
876	PC(P-18:0/18:1)	11.906	772.61609	[M+H]+	C44H86NO7P	glycerophosphocholines	---
877	PC(18:3/18:3)	12.808	778.53607	[M+H]+	C44H76NO8P	Phosphatidylcholines	---
878	PC(18:3/18:3)	13.237	778.53589	[M+Na]+	C44H76NO8P	Phosphatidylcholines	---
879	PC(18:2/18:2)	12.348	782.56757	[M+H]+	C44H80NO8P	Phosphatidylcholines	---
880	PC(18:1/20:1)	12.013	814.62885	[M+H]+	C46H88NO8P	Phosphatidylcholines	---
881	PC(18:1/18:2)	12.096	784.58679	[M+H]+	C44H82NO8P	Phosphatidylcholines	---
882	PC(18:1/16:0)	12.186	760.58374	[M+H]+	C42H82NO8P	Phosphatidylcholines	---
883	PC(18:0/20:4)	12.162	810.59814	[M+H]+	C46H84NO8P	Phosphatidylcholines	---
884	PC(18:0/20:3)	11.936	834.59863	[2M+H]+	C46H86NO8P	Phosphatidylcholines	---
885	PC(18:0/18:2)	12.143	786.59711	[M+H]+	C44H84NO8P	Phosphatidylcholines	---
886	PC(18:0/18:1)	12.139	788.61499	[M+H]+	C44H86NO8P	Phosphatidylcholines	---
887	PC(18:0/18:1)	12.343	788.61444	[M+CH3OH+H]+	C44H86NO8P	Phosphatidylcholines	---
888	PC(18:0/18:1)	13.186	788.62018	[M+2H]2+	C44H86NO8P	Phosphatidylcholines	---
889	PC(18:0/18:1)	13.409	788.62067	[M+NH4]+	C44H86NO8P	Phosphatidylcholines	---
890	PC(18:0/18:1)	13.428	810.59216	[M+Na]+	C44H86NO8P	Phosphatidylcholines	---
891	PC(18:0/18:1)	12.511	810.59198	[2M+H]+	C44H86NO8P	Phosphatidylcholines	---
892	PC(16:0/18:2)	12.145	758.56366	[M+H]+	C42H80NO8P	Phosphatidylcholines	---
893	PC(16:0/18:1)	12.358	760.58344	[M+H]+	C42H82NO8P	Phosphatidylcholines	---
894	PC(16:0/18:1)	13.134	782.56879	[M+Na]+	C42H82NO8P	Phosphatidylcholines	---

895	PC(16:0/18:0)	12.125	762.59741	[M+H] ⁺	C42H84NO8P	Phosphatidylcholines	---
896	PC(16:0/16:0)	12.135	734.5639	[M+H] ⁺	C40H80NO8P	Phosphatidylcholines	---
897	Pazufloxacin	10.732	317.09589	[M-H] ⁻	C16H15FN2O4	Quinoline carboxylic acids	---
898	Palmitoyl glycerol	11.938	313.27188	[M-H2O+H] ⁺	C19H38O4	Monoacylglycerols	---
899	Oxoamide	6.284	193.09659	[M+Na] ⁺	C10H12N2O2	Organooxygen compounds	---
900	Osthole	3.808	267.09592	[M+Na] ⁺	C15H16O3	Coumarins and derivatives	---
901	Ornibactin C8	9.153	737.40863	[M+H] ⁺	C30H56N8O13	Peptides	---
902	Oridonin	9.234	409.18631	[M-H] ⁻	C20H28O6	Kaurane diterpenoids	---
903	Ophiogenin-3-O-alpha-L-rhamnopyranosyl-(1->2)-beta-D-glucopyranoside	8.129	755.41748	[M+H-H2O] ⁺	C39H62O14	Steroidal saponins	---
904	Okaramine J	7.697	525.2868	[M+Na] ⁺	C32H36N4O3	Pyrroloindoles	---
905	Okaramine H	7.479	521.25397	[M+2H] ²⁺	C32H32N4O3	Pyrroloindoles	---
906	Dodecylbenzenesulfonic acid	12.499	325.18146	[M-H] ⁻	C18H30O3S	Benzenesulfonic acids and derivatives	---
907	O-Desmethyltramadol	10.855	250.17685	[M+H] ⁺	C15H23NO2	Cyclohexylphenols	---
908	Octyl acetate	9.955	195.13698	[M+Na] ⁺	C10H20O2	Fatty alcohol esters	---
909	Octaethylene glycol	7.182	393.20746	[M+Na] ⁺	C16H34O9	Dialkyl ethers	---
910	Octadecylamine	12.24	270.31451	[M+H] ⁺	C18H39N	Primary amines	---
911	Octadecanedioic acid	11.492	315.25208	[M+H] ⁺	C18H34O4	Long-chain fatty acids	---
912	Octadeca-9,12-dienal	12.062	265.25079	[M+H] ⁺	C18H32O	Fatty Acyls	---
913	Ochrephilone	13.439	381.17123	[M-H] ⁻	C23H26O5	Ketones	---
914	Obtucarbamate A	7.211	261.08563	[M+Na] ⁺	C11H14N2O4	Phenylcarbamic acid esters	---
915	O-alpha-D-Mannopyranosyl-(1-4)-O-alpha-D-mannopyranosyl-(1-4)-alpha-D-mannopyranose	1.309	503.15836	[M-H] ⁻	C18H32O16	Organooxygen compounds	---
916	O-Adipoylcarnitine	6.554	290.1582	[M+CH3OH+H] ⁺	C13H23NO6	Acyl carnitines	---
917	O-Adipoylcarnitine	7.559	290.15802	[M+H] ⁺	C13H23NO6	Acyl carnitines	---
918	N-Undecanoylglycine	10.066	242.17429	[M-H] ⁻	C13H25NO3	Carboxylic acids and derivatives	---
919	N-Palmitoyl Isoleucine	13.236	368.3143	[M-H] ⁻	C22H43NO3	Amino acids and derivatives	---
920	N-Palmitoyl Alanine	12.824	326.26846	[M-H] ⁻	C19H37NO3	Amino acids and derivatives	---
921	Nonaethylene glycol	7.374	437.23453	[M+Na] ⁺	C18H38O10	Dialkyl ethers	---
922	Nonaethylene glycol	6.892	415.25369	[M+CH3OH+H] ⁺	C18H38O10	Dialkyl ethers	---
923	Nonadecenoic acid	13.121	295.26157	[M-H] ⁻	C19H36O2	Fatty Acyls	---
924	N-Oleoyl Phenylalanine	13.233	428.31509	[M-H] ⁻	C27H43NO3	Amino acids and derivatives	---
925	N-oleoyl leucine	11.589	396.34299	[M+CH3OH+H] ⁺	C24H45NO3	Amino acids and derivatives	---
926	N-Oleoyl isoleucine	13.306	394.33032	[M-H] ⁻	C24H45NO3	Amino acids and derivatives	---
927	N-naphthalen-1-yl-1-pentylindole-3-carboxamide	2.355	379.17996	[M+Na] ⁺	C24H24N2O	Indolecarboxamides and derivatives	---
928	N-Methyldodecylamine	10.538	200.23669	[M+H] ⁺	C13H29N	Secondary amines	---
929	N-Methylcorydaldine	6.566	222.11128	[M+H] ⁺	C12H15NO3	Isoquinolones and derivatives	---

930	N-Methylcalystegine C1	1.318	206.10106	[M+NH4] ⁺	C8H15NO5	Tropane alkaloids	---
931	N-Lauroyl Isoleucine	12.702	312.25214	[M-H] ⁻	C18H35NO3	Carboxylic acids and derivatives	---
932	N-Lactoylvaline	7.189	188.09091	[M-H] ⁻	C8H15NO4	Carboxylic acids and derivatives	---
933	N-lactoyl-Tyrosine	7.073	252.08537	[M-H] ⁻	C12H15NO5	Carboxylic acids and derivatives	---
934	N-lactoyl-Tryptophan	7.93	275.10245	[M-H] ⁻	C14H16N2O4	Carboxylic acids and derivatives	---
935	N-Lactoylleucine	8.077	202.10611	[M-H] ⁻	C9H17NO4	Carboxylic acids and derivatives	---
936	N-lactoyl-Glycine	0.914	146.04346	[M-H] ⁻	C5H9NO4	Carboxylic acids and derivatives	---
937	N-Isobutyl-2,4,12-Octadecatrienamide	12.456	334.30835	[M+H] ⁺	C22H39NO	N-acyl amines	---
938	N-Hydroxy-3,4,5-trimethoxybenzamide	6.332	228.08586	[M+H] ⁺	C10H13NO5	Benzoic acids and derivatives	---
939	N-Hydroxy-3,4,5-trimethoxybenzamide	1.404	228.08583	[M+H-H2O] ⁺	C10H13NO5	Benzoic acids and derivatives	---
940	N-Hydroxy-3,4,5-trimethoxybenzamide	6.241	228.08571	[M+Na] ⁺	C10H13NO5	Benzoic acids and derivatives	---
941	N-Hydroxy-3,4,5-trimethoxybenzamide	6.883	226.0705	[M-H] ⁻	C10H13NO5	Benzoic acids and derivatives	---
942	N-Hexanoylsphingosine	12.133	380.34851	[M+H] ⁺	C24H47NO3	Ceramides	---
943	N-Fructosyl pyroglutamate	2.517	290.08682	[M-H] ⁻	C11H17NO8	N-Fructosyl amino acids	---
944	N-Fructosyl isoleucine	6.199	276.14285	[M-H2O+H] ⁺	C12H23NO7	N-Fructosyl amino acids	---
945	N-Fructosyl isoleucine	4.024	292.13852	[M-H] ⁻	C12H23NO7	N-Fructosyl amino acids	---
946	N-Fructosyl isoleucine	4.299	294.15302	[M+H] ⁺	C12H23NO7	N-Fructosyl amino acids	---
947	N-Formylcytisine	6.382	219.11172	[M+H] ⁺	C12H14N2O2	Cytisine and derivatives	---
948	N-Feruloyloctopamine	8.466	328.11697	[M-H] ⁻	C18H19NO5	Hydroxycinnamic acids and derivatives	---
949	Neotussilagine	9.041	200.1273	[M+Na] ⁺	C10H17NO3	Pyrrolizidines	---
950	Neotrehalose	7.16	341.10687	[M-H] ⁻	C12H22O11	Glycosyl compounds	---
951	Neoline	11.202	460.26727	[M+Na] ⁺	C24H39NO6	Aconitane-type diterpenoid alkaloids	---
952	Neoline	0.18	460.26724	[M+H] ⁺	C24H39NO6	Aconitane-type diterpenoid alkaloids	---
953	Neocoprogen I	11.06	699.35107	[M+CH3OH+H] ⁺	C31H50N6O12	Amino acids and derivatives	---
954	Negletein	9.429	285.07437	[M+H] ⁺	C16H12O5	7-O-methylated flavonoids	---
955	N-Dinitrophenyl-L-Tryptophan	0.536	371.09903	[M+H] ⁺	C17H14N4O6	Dinitroanilines	---
956	Ncg00385798-01_C31H43N7O6_	10.298	608.31604	[M-H] ⁻	C31H43N7O6	Peptides	---
957	Ncg00381227-01_C31H40O10_	10.807	571.25586	[M-H] ⁻	C31H40O10	Limonoids	---
958	Ncg00380873-01_C47H74O16_	8.374	917.48419	[M+H-H2O] ⁺	C47H74O16	Triterpene glycosides	---
959	Ncg00380873-01_C47H74O16_	8.363	917.49097	[M+2H] ²⁺	C47H74O16	Triterpene glycosides	---
960	NCGC00380481-01_C23H28O13S_	6.226	543.11627	[M-H] ⁻	C23H28O13S	Terpene glycosides	---
961	Ncg00380364-01!	8.297	784.48773	[M+H-H2O] ⁺	C41H66O13	Triterpenoids	---
962	Ncg00380251-01!	1.576	415.14218	[M-H] ⁻	C22H24O8	Naphthofurans	---
963	Ncg00380138-01!	6.979	227.13809	[M+Na] ⁺	C11H15NO3	Oxazolidinones	---
964	Ncg00380138-01!	7.335	227.13802	[M+CH3OH+H] ⁺	C11H15NO3	Oxazolidinones	---

965	N-Boc-DL-Histidine	6.182	256.12796	[M+NH4] ⁺	C11H17N3O4	Amino acids and derivatives	---
966	N-Benzylpiperazine	6.972	177.13791	[M+H] ⁺	C11H16N2	Phenylmethanamines	---
967	N-Benzyl-4-((3-Oxo-3-(2-Oxo-2H-Chromen-3-Yl)Propyl)Amino)Benzamide	7.171	425.15335	[M-H] ⁻	C26H22N2O4	Benzamides	---
968	Benzoylphenylalanylphenylalaninol acetate	11.437	467.19254	[M+Na] ⁺	C27H28N2O4	Amino acids and derivatives	---
969	Nakijiquinone R	7.35	452.21063	[M+H] ⁺	C23H33NO6S	Prenylquinones	---
970	Nakijiquinone H	11.646	457.31754	[M+H] ⁺	C26H40N4O3	Prenylquinones	---
971	N-Acetylvaline	6.904	158.08015	[M-H] ⁻	C7H13NO3	Carboxylic acids and derivatives	---
972	N-Acetyltyrosine	6.941	222.07504	[M-H] ⁻	C11H13NO4	Carboxylic acids and derivatives	---
973	N-Acetyltyramine	10.123	178.08507	[M-H] ⁻	C10H13NO2	1-hydroxy-2-unsubstituted benzenoids	---
974	N-Acetyl sphinganine	11.733	344.31485	[M+Na] ⁺	C20H41NO3	Ceramides	---
975	N-Acetylproline	12.113	158.08032	[M+H] ⁺	C7H11NO3	Amino acids and derivatives	---
976	N-Acetyl-L-arginine	2.389	217.12894	[M+H] ⁺	C8H16N4O3	Amino acids and derivatives	---
977	N-Acetyl isoleucine	7.822	172.09554	[M-H] ⁻	C8H15NO3	Carboxylic acids and derivatives	---
978	N-Acetyl asparagine	1.111	219.03412	[M+NH4] ⁺	C6H10N2O4	Amino acids and derivatives	---
979	N2-Isobutyryl-2-Deoxyguanosine	6.437	336.12854	[M-H] ⁻	C14H19N5O5	Purine 2'-deoxyribonucleosides	---
980	N2,N5-Diacetylornithine	6.212	215.10149	[M-H] ⁻	C9H16N2O4	Carboxylic acids and derivatives	---
981	N1,N8-Diacetylspermidine	4.931	230.18544	[M+H] ⁺	C11H23N3O2	Carboxylic acids and derivatives	---
982	N-{2-[(6,7-dimethoxyisoquinolyl)methyl]-4,5-dimethoxyphenyl}(4-fluorophenyl)carbamide	9.489	475.1633	[M-H] ⁻	C27H25FN2O5	Benzylisoquinolines	---
983	N-{3-(3,4-dimethylphenyl)adamantan-1-yl}methyl(3,4,5-trimethoxyphenyl)carboxamide	8.745	508.27371	[M-H2O-H] ⁻	C29H37NO4	Benzamides	---
984	N-[6-amino-1-(4-methoxyphenyl)-2,4-dioxo(1,3-dihydropyrimidin-5-yl)][(3-chlorophenyl)amino]carboxamide	6.84	400.08524	[M-H] ⁻	C18H16ClN5O4	N-phenylureas	---
985	N-[5-[[4-(4-acetyl(hydroxyamino)butylamino)-4-oxobutanoyl]-hydroxyamino]pentyl]-N'-(5-aminopentyl)-N'-hydroxybutanediamide	12.293	545.32697	[M+NH4] ⁺	C24H46N6O8	N-acyl amines	---

986	N-[4-[(9S,13R)-16-hydroxy-7,9,13-trimethyl-5-oxapentacyclo[10.8.0.0.2,9.04,8.013,18]icosa-6,18-dien-6-yl]-2-methylbutyl]acetamide	13.578	478.32791	[M+Na] ⁺	C29H45NO3	Furostanes and derivatives	---
987	(methylethyl)phenyl]-2-(9-methyl-6-oxohydropurin-8-ylthio)butanamide	1.425	386.16394	[M+H] ⁺	C19H23N5O2S	Purinones	---
988	(methylethyl)phenyl]-2-(9-methyl-6-oxohydropurin-8-ylthio)butanamide	1.452	408.14749	[M+H-H2O] ⁺	C19H23N5O2S	Purinones	---
989	bis(trifluoromethyl)phenyl]-2-(2-1,2,3,4-tetrahydroisoquinolyl)acetamide	6.86	437.08377	[M-H2O-H] ⁻	C19H16F6N2O	Amino acids and derivatives	---
990	(trifluoromethyl)phenyl]quinazolin-4-amine	6.303	288.07095	[M-H] ⁻	C15H10F3N3	Quinazolines	---
991	N-[1-(4-methoxy-6-oxopyran-2-yl)-2-methylpropyl]acetamide	6.55	240.12199	[M+H-H2O] ⁺	C12H17NO4	Pyranones and derivatives	---
992	N-[1-(4-methoxy-6-oxopyran-2-yl)-2-methylpropyl]acetamide	6.275	240.12206	[M+H] ⁺	C12H17NO4	Pyranones and derivatives	---
993	N-[1-(4-methoxy-6-oxopyran-2-yl)-2-methylpropyl]acetamide	6.828	240.12201	[M+NH4] ⁺	C12H17NO4	Pyranones and derivatives	---
994	N-[1-(2-Methylbenzyl)-1H-Pyrazol-4-Yl]-3,4-Dihydroisoquinoline-2(1H)-Carbothioamide	7.296	361.14877	[M-H] ⁻	C21H22N4S	Tetrahydroisoquinolines	---
995	N-[1-(2-Methylbenzyl)-1H-Pyrazol-4-Yl]-3,4-Dihydroisoquinoline-2(1H)-Carbothioamide	7.532	361.14865	[M-H2O-H] ⁻	C21H22N4S	Tetrahydroisoquinolines	---
996	N-[(7-Hydroxy-2-Oxo-4-Phenyl-2H-Chromen-8-Yl)Methyl]-D-Leucine	6.328	380.15338	[M-H2O-H] ⁻	C22H23NO5	Neoflavones	---
997	N-[(1E)-2-(2-ethoxyphenyl)-1-azavinyl]-2-[(3,5-dioxo(2H,4H-1,2,4-triazin-6-yl)aminol]acetamide	8.34	331.11633	[2M-H] ⁻	C14H16N6O4	Amino acids and derivatives	---
998	N,N-Dimethyldodecylamine	10.687	214.25157	[M+H] ⁺	C14H31N	Tertiary amines	---
999	N,N-Dimethyldodecylamine	10.364	186.22067	[M+H] ⁺	C12H27N	Tertiary amines	---
1000	N,N-Diethyl-4-Hydroxybenzamide	10.72	192.10085	[M-H] ⁻	C11H15NO2	Benzamides	---
1001	N-(5-Fluoro-3-methyl-1H-indol-1-yl)-4-methyl-2-(pyridin-2-yl)pyrimidine-5-carboxamide	6.68	360.12735	[M-H] ⁻	C20H16FN5O	Pyridinylpyrimidines	---

1002	N-(5-chloro-2-methylphenyl)-2-{4-[(7-methyl-2-oxochromen-4-yl)methyl]piperazinyl}acetamide	1.513	440.17352	[M+H] ⁺	C ₂₄ H ₂₆ ClN ₃ O ₃	Amino acids and derivatives	---
1003	N-(5-chloro-2-methylphenyl)-2-{4-[(7-methyl-2-oxochromen-4-yl)methyl]piperazinyl}acetamide	2.263	440.17346	[M+H- H ₂ O] ⁺	C ₂₄ H ₂₆ ClN ₃ O ₃	Amino acids and derivatives	---
1004	N-(4-Methylquinazolin-2-yl)Guanidine N-(4-acetylphenyl)[2-(2-thienylsulfonyl)(3-1,2,3,4-tetrahydroisoquinolyl)]carboxamide	1.417	202.1066	[M+H] ⁺	C ₁₀ H ₁₁ N ₅	Quinazolines	---
1005	N-(4,5-diphenyl-1H-pyrazolo[3,4-c]pyridazin-3-yl)-N'-phenylurea	1.02	439.08295	[M-H] ⁻	C ₂₂ H ₂₀ N ₂ O ₄ S ₂	Ketones	---
1006	N-(4-(2H,3H-benzo[3,4-e]1,4-dioxin-6-yl)(1,3-thiazol-2-yl))(3,4-dimethoxyphenyl)carboxamide	4.986	407.1637	[M+H] ⁺	C ₂₄ H ₁₈ N ₆ O	Phenylpyridazines	---
1007	N-(3-methoxyphenyl)-9H-purin-6-amine	10.922	397.08716	[2M-H] ⁻	C ₂₀ H ₁₈ N ₂ O ₅ S	Dimethoxybenzenes	---
1008	N-(3-fluoro-4-methylphenyl)-2-(6-oxo-9-phenylhydropurin-8-ylthio)acetamide	7.517	240.08612	[M-H] ⁻	C ₁₂ H ₁₁ N ₅ O	6-aminopurines	---
1009	N-(3-cyanophenyl)-2-(4-hydroxyquinazolin-2-ylthio)acetamide	6.473	408.09338	[M-H] ⁻	C ₂₀ H ₁₆ N ₅ O ₂ S	Substituted imidazoles	---
1010	N-(3-cyanophenyl)-2-(4-hydroxyquinazolin-2-ylthio)acetamide	2.148	337.07486	[M+H] ⁺	C ₁₇ H ₁₂ N ₄ O ₂ S	Quinazolines	---
1011	N-(3-cyanophenyl)-2-(4-hydroxyquinazolin-2-ylthio)acetamide	6.173	337.07486	[2M+H] ⁺	C ₁₇ H ₁₂ N ₄ O ₂ S	Quinazolines	---
1012	N-(3-cyanophenyl)-2-(4-hydroxyquinazolin-2-ylthio)acetamide	3.866	337.07471	[M+2H] ²⁺	C ₁₇ H ₁₂ N ₄ O ₂ S	Quinazolines	---
1013	N-(3-cyanophenyl)-2-(4-hydroxyquinazolin-2-ylthio)acetamide	4.943	337.07468	[M+Na] ⁺	C ₁₇ H ₁₂ N ₄ O ₂ S	Quinazolines	---
1014	N-(3-cyanophenyl)-2-(4-hydroxyquinazolin-2-ylthio)acetamide	6.227	335.05991	[M-H ₂ O-H] ⁻	C ₁₇ H ₁₂ N ₄ O ₂ S	Quinazolines	---
1015	N-(3-cyano-4,5-dimethyl(2-thienyl))-3-(3,4,5-trimethoxyphenyl)propanamide	2.548	375.13861	[M+H] ⁺	C ₁₉ H ₂₂ N ₂ O ₄ S	Anisoles	---
1016	N-(3-chlorophenyl)-2-[4-(morpholin-4-ylcarbonyl)-2-oxohydroquinolyl]acetamide	2.772	426.12198	[M+H] ⁺	C ₂₂ H ₂₀ ClN ₃ O ₄	Quinoline carboxamides	---
1017	N-(3-chlorophenyl)-2-[2-oxo-4-(pyrrolidinylcarbonyl)hydroquinolyl]acetamide	1.874	454.1174	[M-H] ⁻	C ₂₂ H ₂₀ ClN ₃ O ₃	Quinoline carboxamides	---

1018	N-(3-chloro-4-methoxyphenyl)-2-{4-[(7-methyl-2-oxochromen-4-yl)methyl]piperazin-1-yl}acetamide	3.982	456.16922	[M+H] ⁺	C ₂₄ H ₂₆ ClN ₃ O ₄	Amino acids and derivatives	---
1019	N-(3-chloro-4-methoxyphenyl)-2-{4-[(7-methyl-2-oxochromen-4-yl)methyl]piperazin-1-yl}acetamide	2.969	456.16928	[M+H-H ₂ O] ⁺	C ₂₄ H ₂₆ ClN ₃ O ₄	Amino acids and derivatives	---
1020	N-(3-chloro-4-methoxyphenyl)-2-[4-(morpholin-4-ylcarbonyl)-2-oxohydroquinolyl]	1.122	454.11752	[M-H] ⁻	C ₂₃ H ₂₂ ClN ₃ O ₅	Quinoline carboxamides	---
1021	N-(3-chloro-4-methoxyphenyl)-2-[4-(morpholin-4-ylcarbonyl)-2-oxohydroquinolyl]	2.339	456.13242	[M+H] ⁺	C ₂₃ H ₂₂ ClN ₃ O ₅	Quinoline carboxamides	---
1022	N-(3-chloro-4-methoxyphenyl)-2-[4-(morpholin-4-ylcarbonyl)-2-oxohydroquinolyl]	1.573	456.13248	[M+H-H ₂ O] ⁺	C ₂₃ H ₂₂ ClN ₃ O ₅	Quinoline carboxamides	---
1023	N-{3-[(2-hydroxyethyl)methylamino]methyl}(4,5,6,7-tetrahydrobenzo[b]thiophen-2-yl)benzamide	6.342	367.14761	[M+H] ⁺	C ₁₉ H ₂₄ N ₂ O ₂ S	Benzamides	---
1024	N-(3,4-dimethylphenyl)(6-chloro-2-iminochromen-3-yl)carboxamide	6.776	367.14783	[2M+H] ⁺	C ₁₉ H ₂₄ N ₂ O ₂ S	Benzamides	---
1025	N-(2-methyl-3-oxo(2H,4H-benzo[3,4-e]1,4-oxazin-6-yl))(3,4,5-trimethoxyphenyl)carboxamide	1.824	325.07562	[M-H] ⁻	C ₁₈ H ₁₅ ClN ₂ O ₂	Aromatic anilides	---
1026	N-(2-indol-3-ylethyl)-2-[4-(2-methylpropyl)phenyl]propanamide	1.151	417.12875	[M-H] ⁻	C ₁₉ H ₂₀ N ₂ O ₆	Benzoxazinones	---
1027	N-(2-hydroxyethyl)hexadec-9-enamide	1.284	349.22925	[2M+H] ⁺	C ₂₃ H ₂₈ N ₂ O	Bicyclic monoterpenoids	---
1028	N-(2-ethoxyphenyl)-2-[9-(4-methylphenyl)-6-oxohydropurin-8-ylthio]acetamide	12.578	320.25421	[M+Na] ⁺	C ₁₈ H ₃₅ NO ₂	Alkanolamines	---
1029	N-(2-ethoxyphenyl)-2-[9-(4-methylphenyl)-6-oxohydropurin-8-ylthio]acetamide	6.166	436.14386	[M+H-H ₂ O] ⁺	C ₂₂ H ₂₁ N ₅ O ₃ S	Substituted imidazoles	---
1030	N-(2-ethoxyphenyl)-2-[9-(4-methylphenyl)-6-oxohydropurin-8-ylthio]acetamide	2.78	436.14188	[M+H] ⁺	C ₂₂ H ₂₁ N ₅ O ₃ S	Substituted imidazoles	---

1031	N-(2-chlorophenyl)-2-[2-oxo-4-(N-propylcarbamoyl)hydroquinolinyl]acetamide	1.061	396.11142	[M-H]-	C21H20ClN3O3	Quinoline carboxamides	---
1032	N-(2,5-dioxocyclopentyl)acetamide	1.406	156.06485	[M+H-H2O]+	C7H9NO3	1,3-dicarbonyl compounds	---
1033	N-(2,5-difluorophenyl)-2-{4-[(6-ethoxy-2-oxochromen-4-yl)methyl]piperazinyl}acetamide	2.576	458.18356	[M+H]+	C24H25F2N3O4	Amino acids and derivatives	---
1034	N-(2,4-dichlorophenyl)-2-[2-(3-ethoxy-4-hydroxyphenyl)-6-hydroxy-3-azabicyclo[4.4.0]dec-3-yl]acetamide	9.37	491.15329	[M-H]-	C25H30Cl2N2O4	Phenylpiperidines	---
1035	N-(2-(((1S,9R)-octahydro-1H-quinolizin-1-yl)methyl)-3-oxo-1,2,3,4-tetrahydrobenzo[4,5]imidazo[1,2-a]pyrazin-8-yl)propanamide	10.986	432.23602	[M+H-H2O]+	C23H31N5O2	Quinolizines	---
1036	N-(1,3-thiazol-2-yl)(3,4,5-trimethoxyphenyl)carboxamide	0.874	293.06143	[M-H]-	C13H14N2O4S	Benzamides	---
1037	Myrsinone	12.429	293.17746	[M-H2O-H]-	C17H26O4	Prenol lipids	---
1038	Myristic Monoethanolamide	10.463	272.25751	[M+H]+	C16H33NO2	Alkanolamines	---
1039	Myristamine Oxide	10.991	258.2778	[M+H]+	C16H35NO	Long-chain alkyl amine oxides	---
1040	Mycosporine-Glycine	2.063	246.09647	[M+H]+	C10H15NO6	Amino acids and derivatives	---
1041	Murracarpin	8.788	313.10501	[M+Na]+	C16H18O5	Coumarins and derivatives	---
1042	Murracarpin	1.111	329.0737	[M+H]+	C16H18O5	Coumarins and derivatives	---
1043	Muronic acid	11.292	399.27008	[M+H]+	C21H34O5	Gamma butyrolactones	---
1044	Murolic acid	12.143	401.2886	[M+H]+	C21H36O5	Long-chain fatty alcohols	---
1045	m-Toluamide	3.578	136.07509	[M+NH4]+	C8H9NO	Benzene and substituted derivatives	---
1046	Morinin D	6.575	367.1492	[M+NH4]+	C20H24O5	Anisoles	---
1047	Monoolein	13.114	339.28818	[M+H-H2O]+	C21H40O4	Monoacylglycerols	---
1048	Monoethyl phthalate	10.746	193.0482	[M-H]-	C10H10O4	Benzoic acid esters	---
1049	Monoelaidin	13.382	339.28812	[M+H-H2O]+	C21H40O4	Monoacylglycerols	---
1050	Mono-carboxy-isononyl phthalate	9.605	335.14725	[M-H]-	C18H24O6	---	---
1051	Monactin	8.225	768.49176	[M+Na]+	C41H66O12	Macrolides and analogues	---
1052	Monactin	13.462	768.49261	[M+H]+	C41H66O12	Macrolides and analogues	---
1053	Moandaensine C	11.659	629.34705	[M+Na]+	C40H45N4O3	---	---
1054	Mmv688776	2.818	314.10684	[M+Na]+	C17H16ClN3O	Phenylpyrazoles	---
1055	Mmv688514	7.849	264.11139	[M+H]+	C16H13N3O	Benzene and substituted derivatives	---

1056	Mmv688509	6.195	456.20645	[M+NH4] ²⁺	C28H26FN3O2	Phenylpyrroles	---
1057	Mmv688509	2.989	456.20642	[M+H] ⁺	C28H26FN3O2	Phenylpyrroles	---
1058	Mmv688509	3.126	456.20639	[M+H- H2O] ⁺	C28H26FN3O2	Phenylpyrroles	---
1059	Mmv688417	1.108	327.11227	[M+H] ⁺	C16H15ClN6	Pyrazolopyrimidines	---
1060	Mmv688372	8.556	400.15775	[M-H] ⁻	C23H20FN5O	Phenylpyridines	---
1061	Mmv687138	6.537	340.09857	[M+H] ⁺	C19H17NO3S	Benzamides	---
1062	Mmv676476	12.277	379.15347	[M-H] ⁻	C23H24O5	Coumarins and derivatives	---
1063	Mmv676182	8.226	373.21133	[M+H] ²⁺	C22H24N6	Naphthalenes	---
1064	Mmv676008	5.628	442.1022	[M+H] ²⁺	C24H15N3O6	Aromatic anilides	---
1065	Mmv675998	6.375	336.15381	[M+H] ⁺	C17H17N7O	Phenyltriazoles	---
1066	Mmv595321	9.676	457.16669	[M-H] ⁻	C21H26N6O4S	Benzenesulfonamide s	---
1067	Mmv011229	7.601	293.0983	[M+H] ⁺	C14H11F3N4	Trifluoromethylbenz enes	---
1068	Mls002695962	10.984	425.13336	[M+H] ⁺	C22H20N2O7	Camptothecins	---
1069	Mls001148620	7.946	318.16385	[M+H] ²⁺	C19H24ClNO	Diphenylmethanes	---
1070	Mls001148620	6.596	318.16519	[M+H] ⁺	C19H24ClNO	Diphenylmethanes	---
1071	Mls001076763	2.123	344.11642	[M+NH4] ⁺	C18H18ClN3O2	Cytisine and derivatives	---
1072	Mls001076763	2.544	344.11646	[M+H] ⁺	C18H18ClN3O2	Cytisine and derivatives	---
1073	Mls001075064	1.888	354.1424	[M+H] ⁺	C19H19N3O4	Cytisine and derivatives	---
1074	Mls000574971	9.667	309.08487	[M+H] ⁺	C17H12N2O4	Indolonaphthyridine alkaloids	---
1075	Miroprofen	7.762	267.11136	[M+NH4] ⁺	C16H14N2O2	Azoles	---
1076	Microcolin K	8.303	784.48291	[M+H] ⁺	C40H67N5O9	Hybrid peptides	---
1077	MGMG(18:2/0:0)	12.229	561.32532	[M-H2O-H] ⁻	C27H48O9	Glycerolipids	---
1078	Mevinic Acid	12.046	391.2438	[M+Na] ⁺	C23H36O6	Medium-chain hydroxy acids and derivatives	---
1079	Mevalonolactone methylpropyl /-(4- chlorophenyl)-2-methyl- 5-oxo-4-(3,4,5-	2.595	148.09637	[M+H] ⁺	C6H10O3	Delta valerolactones	---
1080	trimethoxyphenyl)-1,4, 6,7,8- pentahydroquinoline-3- methylpropyl /-(4- chlorophenyl)-2-methyl- 5-oxo-4-(3,4,5-	6.925	538.20111	[M-H] ⁻	C30H34ClNO6	Phenylquinolines	---
1081	trimethoxyphenyl)-1,4, 6,7,8- pentahydroquinoline-3- carboxylate	6.923	540.21576	[M+H] ⁺	C30H34ClNO6	Phenylquinolines	---
1082	Methylpedicin	11.385	343.11575	[2M-H] ⁻	C19H20O6	2'-Hydroxychalcones	---
1083	Methylmalondialdehyde	3.47	85.02724	[M-H] ⁻	C4H6O2	Organooxygen compounds	---
1084	Methylglutaric acid	1.637	147.06471	[M+H- H2O] ⁺	C6H10O4	Branched fatty acids	---
1085	Methylglutaric acid methylethyl 2-amino-4- (4-fluorophenyl)-6-	2.512	147.06467	[M+H] ⁺	C6H10O4	Branched fatty acids	---
1086	(hydroxymethyl)-8-oxo- 4H-pyrano[3,2-b]pyran- 3-carboxylate	6.438	374.10706	[M-H] ⁻	C19H18FNO6	Pyranones and derivatives	---

1087	methylethyl 2-amino-4-(4-fluorophenyl)-6-(hydroxymethyl)-8-oxo-4H-pyrano[3,2-b]pyran-3-carboxylate	2.55	393.14828	[M+H] ⁺	C19H18FNO6	Pyranones and derivatives	---
1088	Methylatropine	9.806	327.17816	[M+H] ⁺	C18H26NO3 ⁺	Tropane alkaloids	---
1089	Methyl syringate	1.271	235.05568	[M+Na] ⁺	C10H12O5	Hydroxybenzoic acid derivatives	---
1090	Methyl syringate	1.275	213.07407	[M+NH4] ⁺	C10H12O5	Hydroxybenzoic acid derivatives	---
1091	Methyl neopentyl phthalic acid	9.799	249.10918	[M-H] ⁻	C14H18O4	Benzene and substituted derivatives	---
1092	Methyl 7-Deshydroxypyrogallin-4-Carboxylate	1.188	223.09334	[M+H] ⁺	C13H10O6	Tropolones	---
1093	methyl 4,5,6-trihydroxy-3-(3-methoxy-3-oxoprop-1-en-2-yl)oxycyclohexene-1-carboxylate	6.281	306.11868	[M+H] ⁺	C12H16O8	Beta hydroxy acids and derivatives	---
1094	methyl 4,5,6-trihydroxy-3-(3-methoxy-3-oxoprop-1-en-2-yl)oxycyclohexene-1-carboxylate	2.078	306.11737	[M+H-H2O] ⁺	C12H16O8	Beta hydroxy acids and derivatives	---
1095	Methyl 4-(6,8-dihydroxy-3-methyl-1-oxoisochromen-7-yl)-2,4-dimethoxybutanoate	6.702	370.14847	[M+H-H2O] ⁺	C17H20O8	Isocoumarins and derivatives	---
1096	Methyl 4-(6,8-dihydroxy-3-methyl-1-oxoisochromen-7-yl)-2,4-dimethoxybutanoate	6.911	370.14822	[M+H] ⁺	C17H20O8	Isocoumarins and derivatives	---
1097	methyl 4-(5-chloro-4-hydroxy-3-methoxyphenyl)-2-methyl-5-oxo-1,4,6,7,8-pentahydroquinoline-3-carboxylate	0.888	376.09985	[M-H] ⁻	C19H20ClNO5	Phenylquinolines	---
1098	methyl 4-(4-methoxyphenyl)-2,7,7-trimethyl-5-oxo-1,4,6,7,8-pentahydroquinoline-3-carboxylate	8.077	354.17404	[M-H2O-H] ⁻	C21H25NO4	Phenylquinolines	---
1099	Methyl 3-phenyl-2-(phenylformamido)propanoate	9.222	282.11115	[M-H] ⁻	C17H17NO3	Amino acids and derivatives	---
1100	Methyl 3-[3,4-dihydroxy-2-(3-methylbut-2-enyl)phenyl]-2-[[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]methyl]-4-methoxy-5-oxofuran-2-carboxylate	8.705	521.22076	[M-H] ⁻	C30H34O8	Catechols	---
1101	Methyl 3,4,5-trihydroxycyclohexene-1-carboxylate	4.214	230.10106	[M+H] ⁺	C8H12O5	Cyclic alcohols and derivatives	---

1102	Methyl 3,4,5-trihydroxycyclohexene-1-carboxylate	6.181	230.10104	[M+CH3OH+H] ⁺	C8H12O5	Cyclic alcohols and derivatives	---
1103	Methyl 3-(3,4-dihydroxy-5-phenyloxolan-2-yl)-3-hydroxypropanoate	4.545	300.14267	[M+H] ⁺	C14H18O6	Glycosyl compounds	---
1104	Methyl 3-(3,4-dihydroxy-5-phenyloxolan-2-yl)-3-hydroxypropanoate	6.542	300.14261	[M+2H] ²⁺	C14H18O6	Glycosyl compounds	---
1105	Methyl 3-(3,4-dihydroxy-5-phenyloxolan-2-yl)-3-hydroxypropanoate	3.927	300.14258	[M+Na] ⁺	C14H18O6	Glycosyl compounds	---
1106	Methyl 3-(3-(2,5-dihydroxy-2,2-dimethyl-1-oxo-3aH-imidazo[1,2-a]indol-4-yl)-2-(4-oxoquinazolin-3-yl)propanoate	0.928	509.16864	[M-H] ⁻	C24H24N4O6	Amino acids and derivatives	---
1107	Methyl 2-ethyl-4-[(3R,4R,5S)-5-hydroxy-4,5-dimethyl-2-oxooxolan-3-yl]-2-methyl-3-oxobutanoate	6.159	616.25403	[M+H] ⁺	C35H37NO9	Coumarans	---
1108	Methyl 2-furoate	7.383	125.0222	[M-H] ⁻	C6H6O3	Furans	---
1109	Methyl 2-ethyl-4-[(3R,4R,5S)-5-hydroxy-4,5-dimethyl-2-oxooxolan-3-yl]-2-methyl-3-oxobutanoate	11.135	309.12885	[M+Na] ⁺	C14H22O6	Annonaceous acetogenins	---
1110	Methyl 2-ethyl-4-[(3R,4R,5S)-5-hydroxy-4,5-dimethyl-2-oxooxolan-3-yl]-2-methyl-3-oxobutanoate	7.965	287.14755	[M+CH3OH+H] ⁺	C14H22O6	Annonaceous acetogenins	---
1111	Methyl 2-ethyl-4-[(3R,4R,5S)-5-hydroxy-4,5-dimethyl-2-oxooxolan-3-yl]-2-methyl-3-oxobutanoate	8.341	285.13281	[M-H] ⁻	C14H22O6	Annonaceous acetogenins	---
1112	Methyl 2-[(4-hydroxyphenyl)methylene]-3-oxobenzo[b]furan-5-carboxylate	1.07	295.06421	[M-H] ⁻	C17H12O5	Aurone flavonoids	---
1113	Methyl 2-(4a,6,10a-trihydroxy-1-methyl-5,10-dioxo-3,4-dihydro-1H-benzo[g]isochromen-3-yl)acetate	6.399	368.13208	[M+H-H2O] ⁺	C17H18O8	Naphthopyranones	---
1114	Methyl 2-(4a,6,10a-trihydroxy-1-methyl-5,10-dioxo-3,4-dihydro-1H-benzo[g]isochromen-3-yl)acetate	6.332	368.13205	[M+H] ⁺	C17H18O8	Naphthopyranones	---

1115	methyl 2-(3-methyl-2,6-dioxo-1,3,7-trihydropurin-7-yl)acetate	2.168	261.05951	[M+H-H ₂ O] ⁺	C ₉ H ₁₀ N ₄ O ₄	Amino acids and derivatives	---
1116	methyl 2-(3-methyl-2,6-dioxo-1,3,7-trihydropurin-7-yl)acetate	2.802	261.05945	[M+H] ⁺	C ₉ H ₁₀ N ₄ O ₄	Amino acids and derivatives	---
1117	methyl 2-(3-hydroxy-5-methoxy-9-methyl-8,13-dioxatricyclo[7.3.1.0 ^{2,7}]trideca-2,4,6-triene-4-carbonyl)-3,5-dimethoxybenzoate	1.557	457.15213	[M-H] ⁻	C ₂₄ H ₂₆ O ₉	Benzophenones	---
1118	Methyl 2-(1,3,5-trihydroxy-4a-methyl-8-oxodecahydro-2-naphthalenyl)acrylate	9.06	299.14505	[M+H] ⁺	C ₁₅ H ₂₂ O ₆	Carboxylic acid esters	---
1119	methyl 19-hydroxy-14,18-dimethyl-12-azahexacyclo[10.6.1.1.1.0 ^{2,7} .0 ^{3,8} .0 ^{4,9} .0 ^{5,10} .0 ^{6,11} .0 ^{12,13}]icosa-3,7(20)-diene-3-carboxylate	6.34	392.22046	[M+H] ²⁺	C ₂₃ H ₃₁ NO ₃	Azaspirodecane derivatives	---
1120	methyl 1-[2-(4-fluorophenoxy)ethyl]-5-hydroxy-2-methylindole-3-carboxylate	6.327	388.12225	[M-H] ⁻	C ₁₉ H ₁₈ FN ₂ O ₄	Indolecarboxylic acids and derivatives	---
1121	Methyl 1,4-bis(beta-D-glucopyranosyloxy)-3-(3-methyl-2-buten-1-yl)-2-naphthoate	9.08	655.22412	[M-H] ⁻	C ₂₉ H ₃₈ O ₁₄	Glycosyl compounds	---
1122	methyl (Z)-5-[(1R,4aR,8aR)-5,5,8a-trimethyl-2-methylidene-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl]-3-(acetyloxymethyl)pent-2-enoate	13.451	399.24557	[M+Na] ⁺	C ₂₃ H ₃₆ O ₄	Diterpenoids	---
1123	methyl (Z)-5-[(1R,4aR,8aR)-5,5,8a-trimethyl-2-methylidene-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl]-3-(acetyloxymethyl)pent-2-enoate	8.255	415.22156	[M+H] ²⁺	C ₂₃ H ₃₆ O ₄	Diterpenoids	---
1124	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	7.298	472.27371	[M+NH ₄] ⁺	C ₂₅ H ₃₉ NO ₆	Isoindolones	---

1125	Methyl (2E,3E,5E,7E,9E)-2- Ethylidene-11-[(1R,5R)- 4-Hydroxy-4-(2- Hydroxyethyl)-2-Oxo-6- Oxa-3- Azabicyclo[3.1.0]Hexan- 1-Yl]-4,10-Dimethyl-11- Oxoundeca-3,5,7,9- Methyl (1R,4aS,9S,10S)- 10-Acetyloxy-5,9- Dihydroxy-1,4a- Dimethyl-2-Oxo-7- Propan-2-Yl-10,10a- Dihydro-9H- Phenanthrene-1- Carboxylate	0.912	462.18063	[M-H]-	C22H27NO7	Fatty acid esters	---
1126		9.472	415.17429	[M-H]-	C23H28O7	1-hydroxysteroids	---
1127	Methoxytyrosine	7.575	210.07491	[M-H]-	C10H13NO4	Tyrosine and derivatives	---
1128	Methoxybenzenediol + O-Hex	7.834	347.10059	[M-H]-	C13H18O8	Phenolic glycosides	---
1129	Methoxyacetic acid	6.343	89.02228	[M-H]-	C3H6O3	Carboxylic acids and derivatives	---
1130	Metergoline	8.255	426.21188	[M+Na]+	C25H29N3O2	Indoloquinolines	---
1131	Metergoline	8.255	404.23047	[M+2H]2+	C25H29N3O2	Indoloquinolines	---
1132	Meranzin hydrate	10.769	301.10519	[M+Na]+	C15H18O5	Coumarins and derivatives	---
1133	Meconine	10.767	195.06396	[M+H]+	C10H10O4	Phthalides	---
1134	Maytenin	8.959	421.27753	[M+Na]+	C28H36O3	Cyclic ketones	---
1135	Masitinib	7.406	250.11768	[M+H]+	C28H30N6OS	Aromatic anilides	---
1136	Masitinib	7.707	250.1178	[M+H- H2O]+	C28H30N6OS	Aromatic anilides	---
1137	Marindinin	10.242	233.11626	[M+H]+	C14H16O3	Kavalactones	---
1138	Marchantin E	6.4	471.18106	[M+H]+	C29H26O6	Lignans, neolignans and related compounds	---
1139	Malyngamide J	8.108	608.38043	[2M+H]+	C33H53NO9	Glycosyl compounds	---
1140	Maltoxazine	6.215	180.10098	[M+CH3OH +H]+	C10H13NO2	Pyrrolidines	---
1141	Maltitol	0.934	343.12207	[M-H]-	C12H24O11	Fatty acyl glycosides	---
1142	Maltitol	1.333	367.11935	[M+Na]+	C12H24O11	Fatty acyl glycosides	---
1143	Lyngbyapeptin A	8.846	720.37946	[M+2H]2+	C37H55N5O6S	Amino acids and derivatives	---
1144	LPS(19:0)	8.215	540.32843	[M+2H]2+	C25H50NO9P	Lysophosphatidylseri nes	---
1145	LPS(19:0)	11.591	538.31067	[M-H]-	C25H50NO9P	Lysophosphatidylseri nes	---
1146	LPI(18:2)	11.502	595.2851	[M-H]-	C27H49O12P	Glycerophospholipid s	---
1147	LPI(18:2)	11.346	595.28485	[2M-H]-	C27H49O12P	Glycerophospholipid s	---
1148	LPI(18:1)	11.197	597.30792	[M-H]-	C27H51O12P	Lysophosphatidylino sitols	---
1149	LPI(18:0)	11.049	599.32416	[M-H2O-H]-	C27H53O12P	Lysophosphatidylino sitols	---
1150	LPI(16:0)	11.814	571.2854	[M-H]-	C25H49O12P	Glycerophospholipid s	---
1151	LPG(18:2)	12.372	507.26968	[M-H]-	C24H45O9P	Glycerophospholipid s	---

1152	LPG(18:1)	13.393	509.28558	[M-H]-	C24H47O9P	Lysophosphatidylglycerols	---
1153	LPG(18:0)	12.261	511.30026	[M-H]-	C24H49O9P	Glycerophospholipids	---
1154	LPG(16:0)	13.306	483.26904	[M-H]-	C22H45O9P	Glycerophospholipids	---
1155	LPE(22:6)	11.49	524.27521	[M-H]-	C27H44NO7P	Lysophosphatidylethanolamines	---
1156	LPE(18:1)	12.166	478.29047	[M-H]-	C23H46NO7P	Lysophosphatidylethanolamines	---
1157	LPE(18:0)	11.188	480.3053	[M-H]-	C23H48NO7P	Glycerophospholipids	---
1158	LPE(16:0)	11.935	452.27603	[M-H]-	C21H44NO7P	Glycerophospholipids	---
1159	LPE(16:0)	11.922	476.27301	[M+Na]+	C21H44NO7P	Lysophosphatidylethanolamines	---
1160	LPE(16:0)	11.924	436.28024	[M+H-H2O]+	C21H44NO7P	Lysophosphatidylethanolamines	---
1161	LPE 18:2	11.594	476.27496	[M-H]-	C23H44NO7P	LysoPE	---
1162	LPC(22:6)	11.687	568.33539	[M+CH3OH+H]+	C30H50NO7P	Glycerophospholipids	---
1163	LPC(20:4)	11.736	544.33862	[M+H]+	C28H50NO7P	Glycerophospholipids	---
1164	LPC(19:0)-D5	12.438	576.34515	[M+2H]2+	C27H51D5NO7P	Lysophosphatidylcholines	---
1165	LPC(18:3)	11.868	518.32318	[2M+H]+	C26H48NO7P	Lysophosphatidylcholines	---
1166	LPC(18:2)	11.776	564.32648	[M+HCOO]-	C26H50NO7P	Lysophosphatidylcholines	---
1167	LPC(18:2)	11.923	520.33783	[M+H]+	C26H50NO7P	Lysophosphatidylcholines	---
1168	LPC(18:0)	11.963	524.3689	[M+H]+	C26H54NO7P	Lysophosphatidylcholines	---
1169	LPC(16:1)	11.577	494.3219	[M+H-H2O]+	C24H48NO7P	Glycerophospholipids	---
1170	LPC(16:0)	12.335	496.33731	[M+CH3OH+H]+	C24H50NO7P	Glycerophospholipids	---
1171	LPC(15:0)	10.114	540.32709	[M-H]-	C23H48NO7P	Lysophosphatidylcholines	---
1172	LPC(14:0)	11.284	468.30576	[M+H]+	C22H46NO7P	Lysophosphatidylcholines	---
1173	LPC 18:3	11.39	562.31104	[M+FA-H]-	C26H48NO7P	LysoPC	---
1174	LPC 18:2	11.96	564.32697	[M-H]-	C35H43N5O2	LysoPC	---
1175	Lobetyolin	8.823	441.17279	[2M-H]-	C20H28O8	---	---
1176	Lobarin	7.833	473.18475	[M-H]-	C25H30O9	Diarylethers	---
1177	Lividic acid	3.225	518.24207	[M+H]+	C27H32O9	Deposides and deposidones	---
1178	Lirioresinol A	6.341	441.1517	[M+H]+	C22H26O8	Furanoid lignans	---
1179	Liquiritin apioside	4.346	549.16217	[M-H]-	C26H30O13	Flavonoid O-glycosides	---
1180	Liquiritin apioside	6.423	549.16248	[M-H2O-H]-	C26H30O13	Flavonoid O-glycosides	---
1181	Lignocaine N-oxide	10.075	251.17809	[M+H]+	C14H22N2O2	Amino acids and derivatives	---
1182	Licochalcone C	7.093	337.14789	[M-H]-	C21H22O4	Retrochalcones	---
1183	Licoagroside B	11.338	431.18173	[M-H]-	C18H24O12	Saccharolipids	---
1184	Leu-Ser	6.33	201.12245	[M+NH4]+	C9H18N2O4	Peptides	---
1185	Leupeptin Pr-LL	13.227	441.31647	[M+Na]+	C21H40N6O4	Peptides	---
1186	Leu-Ile-Arg	11.917	401.28873	[M+H]+	C18H36N6O4	Peptides	---
1187	Leu-Ile-Arg	12.335	401.28473	[M+Na]+	C18H36N6O4	Peptides	---
1188	Leucylvaline	6.492	229.15384	[M-H]-	C11H22N2O3	Peptides	---
1189	Leucyl-Isoleucine	7.019	243.16916	[M-H]-	C12H24N2O3	Carboxylic acids and derivatives	---
1190	L-DOPA 3'-glucoside	6.651	358.11179	[M-H]-	C15H21NO9	Carboxylic acids and derivatives	---

1191	Lauryldiethanolamine	12.176	274.27319	[M+H] ⁺	C16H35NO2	Alkanolamines	---
1192	Lauryl Ether Sulphate	12.225	309.17181	[M-H] ⁻	C14H30O5S	Sulfuric acid monoesters	---
1193	Lauryl Diethanolamide	11.555	288.25156	[M+H] ⁺	C16H33NO3	N-acyl amines	---
1194	Lauramine oxide	10.315	230.24678	[M+H] ⁺	C14H31NO	Long-chain alkyl amine oxides	---
1195	Lapiferin	8.097	377.23209	[M+H] ²⁺	C22H34O6	Fatty acid esters	---
1196	Laminaripentaose	5.575	851.27045	[M+H] ⁺	C30H52O26	Oligosaccharides	---
1197	Lagochilin	8.226	379.24615	[M+2H] ²⁺	C20H36O5	Diterpenoids	---
1198	Lactoquinomycin A	2.994	458.18344	[M+CH3OH +H] ⁺	C24H27NO8	Benzoisochromanequ inones	---
1199	Lactoquinomycin A	1.482	458.18384	[M+H] ⁺	C24H27NO8	Benzoisochromanequ inones	---
1200	Lactobionic acid	12.263	357.14496	[M+H] ⁺	C12H22O12	Fatty acyl glycosides	---
1201	Lactiflorin	2.612	461.14847	[M-H] ⁻	C23H26O10	Benzoic acid esters	---
1202	Lacidipine	11.44	454.22327	[M-H] ⁻	C26H33NO6	Cinnamic acid esters	---
1203	L,L-Cyclo(prolylalanyl)	6.409	169.09685	[M+NH4] ⁺	C8H12N2O2	Carboxylic acids and derivatives	---
1204	Kinetin Riboside	6.235	346.11197	[M-H] ⁻	C15H17N5O5	Purine nucleosides	---
1205	Khivorine	7.162	587.28394	[M+H] ⁺	C32H42O10	Limonoids	---
1206	Khivorine	7.166	585.26764	[M-H] ⁻	C32H42O10	Limonoids	---
1207	Khayanthone	10.466	569.27661	[M-H] ⁻	C32H42O9	Limonoids	---
1208	Kalopanaxsaponin H	10.376	913.51154	[M+H] ⁺	C47H76O17	Triterpenoids	---
1209	JWH-015	6.973	328.17377	[M+H] ⁺	C23H21NO	Naphthoylindoles	---
1210	Junosine	1.351	326.14236	[M+H] ⁺	C19H19NO4	Quinolines and derivatives	---
1211	Jasmine ketolactone	10.12	207.10057	[M-H] ⁻	C12H16O3	Oxocins	---
1212	Ivermectin	8.705	892.53723	[M+2H] ²⁺	C48H74O14	Milbemycins	---
1213	Isovalerylglutamic acid	7.868	230.10104	[M-H] ⁻	C10H17NO5	Carboxylic acids and derivatives	---
1214	isosakuranetin-7-O- neohesperidoside	1.421	593.18964	[M-H] ⁻	C28H34O14	Flavonoid-7-O- glycosides	---
1215	Isolongifolol	13.147	240.23055	[M+H] ⁺	C15H26O	Sesquiterpenoids	---
1216	Isoleucylvaline	6.545	231.1698	[M+CH3OH +H] ⁺	C11H22N2O3	Peptides	---
1217	Isoleucylvaline	7.662	231.16975	[M+H] ⁺	C11H22N2O3	Peptides	---
1218	Isoleucyl-Prolyl- Arginine	12.233	385.25476	[M+CH3OH +H] ⁺	C17H32N6O4	Peptides	---
1219	Isoindoline	6.308	120.08067	[M+NH4] ⁺	C8H9N	Isoindoles and derivatives	---
1220	Isoindoline	7.001	120.08061	[M+H] ⁺	C8H9N	Isoindoles and derivatives	---
1221	Isoindolin-1-one	7.121	134.05974	[M+H] ⁺	C8H7NO	Isoindoles and derivatives	---
1222	Isoflavone base + 1O, 1MeO, O-Pen-Hex	6.598	561.16168	[M-H2O-H] ⁻	C27H30O13	Isoflavone O- glycosides	---
1223	Isoflavone base + 1O, 1MeO, O-Hex-Hex	1.323	637.18018	[M-H] ⁻	C28H32O14	Isoflavone O- glycosides	---
1224	Isobutyryl-Carnitine	6.318	232.15289	[M+H] ⁺	C11H21NO4	Acyl carnitines	---
1225	Isobavachin	6.558	323.13333	[M-H] ⁻	C20H20O4	8-prenylated flavans	---
1226	Isbufylline	4.789	237.13376	[M+H] ⁺	C11H16N4O2	Xanthines	---
1227	iodinated analogue of makaluvone	11.332	329.00278	[M+H] ⁺	C11H10IN2O2	Pyrrolo[4,3,2- de]quinolines	---
1228	Indole + 1O, 1carboxy, O-Hex	7.672	338.08646	[M-H] ⁻	C15H17NO8	Indole and derivatives	---
1229	Indigo	9.666	263.08038	[M+H] ⁺	C16H10N2O2	Indolines	---
1230	Indane	11.459	119.08517	[M+H] ⁺	C9H10	Indanes	---
1231	Inaequalisine_A	8.319	443.27057	[M+H] ²⁺	C29H35N2O2	---	---
1232	Illicicolin A	6.486	391.20554	[2M+H] ⁺	C23H31ClO3	Sesquiterpenoids	---
1233	Illicicolin A	9.661	389.18481	[M-H] ⁻	C23H31ClO3	Sesquiterpenoids	---
1234	Icos-2-enoic acid	13.274	309.27737	[M-H] ⁻	C20H38O2	Fatty Acyls	---
1235	Icos-19-Ene-1,2,4-Triol	10.989	346.32941	[M+H] ⁺	C20H40O3	Long-chain fatty alcohols	---

1236	Icos-19-Ene-1,2,4-Triol	11.607	346.32932	[M+H-H ₂ O] ⁺	C ₂₀ H ₄₀ O ₃	Long-chain fatty alcohols	---
1237	Hypothallin	0.901	517.23322	[2M-H] ⁻	C ₂₉ H ₃₂ N ₂ O ₄	Amino acids and derivatives	---
1238	Hydroxysuberic acid	7.957	189.07463	[M-H] ⁻	C ₈ H ₁₄ O ₅	Dicarboxy fatty acids	---
1239	Hydroxycotinine	6.482	193.0966	[M+H] ⁺	C ₁₀ H ₁₂ N ₂ O ₂	Pyrrolidinylpyridines	---
1240	Hydratoperidin	8.747	648.36328	[M+2H] ²⁺	C ₃₉ H ₅₂ O ₈	Terpene lactones	---
1241	Huperzine A	7.006	265.12787	[M+Na] ⁺	C ₁₅ H ₁₈ N ₂ O	Quinolones and derivatives	---
1242	Hovenidulcioside A1	8.665	853.46271	[M+2H] ²⁺	C ₄₄ H ₆₈ O ₁₆	Diterpene glycosides	---
1243	Homocysteine thiolactone	1.11	118.03461	[M+H] ⁺	C ₄ H ₇ NOS	Amino acids and derivatives	---
1244	Histidyltyrosine	8.343	317.12152	[M-H] ⁻	C ₁₅ H ₁₈ N ₄ O ₄	Peptides	---
1245	Histidylproline	4.241	235.11812	[M+H-H ₂ O] ⁺	C ₁₁ H ₁₆ N ₄ O ₃	Peptides	---
1246	Histidylproline	6.476	253.12808	[M+Na] ⁺	C ₁₁ H ₁₆ N ₄ O ₃	Peptides	---
1247	Histamine dihydrochloride	1.115	221.99214	[M+2H] ²⁺	C ₅ H ₁₁ Cl ₂ N ₃	Primary amines	---
1248	Hirsutenone	1.319	327.12473	[M+H-H ₂ O] ⁺	C ₁₉ H ₂₀ O ₅	Linear diarylheptanoids	---
1249	Hexyl dodecanoate	13.224	283.26276	[M-H] ⁻	C ₁₈ H ₃₆ O ₂	Fatty Acyls	---
1250	Hexyl decanoate	12.522	255.231	[M-H] ⁻	C ₁₆ H ₃₂ O ₂	Fatty Acyls	---
1251	Hexosyl LPE 16:0	11.521	614.32611	[M-H] ⁻	C ₂₇ H ₅₄ NO ₁₂ P	LysoHexPE	---
1252	Hexopyranoside, 1-[6-[dodecahydro-5-hydroxy-3-(1-hydroxy-1-methylethyl)-6a,9b-dimethylindeno[5,4-b]pyran-7-yl]-3,4,4a,7,8,8a-hexahydro-4a-methyl-2H-1-benzopyran-2-yl]-1-methylethyl 2-Hexopyranose, 1-O-[(3beta,5xi,9xi,18xi)-3-[(3-O-hexopyranosylhexopyranuronosyl)oxy]-28-oxocolean-12-en-28-yl]-	8.52	716.43073	[M+2H] ²⁺	C ₃₈ H ₆₃ NO ₁₀	Triterpenoids	---
1253	Hexopyranosylhexopyranuronosyl)-28-oxocolean-12-en-28-yl]-	9.466	955.48584	[M-H] ⁻	C ₄₈ H ₇₆ O ₁₉	Triterpene glycosides	---
1254	Hexadecanamide	10.315	256.26224	[M+H] ⁺	C ₁₆ H ₃₃ NO	Fatty amides	---
1255	HEPES	6.196	239.10185	[M+H] ⁺	C ₈ H ₁₈ N ₂ O ₄ S	N-alkylpiperazines	---
1256	Hederoside F	10.45	819.44678	[M+H] ⁺	C ₄₂ H ₆₈ O ₁₄	Triterpene glycosides	---
1257	Harmanine	7.469	199.08546	[M+H] ⁺	C ₁₂ H ₁₀ N ₂ O	Organooxygen compounds	---
1258	Haploside C	2.009	695.18396	[M-H] ⁻	C ₃₁ H ₃₆ O ₁₈	Flavonoid O-glycosides	---
1259	Haematoporphyrin	13.013	597.35663	[M+H] ⁺	C ₃₄ H ₃₈ N ₄ O ₆	Porphyrins	---
1260	h_62_furazabol-m	6.651	369.21109	[2M+H] ⁺	C ₂₀ H ₃₀ N ₂ O ₃	Estrane steroids	---
1261	Gymnemic Acid II	8.644	831.45105	[M+2H] ²⁺	C ₄₃ H ₆₈ O ₁₄	Triterpene glycosides	---
1262	Grossamide or its isomer (Not validated)	9.482	623.23364	[M-H] ⁻	C ₃₆ H ₃₆ N ₂ O ₈	Arylbenzofuran flavonoids	---
1263	Graveolide	10.06	266.17096	[M+NH ₄] ⁺	C ₁₅ H ₂₀ O ₃	Sesquiterpene lactones	---
1264	Gramicidin	12.753	941.54303	[M+H] ⁺	C ₉₉ H ₁₄₀ N ₂₀ O ₁₇	Peptides	---
1265	Goniomedine A	10.819	649.37225	[M+Na] ⁺	C ₄₀ H ₄₉ N ₄ O ₄	Pleiocarpaman alkaloids	---
1266	Glycycoumarin	6.274	367.12201	[M-H] ⁻	C ₂₁ H ₂₀ O ₆	Hydroxyisoflavonoids	---

1267	Glutamyltyrosine	7.6	309.10489	[M-H]-	C14H18N2O6	Tyrosine and derivatives	---
1268	Glutamyltryptophan	7.662	332.12338	[M-H]-	C16H19N3O5	Peptides	---
1269	Glutamylthreonine	9.777	249.1088	[M+Na]+	C9H16N2O6	Peptides	---
1270	Glutamyl-S-(C3H7S)-Cysteinylglycine	6.488	380.09897	[M-H]-	C13H23N3O6S2	Peptides	---
1271	Glutamylphenylalanine	6.926	295.12781	[M+H]+	C14H18N2O5	Amino acids and derivatives	---
1272	Glutamylleucine	6.661	259.12781	[M-H]-	C11H20N2O5	Peptides	---
1273	Glutamylleucine	6.687	261.14355	[M+H]+	C11H20N2O5	Peptides	---
1274	Glutaminyl-Isoleucyl-Lysine	7.183	388.25223	[M+NH4]+	C17H33N5O5	Peptides	---
1275	Glutaminylarginine	10.341	301.16376	[M-H]-	C11H22N6O4	Carboxylic acids and derivatives	---
1276	Glutamic acid, 1-[5'-hydroxy-2,6'-dimethyl-5-(1-methylethenyl)spiro[cyclopentane-1,3'-[7]oxabicyclo[4.1.0]heptan-2'-yl] ester	10.98	404.20532	[M+NH4]+	C20H31NO6	Amino acids and derivatives	---
1277	Glu-CA	7.696	520.32965	[M+NH4]+	C29H47NO8	ClassyFy Status	---
1278	Glomellic acid	6.283	490.20993	[M+H]+	C25H28O9	Depsides and depsidones	---
1279	Glochidone putative	10.38	423.35983	[M+H]+	C30H46O	Triterpenoids	---
1280	Gitoxigenin Diacetate	13.345	492.29556	[M+2H]2+	C27H38O7	Cardenolides and derivatives	---
1281	Germerine	8.487	694.41711	[M+2H]2+	C37H59NO11	Cerveratrum-type alkaloids	---
1282	Germanasim E	8.555	681.16266	[2M-H]-	C29H32O16	Isoflavonoid O-glycosides	---
1283	Gentiatibetine	6.296	166.08559	[M+NH4]+	C9H11NO2	Pyranopyridines	---
1284	Gentiatibetine	7.569	166.08553	[M+H-H2O]+	C9H11NO2	Pyranopyridines	---
1285	Gentiatibetine	7.027	166.08553	[M+H]+	C9H11NO2	Pyranopyridines	---
1286	Gelomulide N	11.198	415.20956	[M-H2O+H]+	C24H32O7	Naphthofurans	---
1287	Garcinolic Acid	7.891	669.30414	[M+H]+	C38H46O9	Dibenzopyrans	---
1288	gamma-Glutamylmethionine	6.274	277.08411	[M-H]-	C10H18N2O5S	Peptides	---
1289	gamma-Glutamylmethionine	6.295	279.09964	[M+H]+	C10H18N2O5S	Peptides	---
1290	gamma-Glutamylhistidine	6.73	283.10138	[M-H]2-	C11H16N4O5	Peptides	---
1291	gamma-Glutamylhistidine	1.556	283.10123	[M-H]-	C11H16N4O5	Peptides	---
1292	Gabexate	7.494	322.1749	[M+CH3OH+H]+	C16H23N3O4	Benzoic acid esters	---
1293	G(8-O-4)FA sulfate	6.227	469.07983	[2M-H]-	C20H22O11S	Lignols	---
1294	Furostane base -2H + O-Hex	10.092	639.37183	[M+HCOO]-	C33H54O9	Steroidal saponins	---
1295	Furostane base -1H2O -2H + 1O, O-Hex, O-PendHex	10.177	915.45496	[M-H]-	C44H70O17	Steroidal saponins	---
1296	Fumonisin A1	8.885	764.40247	[M+2H]2+	C36H61NO16	Fumonisin	---
1297	FT-sulfone; C6H9F3O4S	6.426	233.01088	[2M-H]-	C6H9F3O4S	PFSA	---
1298	Fridamycin A	5.779	485.14841	[M-H2O-H]-	C25H26O10	Anthraquinones	---
1299	Fridamycin A	3.657	485.14844	[M-H]-	C25H26O10	Anthraquinones	---
1300	Forsythoside B	1.476	755.23975	[M-H]-	C34H44O19	Oligosaccharides	---
1301	Formamide, N-[(1Z)-2-(4-methoxyphenyl)ethenyl]-	6.683	178.08582	[M+H]+	C10H11NO2	Phenol ethers	---

1302	Fluticasone propionate	8.945	523.17529	[M+Na] ⁺	C25H31F3O5S	Steroid esters	---
1303	Fluorocurarine chloride	2.853	343.16037	[M+CH3OH+H] ⁺	C20H23ClN2O	Strychnos alkaloids	---
1304	Flumethasone pivalate	6.343	495.25424	[M+CH3OH+H] ⁺	C27H36F2O6	Gluco/mineralocorticoids, progestogens and derivatives	---
1305	Flumequine	2.087	262.09079	[M+H] ⁺	C14H12FNO3	Quinoline carboxylic acids	---
1306	flufenacet ESA	6.156	274.05499	[M-H] ⁻	C11H14FNO4S	Anilides	---
1307	Flazine	9.673	307.07004	[M-H] ⁻	C17H12N2O4	Harmala alkaloids	---
1308	Flavonol base + 3O, O-Hex-Pen	1.181	415.1059	[M-H] ⁻	C21H20O9	Flavonol O-glycosides-Flavonol + 3O	---
1309	Flavanol base + 5O	0.899	305.06219	[M-H] ⁻	C15H14O7	Flavanol O-glycosides	---
1310	Fissinolide	9.228	511.23688	[M-H] ⁻	C29H36O8	Limonoids	---
1311	Feruloyl dehydrotyramine	8.456	312.12061	[M+H] ⁺	C18H17NO4	Hydroxycinnamic acids and derivatives	---
1312	Ferrudiol	6.189	506.18454	[M+H] ⁺	C28H24O8	Benzoic acid esters	---
1313	Fasciculic acid B	11.254	659.40979	[M+Na] ⁺	C36H60O9	Triterpenoids	---
1314	Famciclovir	6.2	322.14893	[M+H] ⁺	C14H19N5O4	Purines and purine derivatives	---
1315	FA 9:0 + 1O, sulfate	7.415	253.06943	[M-H] ⁻	C6H15N4O5P	Sulfate containing metabolites	---
1316	FA 18:2+4O	8.832	343.20953	[M-H] ⁻	C18H32O6	Oxidized fatty acids	---
1317	FA 18:2+3O	9.729	327.21533	[M-H] ⁻	C18H32O5	Oxidized fatty acids	---
1318	euphodendroidin W	7.264	587.28131	[M+H] ⁺	C30H44O10	Jatrophane and cyclojatrophane diterpenoids	---
1319	Ethylene dodecanedioate	11.97	257.17316	[M+H] ⁺	C14H24O4	Macrolides and analogues	---
1320	Ethyl chrysanthemate	10.311	214.17874	[M+H] ⁺	C12H20O2	Monocyclic monoterpenoids	---
1321	ethyl 7-(4-chlorophenyl)-2-methyl-5-oxo-4-(3,4,5-trimethoxyphenyl)-1,4,6,7,8-pentahydroquinoline-3-carboxylate	4.129	534.16394	[M+Na] ⁺	C28H30ClNO6	Phenylquinolines	---
1322	ethyl 7-(4-chlorophenyl)-2-methyl-5-oxo-4-(3,4,5-trimethoxyphenyl)-1,4,6,7,8-pentahydroquinoline-3-carboxylate	3.904	534.16406	[M+NH4] ⁺	C28H30ClNO6	Phenylquinolines	---
1323	ethyl 7-(4-chlorophenyl)-2-methyl-5-oxo-4-(3,4,5-trimethoxyphenyl)-1,4,6,7,8-pentahydroquinoline-3-carboxylate	4.806	534.16388	[M+H] ⁺	C28H30ClNO6	Phenylquinolines	---
1324	ethyl 5-hydroxy-2-methyl-1-[2-(4-propylphenoxy)ethyl]benzo[g]indole-3-carboxylate	1.302	432.22028	[M+CH3OH+H] ⁺	C27H29NO4	Indolecarboxylic acids and derivatives	---
1325	ethyl 3-indol-3-yl-2-(2,2,3,3-tetrafluoropropanoylamino)propanoate	6.282	395.0798	[M-H] ⁻	C16H16F4N2O3	Amino acids and derivatives	---

1326	ethyl 3-ethyl-4-hydroxy-2-oxohydroquinoline-6-carboxylate	9.748	260.091	[M-H]-	C14H15NO4	Hydroxyquinolines	---
1327	ethyl 3-{N-[2-(4-chlorophenyl)acetamino]carbamoyl}propanoate	1.112	313.09589	[M+NH4]+	C14H17ClN2O4	Phenylacetamides	---
1328	ethyl 2-{3-methyl-7-[(3-methylphenyl)methyl]-2,6-dioxo-1,3,7-trihydropurin-8-ylthio}acetate	14.001	387.11243	[M-H]-	C18H20N4O4S	Xanthines	---
1329	ethyl 2-[(3-methylphenyl)carbamoyl]aminolacetate	9.512	244.09576	[M+Na]+	C12H15NO3	Benzamides	---
1330	Ethyl 2,3-dioxo-1,4-dihydroquinoline-4-carboxylate	8.459	232.05913	[M-H]-	C12H11NO4	Hydroquinolones	---
1331	Ethyl 2,3-dioxo-1,4-dihydroquinoline-4-carboxylate	7.576	234.07275	[M+CH3OH+H]+	C12H11NO4	Hydroquinolones	---
1332	(adamantan-1-ylcarbamoyl)amino-3-indol-3-ylpropanoate	8.165	439.22214	[M-H]-	C24H30N2O3	Amino acids and derivatives	---
1333	ethyl 1-(2-ethylthioethyl)-5-hydroxy-2-methylbenzo[g]indole-3-carboxylate	8.558	356.13248	[M-H]-	C20H23NO3S	Indolecarboxylic acids and derivatives	---
1334	Ethyl (S)-3-hydroxybutyrate glucoside	6.921	293.12262	[M-H]-	C12H22O8	Fatty Acyls	---
1335	Ethenodeoxyadenosine	2.295	276.10693	[M+H]+	C12H13N5O3	Purines and purine derivatives	---
1336	Ethenodeoxyadenosine	2.603	276.10684	[M+H-H2O]+	C12H13N5O3	Purines and purine derivatives	---
1337	Estradiol 17-sulfate	6.532	351.12775	[M-H]-	C18H24O5S	Steroids and steroid derivatives	---
1338	Erythrin	9.69	413.17694	[M+Na]+	C25H26O4	Isoflavones	---
1339	Erucamide	13.146	338.3403	[M+H]+	C22H43NO	Fatty amides	---
1340	Eriodictyol 7,3'-Dimethyl Ether	10.027	315.08548	[M-H]-	C17H16O6	7-O-methylated flavonoids	---
1341	epsilon-Maleimido-lysine	4.344	242.11211	[M+CH3OH+H]+	C10H15N3O4	Carboxylic acids and derivatives	---
1342	Epigallocatechin gallate	8.903	353.15546	[M+Na]+	C16H26O7	Glycosyl compounds	---
1343	Epiandrosterone sulfate	6.853	369.17563	[M-H]-	C19H30O5S	Steroids and steroid derivatives	---
1344	Enrofloxacin	8.006	360.17429	[M+H]+	C19H22FN3O3	Quinoline carboxylic acids	---
1345	Eltoprazine	6.755	221.12718	[M+H]+	C12H16N2O2	Diazinanes	---
1346	Eltoprazine	6.468	221.12794	[M+CH3OH+H]+	C12H16N2O2	Diazinanes	---
1347	Eltoprazine	6.525	221.12726	[M+Na]+	C12H16N2O2	Diazinanes	---
1348	Ehretioside B	2.31	312.11023	[M+H]+	C14H17NO7	Glycosyl compounds	---
1349	Ehretioside B	6.647	350.06674	[M+2H]2+	C14H17NO7	Glycosyl compounds	---
1350	Echinoside B	6.222	467.13715	[M-H2O-H]-	C25H24O9	P-terphenyls	---
1351	Echimidine N-oxide	11.415	414.21219	[M+H]+	C20H31NO8	Alkaloids and derivatives	---
1352	Dronedarone	12.472	557.30603	[M+H]+	C31H44N2O5S	Ketones	---

1353	D-Pipecolic acid	1.15	130.08588	[M+H-H ₂ O] ⁺	C ₆ H ₁₁ NO ₂	Carboxylic acids and derivatives	---
1354	Donepezil	9.801	380.22546	[M+NH ₄] ⁺	C ₂₄ H ₂₉ NO ₃	N-benzylpiperidines	---
1355	Dodecyl sulfate	11.816	265.1463	[M-H] ⁻	C ₁₂ H ₂₆ O ₄ S	Sulfuric acid monoesters	---
1356	Disaccharides ((2Methyl-Hex)-Pen)	3.214	385.1333	[M-H] ⁻	C ₁₃ H ₂₄ O ₁₀	Sugars	---
1357	Diperocaine	1.355	434.18573	[M+H] ⁺	C ₂₂ H ₂₈ ClN ₃ O ₄	Phenylcarbamic acid esters	---
1358	Di-N-propylamine	13.329	102.12777	[M+H] ⁺	C ₆ H ₁₅ N	Organonitrogen compounds	---
1359	Dimethyl-3-hydroxypyrid-4-one	8.059	140.06979	[M+H] ⁺	C ₇ H ₉ NO ₂	Pyridines and derivatives	---
1360	Dimethyl myristamine dimethyl (2E,6E,11Z)-19-(2-amino-2-oxoethyl)-9,13-dihydroxy-8-methoxy-10,12,14-trimethyl-15-oxohenicosa-2,6,11-trienedionate	11.349	242.28285	[M+H] ⁺	C ₁₆ H ₃₅ N	Tertiary amines	---
1361		12.456	554.3324	[M+2H] ²⁺	C ₂₉ H ₄₇ NO ₉	Fatty acid methyl esters	---
1362	Dimethenamide ESA	2.506	322.07492	[M+H] ⁺	C ₁₂ H ₁₉ NO ₅ S ₂	Heteroaromatic compounds	---
1363	Dimerum acid	7.598	485.25763	[2M+H] ⁺	C ₂₂ H ₃₆ N ₄ O ₈	Cyclic carboximidic acids	---
1364	Dihydrokawain-5-Ol	6.587	287.06818	[M+H] ⁺	C ₁₄ H ₁₆ O ₄	Kavalactones	---
1365	Dihydrogedunin	8.625	483.24158	[M-H] ⁻	C ₂₈ H ₃₆ O ₇	Limonoids	---
1366	Dihydrobenzoic acid pentose	6.309	285.05966	[M-H ₂ O-H] ⁻	C ₁₂ H ₁₄ O ₈	Phenolic glycosides	---
1367	Diflufenzopyr	6.327	333.08099	[M-H ₂ O-H] ⁻	C ₁₅ H ₁₂ F ₂ N ₄ O ₃	N-phenylureas	---
1368	Diflufenzopyr	13.595	333.08099	[M-H] ⁻	C ₁₅ H ₁₂ F ₂ N ₄ O ₃	N-phenylureas	---
1369	Diferuloyl glycerol	3.164	443.1369	[M-H] ⁻	C ₂₃ H ₂₄ O ₉	Coumaric acids and derivatives	---
1370	Dibutylamine	7.182	130.15858	[M+H] ⁺	C ₈ H ₁₉ N	Organonitrogen compounds	---
1371	Diaveridine	9.949	261.13394	[M+H] ⁺	C ₁₃ H ₁₆ N ₄ O ₂	Dimethoxybenzenes	---
1372	Dianthosaponin C	8.427	633.36371	[M+2H] ²⁺	C ₃₅ H ₅₄ O ₁₀	Triterpenoids	---
1373	Dianthosaponin C	8.05	635.37988	[M+H] ⁺	C ₃₅ H ₅₄ O ₁₀	Triterpenoids	---
1374	Dianthosaponin C	8.051	652.40778	[M+NH ₄] ⁺	C ₃₅ H ₅₄ O ₁₀	Triterpenoids	---
1375	Dianthosaponin C	8.052	673.33752	[M+CH ₃ OH+H] ⁺	C ₃₅ H ₅₄ O ₁₀	Triterpenoids	---
1376	Dianthosaponin C	8.126	635.38318	[M+H-H ₂ O] ⁺	C ₃₅ H ₅₄ O ₁₀	Triterpenoids	---
1377	Diaminopropane	6.464	125.07066	[M+H] ⁺	C ₆ H ₈ N ₂ O	Benzene and substituted derivatives	---
1378	Diacetone ketogulonic acid	7.001	311.13275	[M-H] ⁻	C ₁₂ H ₂₄ O ₉	Sugar acids and derivatives	---
1379	DGMG(18:3)	11.062	721.36133	[M-H] ⁻	C ₃₃ H ₅₆ O ₁₄	Lipids	---
1380	Despropylspiroxamine	11.772	256.2261	[M+NH ₄] ⁺	C ₁₅ H ₂₉ NO ₂	Ketals	---
1381	D-erythro-Sphingosine C-20	13.011	310.30865	[M+H-H ₂ O] ⁺	C ₂₀ H ₄₁ NO ₂	Alkanolamines	---
1382	Deoxyloganic acid (Not validated)	7.306	359.13281	[M-H] ⁻	C ₁₆ H ₂₄ O ₉	Iridoid glycosides	---
1383	Deoxykhivorin	9.218	593.36469	[M+H] ⁺	C ₃₂ H ₄₂ O ₉	Naphthopyrans	---
1384	Deoxykhivorin	8.13	593.36456	[2M+H] ⁺	C ₃₂ H ₄₂ O ₉	Naphthopyrans	---
1385	Denatonium_TP222	10.062	222.14746	[M] ⁺	C ₁₃ H ₂₀ NO ₂	Amino acids and derivatives	---
1386	Demethyleneberberine	9.918	347.1084	[M+H] ⁺	C ₁₉ H ₁₈ NO ₄ ⁺	Protoberberine alkaloids and derivatives	---
1387	Dehydroxynocardamine	12.747	585.3584	[M+H] ⁺	C ₂₇ H ₄₈ N ₆ O ₈	Macrolactams	---

1388	Dehydrowarfarin	6.128	305.08536	[M-H]-	C19H14O4	Coumarins and derivatives	---
1389	Dehydrosalsolidine	6.468	206.11671	[M+H]+	C12H15NO2	Dihydroisoquinolines	---
1390	Dehydrophytosphingosine	10.601	316.28308	[M+H]+	C18H37NO3	Lipids	---
1391	Dehydro-P-Cymene	10.798	133.10069	[M+NH4]+	C10H12	Benzene and substituted derivatives	---
1392	Dehydro-P-Cymene	9.477	133.10065	[M+H]+	C10H12	Benzene and substituted derivatives	---
1393	Dehydroepiandrosterone 3-glucuronide	12.292	463.23343	[M-H2O-H]-	C25H36O8	Steroids and steroid derivatives	---
1394	Dehydroabietylamine acetate	12.024	345.26202	[M+H]+	C22H34NO2	Hydrophenanthrenes	---
1395	Dehydroabietamide	6.768	300.20035	[M+NH4]+	C20H29NO	Diterpenoids	---
1396	Decarestrictine D	8.77	239.08783	[M+Na]+	C10H16O5	Oxocins	---
1397	Decahydrogambogic Acid	12.149	637.37488	[M-H]-	C38H54O8	Dibenzopyrans	---
1398	Decahydrogambogic Acid	8.49	677.39008	[M+2H]2+	C38H54O8	Dibenzopyrans	---
1399	Deacetylgedunin	8.171	439.21524	[M-H]-	C26H32O6	Limonoids	---
1400	Cyproterone acetate	6.441	417.18463	[2M+H]+	C24H29ClO4	Gluco/mineralocorticoids, progestogens and derivatives	---
1401	Cyclopentylamine	3.137	86.09673	[M+H]+	C5H11N	Organonitrogen compounds	---
1402	Cyclohepta[b]pyrrole-3-propanoic acid, alpha-	6.276	309.11752	[M-H]-	C17H14N2O4	1,4-benzodiazepines	---
1403	(acetylamino)-1,4-dihydro-4-oxo-	7.572	275.10126	[M+Na]+	C14H14N2O4	Amino acids and derivatives	---
1404	Cyclo(Pro-Val)	7.277	197.12788	[M+H]+	C10H16N2O2	Amino acids and derivatives	---
1405	Cyclo(Pro-Thr)	6.328	199.10684	[M+CH3OH+H]+	C9H14N2O3	Amino acids and derivatives	---
1406	Cyclo(Pro-Leu)	8.261	211.14334	[M+H]+	C11H18N2O2	Amino acids and derivatives	---
1407	Cyaonoside B	10.542	939.49084	[M-H]-	C48H76O18	Triterpene glycosides	---
1408	Crotamiton	12.256	204.13757	[M+H]+	C13H17NO	Anilides	---
1409	Creatine riboside	6.337	264.12167	[M+H]+	C9H17N3O6	Organooxygen compounds	---
1410	Corymbosin	0.972	357.10159	[M-H]-	C19H18O7	7-O-methylated flavonoids	---
1411	Corylifol A	6.905	389.17712	[M+H]+	C25H26O4	Isoflavones	---
1412	Corylifol A	9.69	389.17938	[M-H]-	C25H26O4	Isoflavones	---
1413	Corchorifatty Acid F	9.717	351.21249	[M+CH3OH+H]+	C18H32O5	Lineolic acids and derivatives	---
1414	Corchorifatty acid D	12.563	307.19247	[M-H]-	C18H28O4	Fatty Acyls	---
1415	Conglobatin	8.592	516.30615	[M+2H]2+	C28H38N2O6	Macrolides and analogues	---
1416	Conduritol epoxide	1.006	161.04295	[M-H2O-H]-	C6H10O5	Oxepanes	---
1417	Communesin B	11.457	531.27209	[M+H]+	C32H36N4O2	Alpha carbolines	---
1418	Columbamide A	6.402	488.23447	[M+NH4]+	C23H41Cl2NO4	N-acyl amines	---
1419	Codiapeltine B	12.863	727.27264	[M+H]+	C41H42O12	Rhamnofolane and daphnane diterpenoids	---
1420	Clovamide	1.039	404.10187	[M-H2O-H]-	C18H17NO7	Amino acids and derivatives	---

1421	Citric acid (Not validated, isomer of 228)	9.147	191.01775	[M-H]-	C6H8O7	Tricarboxylic acids and derivatives	---
1422	Citraconic anhydride	1.702	111.00643	[M-H]-	C5H4O3	Dihydrofurans	---
1423	cis-Aconitic anhydride	2.074	154.99641	[M-H]-	C6H4O5	Carboxylic acids and derivatives	---
1424	cis-6-Nitro-p-mentha-1(7),2-diene	10.745	180.10062	[M-H]-	C10H15NO2	Prenol lipids	---
1425	Cimiracemoside D	8.146	701.38965	[M+Na]+	C37H58O11	Cucurbitacin glycosides	---
1426	Cimiracemoside D	8.146	679.40552	[2M+H]+	C37H58O11	Cucurbitacin glycosides	---
1427	Cimicidanol-3-O-alpha-L-arabinoside	8.722	617.36346	[M+H]+	C35H52O9	Cycloartanols and derivatives	---
1428	Cholylvaline	12.594	530.34412	[M+H]+	C29H49NO6	Glycinated bile acids and derivatives	---
1429	Cholylasparagine	8.265	545.31537	[M+2H]2+	C28H46N2O7	Glycinated bile acids and derivatives	---
1430	Chenodeoxycholythreonine	13.403	516.32562	[M+2H]2+	C28H47NO6	Glycinated bile acids and derivatives	---
1431	Chenodeoxycholyglutamic acid	8.625	544.32031	[M+2H]2+	C29H47NO7	Glycinated bile acids and derivatives	---
1432	Chenodeoxycholyglutamic acid	7.545	504.33475	[M+CH3OH+H]+	C29H47NO7	Glycinated bile acids and derivatives	---
1433	Chenodeoxycholylcysteine	7.274	496.30841	[M+H]+	C27H45NO5S	Glycinated bile acids and derivatives	---
1434	Caucasicoside A	8.355	589.3407	[M+2H]2+	C33H50O10	Steroidal saponins	---
1435	Carnequinazoline A	9.135	329.19809	[M+H]+	C18H21N3O2	Quinazolines	---
1436	Card-20(22)-enolide, 3-(beta-D-glucopyranosyloxy)-5,14-dihydroxy-, (3alpha,5beta,8xi,9xi)-	6.526	575.27936	[M+2H]2+	C29H44O10	Cardenolides and derivatives	---
1437	Card-20(22)-enolide, 1,3-bis(acetyloxy)-14,15-epoxy-7,21-dihydroxy-4,4,8-trimethyl-, (1alpha,3alpha,7alpha,9xi,13alpha,15beta,17alpha)-	10.057	591.2854	[M-H]-	C30H42O9	Limonoids	---
1438	Carbapenem	13.627	110.06	[M+H]+	C6H7NO	Lactams	---
1439	Carbapenem	7.682	110.06002	[M+NH4]+	C6H7NO	Lactams	---
1440	Caramboxin	2.849	256.08029	[M+H-H2O]+	C11H13NO6	Amino acids and derivatives	---
1441	Caramboxin	6.897	254.06523	[M-H]-	C11H13NO6	Amino acids and derivatives	---
1442	Capric dimethyl amine oxide	9.572	202.2157	[M+H]+	C12H27NO	Long-chain alkyl amine oxides	---
1443	Canrenone	12.709	339.19705	[M-H]-	C22H28O3	Steroid lactones	---
1444	Calystegine B5	1.507	176.09114	[M+H]+	C7H13NO4	Tropane alkaloids	---
1445	Calystegine A7	6.753	158.08014	[M-H]-	C7H13NO3	Tropane alkaloids	---
1446	Calystegine A6	7.787	158.08012	[M-H]-	C7H13NO3	Tropane alkaloids	---
1447	Cadabicyclone	12.47	249.1476	[M-H]-	C15H22O3	Prenol lipids	---
1448	C17-Sphinganine	10.526	288.2886	[M+H]+	C17H37NO2	Alkanolamines	---
1449	C17 Sphingosine	13.158	268.26202	[M+H-H2O]+	C17H35NO2	Alkanolamines	---

1450	Butanoic acid, 2-methyl-, (3aS,6R,7S,8S,8aR)- octahydro-7-hydroxy-6- methyl-3-methylene-2,5- dioxo-7-[(2E)-1-oxo-2- buten-1-yl]-2H- cyclohepta[b]furan-8-yl ester	11.82	377.15924	[M-H]-	C20H26O7	Terpene lactones	---
1451	Butanoic acid, 2-methyl-, (10Z)-6-formyl- 2,3,3a,4,5,8,9,11a- octahydro-5-hydroxy-10- (hydroxymethyl)-3- methylene-2- oxocyclodeca[b]furan-4- yl ester	9.697	401.15717	[M+H- H2O]+	C20H26O7	Germacranolides and derivatives	---
1452	Butacaine	10.688	307.23398	[M+NH4]+	C18H30N2O2	Benzoic acid esters	---
1453	Bungeiside C	6.414	475.14349	[2M-H]-	C19H26O11	Glycosyl compounds	---
1454	Bumetanide	6.815	363.10614	[2M-H]-	C17H20N2O5S	Diphenylethers 3-(3-	---
1455	Bourgeanic acid	12.06	387.30872	[M+H- H2O]+	C22H42O5	hydroxyalkanoyloxy)	---
1456	bottromycin A2 acid	8.621	809.4386	[M+2H]2+	C41H60N8O7S	alkanoic acids Hybrid peptides	---
1457	Boc-glycine	3.376	176.09119	[M+H]+	C7H13NO4	Amino acids and derivatives	---
1458	Bistris	1.386	210.13234	[M+H]+	C8H19NO5	Alkanolamines	---
1459	Bis(2- ethylhexyl)phosphate	12.589	321.21783	[M-H]-	C16H35O4P	Dialkyl phosphates	---
1460	Bio2_000792	13.475	391.1192	[M+Na]+	C21H20O6	Linear diarylheptanoids	---
1461	Biflavonoid-flavone base + 3O and flavone base + 2O + 1MeO	8.342	551.09668	[M-H]-	C31H20O10	Biflavonoids	---
1462	BiakamideA,B	6.439	512.26923	[M+H]+	C26H42ClN3O3 S	Aromatic monoterpenoids	---
1463	Betulalbuside A	9.051	355.17032	[M+Na]+	C16H28O7	Fatty acyl glycosides	---
1464	beta-TOXICAROL	13.395	409.23325	[M-H]-	C23H22O7	Rotenones	---
1465	beta-D-Glucopyranoside, 4-ethenylphenyl 6-O-(6- deoxy-alpha-L- mannopyranosyl)-	8.54	427.15741	[M-H]-	C20H28O10	Glycosyl compounds	---
1466	beta-D-Glucopyranoside, 2-hydroxy-4-(2-propen- 1-yl)phenyl 6-O-beta-D- glucopyranosyl-	6.006	473.14835	[M-H]-	C21H30O12	Glycosyl compounds	---
1467	beta-D-Glucopyranoside, (1aS,1bS,2S,5aR,6S,6aS) -6-[[3-O-acetyl-6-deoxy- 2-O-[(2E)-3-(4- hydroxyphenyl)-1-oxo-2- propen-1-yl]-alpha-L- mannopyranosyl]oxy]- 1a,1b,2,5a,6,6a- hexahydro-1a- (hydroxymethyl)oxireno[4,5]cyclopenta[1,2- c]dvran-2-yl, 2-acetate	6.129	737.23236	[M-2H]2-	C34H42O18	Hydroxycinnamic acid esters	---

	beta-D-Glucopyranose, 1-O-						
1468	[(2alpha,3beta,5xi,9xi,18xi)-2,3,19,24-tetrahydroxy-24,28-dioxoolean-12-en-28-yl]-Benzyl alcohol + Hex-Hex	8.852	698.40881	[M+2H] ²⁺	C36H56O12	Triterpenoids	---
1469	Benzyl alcohol + Hex-Hex	6.909	431.15411	[M-H] ⁻	C19H28O11	Alkyl benzyl hexosides	---
1470	Benzothiazole	10.03	136.02089	[M+H] ⁺	C7H5NS	Benzothiazoles	---
1471	Benzonate	12.809	604.36841	[M+H] ⁺	C30H53NO11	Benzoic acid esters	---
	Benzoic acid, 4-hydroxy-, 1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-8-[[[(2E)-2-methyl-1-oxo-2-buten-1-yl]oxy]-4-azulenyl ester						
1472	Benzoic acid, 2-hydroxy-4-methoxy-6-(2-phenylethyl)-Benzoic acid + 2O, O-Hex	7.296	455.24673	[M+H] ⁺	C27H36O6	Sesquiterpenoids	---
1473	Benzoic acid + 1O, 2MeO, O-Hex	1.576	271.10126	[M-H] ⁻	C16H16O4	Stilbenes	---
1474	Benzoic acid + 1O, 2MeO, O-Hex	6.387	315.0708	[M-H] ⁻	C13H16O9	Phenolic glycosides	---
1475	Benzododecinium	6.535	359.09576	[M-H] ⁻	C15H20O10	Phenolic glycosides	---
1476	Benzododecinium	11.485	304.29819	[M] ⁺	C21H38N ⁺	Phenylmethanamines	---
1477	Benzo[c]cinnoline	7.488	181.07504	[M+H] ⁺	C12H8N2	Diazanaphthalenes	---
1478	Benidipine	6.682	504.21732	[M-H] ⁻	C28H31N3O6	N-benzylpiperidines	---
1479	Benfluorex Hydrochloride	6.804	352.14755	[M+H] ⁺	C19H21ClF3NO ₂	Benzoic acid esters	---
1480	Barceloneic acid A	7.306	338.12027	[M+H] ⁺	C16H16O7	Diphenylethers	---
1481	Azaleatin 3-rutinoside	8.233	623.15698	[M-H] ⁻	C28H32O16	Flavonoids	---
1482	axinastatin 3	8.865	781.45947	[M+2H] ²⁺	C40H60N8O8	Peptides	---
1483	Austrobuxusin I	7.948	591.35486	[M+H] ⁺	C33H50O9	Tricarboxylic acids and derivatives	---
1484	Austrobuxusin I	7.948	613.33795	[M+2H] ²⁺	C33H50O9	Tricarboxylic acids and derivatives	---
1485	Auraptene	11.915	297.15085	[M-H] ⁻	C19H22O3	Terpene lactones	---
1486	Asteriscunolide D	6.24	264.16229	[M+NH4] ²⁺	C15H18O3	Butenolides	---
1487	Aspterric acid	14.921	265.14621	[M-H] ⁻	C15H22O4	Alpha hydroxy acids and derivatives	---
1488	Aspochalasin K	7.374	432.27795	[M+NH4] ⁺	C25H39NO5	Isoindolones	---
1489	Aspergamid B	2.984	486.17911	[M+H] ⁺	C26H29N3O4	2,2-dimethyl-1-benzopyrans	---
1490	Asparagine propyl ester	1.512	175.10693	[M+H] ⁺	C7H14N2O3	---	---
1491	Ascochlorin	6.87	403.1694	[M-H2O-H] ⁻	C23H29ClO4	Aldehydes	---
1492	Arvenin I	8.517	721.38446	[M+2H] ²⁺	C38H56O13	Steroidal saponins	---
1493	Armilarisin A	8.186	233.04378	[M-H2O-H] ⁻	C12H10O5	Coumarins and derivatives	---
1494	Aristolochic acid C	0.624	328.04431	[M+H] ⁺	C16H9NO7	Aristolochic acids and derivatives	---
1495	Aristolochic acid C	5.925	328.04413	[M+CH3OH+H] ⁺	C16H9NO7	Aristolochic acids and derivatives	---
1496	Aristolochic acid C	0.299	328.04306	[2M+H] ⁺	C16H9NO7	Aristolochic acids and derivatives	---
1497	arisanetetralone	12.353	365.13397	[M+Na] ⁺	C20H22O5	Aryltetralin lignans	---
1498	Arginylisoleucine	4.047	288.20166	[M+H] ⁺	C12H25N5O3	Peptides	---
1499	Arginylasparagine	9.161	289.16339	[M+H] ⁺	C10H20N6O4	Peptides	---
1500	Arachidoyl Ethanolamide	11.732	356.35095	[M+H] ⁺	C22H45NO2	Alkanolamines	---

1501	Apratoxin A	12.734	840.50055	[M+2H] ²⁺	C45H69N5O8S	Cyclic depsipeptides	---
1502	Apodanthoside (Not validated)	6.869	401.10666	[M-H] ⁻	C17H22O11	Iridoid glycosides	---
1503	Apixaban	1.436	460.19949	[M+H] ⁺	C25H25N5O4	Phenylpiperidines	---
1504	Apixaban	1.567	460.19949	[M+Na] ⁺	C25H25N5O4	Phenylpiperidines	---
1505	Apitolisib	1.409	499.22089	[M+H] ⁺	C23H30N8O3S	Thienopyrimidines	---
1506	Apimaysin	6.202	559.14679	[2M-H] ⁻	C27H28O13	Flavonoid C-glycosides	---
1507	Apicidin	13.261	624.375	[M+2H] ²⁺	C34H49N5O6	Peptides	---
1508	Apicidin	13.245	624.37897	[M+H] ⁺	C34H49N5O6	Peptides	---
1509	Anwulignan	12.498	327.17749	[M-H ₂ O-H] ⁻	C20H24O4	Dibenzylbutane lignans	---
1510	Anthraquinone base + 1O, MeOH, O-Hex-Pen	6.301	547.14795	[M-H] ⁻	C26H28O13	Anthraquinones-aglycone+1O+1MeOH	---
1511	Antcin K	8.23	487.30234	[M-H] ⁻	C29H44O6	Steroids and steroid derivatives	---
1512	Angustoline	6.373	354.12079	[M+H] ⁺	C20H17N3O2	Beta carbolines	---
1513	Angolensin	1.511	295.09436	[M+H] ⁺	C16H16O4	Alpha-methyldeoxybenzoin flavonoids	---
1514	Angeloylgomisin H	10.805	499.22632	[M-H] ⁻	C28H36O8	Hydrolyzable tannins	---
1515	Andrachcinidine	12.42	228.19456	[M+NH ₄] ⁺	C13H25NO2	Piperidines	---
1516	Andrachcinidine	10.842	228.19453	[M+H] ⁺	C13H25NO2	Piperidines	---
1517	Anabasamine	6.248	254.16635	[M+H] ⁺	C16H19N3	Bipyridines and oligopyridines	---
1518	Amorphin	1.327	727.22272	[M+H] ⁺	C34H40O16	Flavonoid O-glycosides	---
1519	Amorolfine hydrochloride	11.565	354.25964	[M+Na] ⁺	C21H36ClNO	Phenylpropanes	---
1520	Altretamine	10.843	211.16817	[M+NH ₄] ⁺	C9H18N6	Tertiary amines	---
1521	alpha-Methyl-4-carboxyphenylglycine	1.029	208.06227	[M-H] ⁻	C10H11NO4	Carboxylic acids and derivatives	---
1522	alpha-Hydroxyhippuric acid alpha-D-Glucopyranoside, O-beta-D-glucopyranosyl-(1->2)-6-O-[(2E)-2-methyl-1-oxo-2-buten-1-yl]-alpha-D-glucopyranosyl O-beta-D-glucopyranosyl-(1->2)-alpha-D-Glucopyranoside, 4-O-[(2E)-1-oxo-3-phenyl-2-propen-1-yl]-beta-D-fructofuranosyl alpha-D-Glucopyranoside, 3,6-bis-O-[(2E)-3-(4-hydroxy-3-methoxyphenyl)-1-oxo-2-propen-1-yl]-beta-D-fructofuranosyl alpha-D-Glucopyranoside, 3,6-bis-O-[(2E)-3-(4-hydroxy-3-methoxyphenyl)-1-oxo-2-propen-1-yl]-beta-D-fructofuranosyl	1.257	218.04211	[M+CH ₃ OH+H] ⁺	C9H9NO4	Benzamides	---
1523	alpha-Hydroxyhippuric acid alpha-D-Glucopyranoside, O-beta-D-glucopyranosyl-(1->2)-6-O-[(2E)-2-methyl-1-oxo-2-buten-1-yl]-alpha-D-glucopyranosyl O-beta-D-glucopyranosyl-(1->2)-alpha-D-Glucopyranoside, 4-O-[(2E)-1-oxo-3-phenyl-2-propen-1-yl]-beta-D-fructofuranosyl alpha-D-Glucopyranoside, 3,6-bis-O-[(2E)-3-(4-hydroxy-3-methoxyphenyl)-1-oxo-2-propen-1-yl]-beta-D-fructofuranosyl	5.246	766.29559	[M+H] ⁺	C29H48O22	Saccharolipids	---
1524	alpha-Hydroxyhippuric acid alpha-D-Glucopyranoside, O-beta-D-glucopyranosyl-(1->2)-6-O-[(2E)-2-methyl-1-oxo-2-buten-1-yl]-alpha-D-glucopyranosyl O-beta-D-glucopyranosyl-(1->2)-alpha-D-Glucopyranoside, 4-O-[(2E)-1-oxo-3-phenyl-2-propen-1-yl]-beta-D-fructofuranosyl	6.203	490.18951	[M+H] ⁺	C21H28O12	Cinnamic acid esters	---
1525	alpha-Hydroxyhippuric acid alpha-D-Glucopyranoside, O-beta-D-glucopyranosyl-(1->2)-6-O-[(2E)-2-methyl-1-oxo-2-buten-1-yl]-alpha-D-glucopyranosyl O-beta-D-glucopyranosyl-(1->2)-alpha-D-Glucopyranoside, 4-O-[(2E)-1-oxo-3-phenyl-2-propen-1-yl]-beta-D-fructofuranosyl	2.487	693.20593	[M-H] ⁻	C32H38O17	Coumaric acids and derivatives	---
1526	alpha-Hydroxyhippuric acid alpha-D-Glucopyranoside, O-beta-D-glucopyranosyl-(1->2)-6-O-[(2E)-2-methyl-1-oxo-2-buten-1-yl]-alpha-D-glucopyranosyl O-beta-D-glucopyranosyl-(1->2)-alpha-D-Glucopyranoside, 4-O-[(2E)-1-oxo-3-phenyl-2-propen-1-yl]-beta-D-fructofuranosyl	3.19	693.20612	[M-2H] ²⁻	C32H38O17	Coumaric acids and derivatives	---

1527	alpha-(4-Fluorophenyl)- 4-(5-fluoro-2- pyrimidinyl)-1- diperazine butanol	6.978	349.18161	[M+Na]+	C18H22F2N4O	Diazinanes	---
1528	Aloeresin	12.499	393.16916	[M-H]-	C19H22O9	Glycosyl compounds	---
1529	Alibendol	9.108	274.10635	[M+Na]+	C13H17NO4	Hydroxybenzoic acid derivatives	---
1530	Alibendol	11.875	252.11873	[M+H]+	C13H17NO4	Hydroxybenzoic acid derivatives	---
1531	Alanylisoleucine	6.371	201.1225	[M-H]-	C9H18N2O3	Peptides	---
1532	AKOS032436253	11.5	502.28964	[M+H]+	C30H40NNaO4	Aryl alkyl ketones	---
1533	AKOS030242091	12.582	511.20648	[M+Na]+	C25H32N2O8	Ibogan-type alkaloids	---
1534	Aerugine	2.498	210.06007	[M+NH4]+	C10H11NO2S	Aralkylamines	---
1535	Acridinic acid	7.4	216.03111	[M-H]-	C11H7NO4	Quinoline carboxylic acids	---
1536	Acetyltributyl citrate	12.585	425.21207	[M+Na]+	C20H34O8	Tetracarboxylic acids and derivatives	---
1537	Acetylsulfathiazole	5.954	298.0332	[M+CH3OH +H]+	C11H11N3O3S2	Benzenesulfonamide s	---
1538	Acetyl-Leucyl-Valyl- Argininal	12.569	413.28598	[M+H]+	C19H36N6O4	Peptides	---
1539	Acetyl-Leucyl-Valyl- Argininal	12.643	413.28418	[M+Na]+	C19H36N6O4	Peptides	---
1540	Acetylleucine (isomer of 164)	7.978	172.09555	[M-H]-	C8H15NO3	Leucine and derivatives	---
1541	Acetylcytisine	6.415	233.12729	[M+H]+	C13H16N2O2	Amino acids and derivatives	---
1542	Acetoacetaldehyde	2.049	85.02725	[M-H2O-H]-	C4H6O2	Organooxygen compounds	---
1543	9-Pentadecenoic acid	11.446	239.19948	[M-H]-	C15H28O2	Fatty Acyls	---
1544	9"-O-Z-p-coumaroyl-9"- O-E-p-coumaroyl- (7S,8S)-guaiaacylglycerol 8-O-4'-coniferyl ether	1.202	683.21112	[M-H]-	C38H36O12	Lignans, neolignans and related compounds	---
1545	9"-O-E-p-Coumaroyl-9"- O-Z-p-coumaroyl- (7R,8S)-guaiaacylglycerol 8-O-4'-coniferyl ether 9-hydroxy-5b,8,11a- trimethyl-1-prop-1-en-2- yl-	9.224	667.22095	[M-H]-	C38H36O11	Lignans, neolignans and related compounds	---
1546	1,2,3,4,5,6,7,7a,9,10,11,1 1b,12,13,13a,13b- hexadecahydrocyclopent a[a]chrysene-3a,5a,8- tricarboxylic acid 9-hydroxy-5b,8,11a- trimethyl-1-prop-1-en-2- yl-	6.814	551.28046	[M-H]-	C30H44O7	Triterpenoids	---
1547	1,2,3,4,5,6,7,7a,9,10,11,1 1b,12,13,13a,13b- hexadecahydrocyclopent a[a]chrysene-3a,5a,8- tricarboxylic acid	6.575	555.27454	[M+H]+	C30H44O7	Triterpenoids	---

1548	9-nydroxy-2,6,12-trimethyl-12-[2-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyethyl]-15-oxatetracyclo[8.4.1.01,10.02,7]pentadecane-6-carboxylic acid	9.108	515.28137	[2M+H] ⁺	C26H42O10	Fatty acyl glycosides	---
1549	9-F1-phytoprostane	11.119	327.21536	[M-H] ⁻	C18H32O5	Fatty Acyls	---
1550	9a-12a-Octadecadiynoic acid	10.61	277.21439	[M+H] ⁺	C18H28O2	Long-chain fatty acids	---
1551	9,19-Cyclolanost-24-en-26-oic acid, 3-[(2-O-hexopyranosyl)pentopyranosyl]oxy]-12,15-dihydroxy-, (3beta,8xi,9beta,24F)-	12.887	765.4411	[M+H] ⁺	C41H66O14	Steroidal saponins	---
1552	9,19-Cyclolanost-24-en-26-oic acid, 3-[(2-O-hexopyranosyl)pentopyranosyl]oxy]-12,15-dihydroxy-, (3beta,8xi,9beta,24F)-	8.606	765.44037	[M+2H] ²⁺	C41H66O14	Steroidal saponins	---
1553	9,13-Epoxy-3,18-dihydroxy-15,16-labdanolide	12.372	397.22397	[M-H] ⁻	C20H32O5	Gamma butyrolactones	---
1554	9,10-DiHODE	10.693	311.22113	[M-H] ⁻	C18H32O4	Fatty Acyls	---
1555	9-(Methoxycarbonyl)dec-9-enoic acid	10.798	229.14236	[M+H] ⁺	C12H20O4	Medium-chain fatty acids	---
1556	9-(4-methylphenyl)-8-[(4-methylphenyl)methylthio]hyd dropurin-6-one 9-(4-hydroxyphenyl)-3,3,6,6-tetramethyl-10-phenyl-2,3,4,5,6,7,9,10-octahydroac ridine-1,8-dione	6.818	361.11136	[M-H] ⁻	C20H18N4OS	Substituted imidazoles	---
1557	9-(2,3-dihydroxypropoxy)-9-oxononanoic acid	6.33	464.22156	[M+H] ⁺	C29H31NO3	Phenylquinolines	---
1558	8-O-Acetylharpagide	8.461	261.13232	[M-H] ⁻	C12H22O6	Medium-chain fatty acids	---
1559	8-Methylquinoline	2.476	424.17886	[M+H] ⁺	C17H26O11	Iridoid O-glycosides	---
1560	8-Hydroxy-9,10-epoxystearic acid	6.696	144.0802	[M+H] ⁺	C10H9N	Quinolines and derivatives	---
1561	8-Hydroxy-9,10-epoxystearic acid	11.482	337.23325	[M+Na] ⁺	C18H34O4	Lineolic acids and derivatives	---
1562	8-Hydroxy-9,10-epoxystearic acid	11.498	297.24054	[M+H-H2O] ⁺	C18H34O4	Lineolic acids and derivatives	---
1563	8-Hydroxy-9,10-epoxystearic acid	10.329	356.27612	[M+H] ⁺	C18H34O4	Lineolic acids and derivatives	---
1564	8-Daucene-2,4,6-triol, O-(4-Hydroxybenzoyl), 2-Ac	10.375	455.18701	[M+Na] ⁺	C24H32O6	Sesquiterpenoids	---
1565	8-Daucene-2,4,6-triol, O-(4-Hydroxybenzoyl), 2-Ac	6.436	455.18729	[2M+H] ²⁺	C24H32O6	Sesquiterpenoids	---
1566	8-Acetamido-2-methyl-7-oxononanoic acid	7.217	244.1537	[M+H] ⁺	C12H21NO4	Medium-chain fatty acids	---

1567	8-[2-(3,4-dimethoxy-2,5-dimethoxyoxolan-3-yl)ethyl]-4a,7,8-trimethylspiro[2,3,5,6,7,8-a-hexahydro-1H-naphthalene-4,2'-naphthalene]-2,3-diol	12.282	429.24689	[M+H] ⁺	C22H38O8	Glycosyl compounds	---
1568	8:1+2O fatty acyl hexoside	7.576	321.15384	[M-H] ⁻	C14H26O8	Fatty acyl hexosides	---
1569	8,9-Dihydroxy-1,5,6,10B-tetrahydropyrrolo[2,1-A]isoquinolin-3(2H)-one	6.368	220.09628	[M+NH4] ⁺	C12H13NO3	Tetrahydroisoquinolines	---
1570	8,8-Dimethyl-2-phenyl-4H,8H-benzo[1,2-b:3,4-b']dipyran-4-one	6.816	303.10632	[M-H] ⁻	C20H16O3	Pyranoflavonoids	---
1571	8-(3-methoxy-2-(methoxycarbonyl)phenyl)octanoic acid	12.185	307.15674	[M-H] ⁻	C17H24O5	Methoxybenzoic acids and derivatives	---
1572	8-(2-Hydroxy-3-methoxy-3-methylbutyl)-7-methoxy-1-benzopyran-2-one	8.911	315.12061	[M+Na] ⁺	C16H20O5	Coumarins and derivatives	---
1573	8-(2,4-dihydroxy-6-pentyl-phenoxy)-6-hydroxy-3-pentylisocoumarin	7.237	425.20096	[M-H] ⁻	C25H30O6	Isocoumarins and derivatives	---
1574	7-O-Methylbavachin	12.358	337.19772	[M-H] ⁻	C21H22O4	6-prenylated flavans	---
1575	7-O-Methyl morroniside	6.003	438.19437	[M+Na] ⁺	C18H28O11	Glycosyl compounds	---
1576	7-O-Methyl morroniside	6.198	438.19434	[M+H] ⁺	C18H28O11	Glycosyl compounds	---
1577	7-Hydroxy-5-methylflavone	1.554	251.07564	[M-H] ⁻	C16H12O3	Flavones	---
1578	7-hydroxy-4-methyl-1,4,4a,5,6,8a-hexahydropyrimido[4,5-d]pyrimidin-2(3H)-one	2.321	207.08546	[M+H] ⁺	C7H12N4O2	Pyrimidones	---
1579	7-Hexadecynoic acid	12.117	251.19942	[M-H] ⁻	C16H28O2	Fatty Acyls	---
1580	7-Deshydroxypyrogallin-4-carboxylic acid	7.037	247.02672	[M-H] ⁻	C12H8O6	Tropolones	---
1581	7-Deacetoxy-7-Oxokhivorin	9.689	541.24579	[M-H] ⁻	C30H38O9	Naphthopyrans	---
1582	7-Benzofurancarboxylic acid, 2,3-dihydro-2-(1-hydroxy-1-methylethyl)-4-methoxy-6-(2-phenylethyl)-	11.803	379.15005	[M+Na] ⁺	C21H24O5	Stilbenes	---
1583	7-Benzofurancarboxylic acid, 2,3-dihydro-2-(1-hydroxy-1-methylethyl)-4-methoxy-6-(2-phenylethyl)-	13.384	355.15582	[M-H] ⁻	C21H24O5	Stilbenes	---

1584	7-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy-6-[[[(2S,3R,4S,5R)-3,4,5-trihydroxyoxan-2-yl]oxymethyl]oxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)-2,3-7-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy-6-[[[(2S,3R,4S,5R)-3,4,5-trihydroxyoxan-2-yl]oxymethyl]oxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)-2,3-7,2'-Dihydroxyflavone 7,2',3'-Trimethoxyflavanone 6-Oxopiperidine-2-carboxylic acid	4.893	711.21454	[M-H]-	C32H40O18	Flavonoid O-glycosides	---
1585	7,2',3'-Trimethoxyflavanone 6-Oxopiperidine-2-carboxylic acid	5.205	711.21466	[M-H ₂ O-H]-	C32H40O18	Flavonoid O-glycosides	---
1586	6-O-[2",3"-dicinnamoyl-4"-acetyl-alpha-L-rhamnopyranosyl]-catalpol	9.345	253.04843	[M-H]-	C15H10O4	Flavones	---
1587	6"-O-(3-Hydroxy-3-Methylglutaroyl)Astragal in	11.89	337.10272	[M+Na]+	C18H18O5	7-O-methylated flavonoids	---
1588	6-n-Propyluracil	1.522	144.06511	[M+CH ₃ OH+H]+	C6H9NO3	Carboxylic acids and derivatives	---
1589	6-Nitroveratraldehyde	5.883	811.28156	[M+H]+	C41H46O17	Cinnamic acid esters	---
1590	6-Methyl-2-pyridinecarboxylic acid	2.364	591.13611	[M-H]-	C27H28O15	Flavonol O-glycosides	---
1591	6-methyl-2-[4-benzylpiperazinyl]-3-hydroxypyrimidin-4-one	6.223	155.08121	[M+H]+	C7H10N2O2	Diazines	---
1592	6-methyl-1-[(3-nitrophenyl)amino]furan	6.944	210.03876	[M-H]-	C9H9NO5	Nitrophenyl ethers	---
1593	o[2,3-h]chromen-8-one	6.748	138.05458	[M+H-H ₂ O]+	C7H7NO2	Pyridines and derivatives	---
1594	6-methoxy-4-oxo-4H-chromene-3-carbaldehyde	9.059	307.14981	[M+Na]+	C16H20N4O	N-arylpiperazines	---
1595	6-hydroxyoct-1-enoylglycine	0.159	359.06204	[M+Na]+	C18H12N2O5	Angular furanocoumarins	---
1596	6-Hydroxymethyl-2,2-dimethyl-dihydro-furo(3,4-d)(1,3)dioxol-4-one	8.155	205.04874	[M+H]+	C11H8O4	Chromones	---
1597	6-Hydroxy-8-(/-hydroxy-2-oxochromen-8-yl)-7-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-6-oxochromen-2-one	1.534	216.12195	[M+H]+	C10H17NO4	Carboxylic acids and derivatives	---
1598	6-Hydroxy-3,4-dihydro-2(1H)-quinolinone	2.365	189.07469	[M+H-H ₂ O]+	C8H12O5	Ketals	---
1599	6-Hydroxy-3,4-dihydro-2(1H)-quinolinone	6.216	499.09152	[M-H]-	C24H20O12	Coumarin glycosides	---
1600	6-Hydroxy-3,4-dihydro-2(1H)-quinolinone	8.78	164.07004	[M+H]+	C9H9NO2	Quinolines and derivatives	---

1601	6-Hydroxy-2,6,10,10-tetramethyl-1-oxaspiro[4.5]dec-8-yl 6-O-[(2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)tetrahydro-2-furanyl]-beta-D-glucopyranoside	8.782	567.2627	[2M-H]-	C24H42O12	Glycosyl compounds	---
1602	6-Feruloylcatalpol	1	537.16327	[M-H]-	C25H30O13	Coumaric acids and derivatives	---
1603	6-ethyl-3-(4-isopropoxyphenyl)-4-oxo-4H-chromen-7-yl	6.92	389.14062	[M+Na]+	C22H22O5	Isoflavones	---
1604	6-ethoxy-4-[(4-hydroxyquinazolin-2-ylthio)methyl]chromen-2-one	1.06	379.07983	[M-H]-	C20H16N2O4S	Coumarins and derivatives	---
1605	6-chloro-4-hydroxychromen-2-one	8.985	196.99994	[M+CH3OH+H]+	C9H5ClO3	4-hydroxycoumarins	---
1606	6-chloro-2-(trichloromethyl)chromen-4-one	0.768	164.93298	[M-H+Cl]-	C10H4Cl4O2	Chromones	---
1607	6-Carbomethoxy-7-isobutyroxy-cumarin	3.691	308.11182	[M+H]+	C15H14O6	Coumarins and derivatives	---
1608	6-Carbomethoxy-7-isobutyroxy-cumarin	3.98	308.11182	[M+H-H2O]+	C15H14O6	Coumarins and derivatives	---
1609	6-aminododecanedioic acid, chloride	9.801	244.15311	[M-H]-	C12H23NO4	Medium-chain fatty acids	---
1610	6-amino-4-(4-hydroxyphenyl)-3-propyl-4H-pyrano[3,2-d]pyrazole-5-carbonitrile	9.301	295.11978	[M-H]-	C16H16N4O2	1-hydroxy-2-unsubstituted benzenoids	---
1611	6alpha-isobutyryloxy-1-hydroxy-4alphaH-1,10-secoeudesman-5(10),11(13)-dien-12,8beta-olide	6.389	359.18008	[M+NH4]+	C19H28O5	Terpene lactones	---
1612	6-{7-Acetoxy-5-chloro-3-[(1E,3E)-3,5-dimethyl-1,3-heptadien-1-yl]-7-methyl-6,8-dioxo-7,8-dihydro-2(6H)-isoquinolinylnorleucine	6.219	519.22833	[2M+H]+	C27H35ClN2O6	Azaphilones	---
1613	6-{7-Acetoxy-5-chloro-3-[(1E,3E)-3,5-dimethyl-1,3-heptadien-1-yl]-7-methyl-6,8-dioxo-7,8-dihydro-2(6H)-isoquinolinylnorleucine	6.272	519.22845	[M+H]+	C27H35ClN2O6	Azaphilones	---
1614	6-[2-hydroxy-3-methoxy-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybutyl]-5,7-dimethoxychromen-2-one	9.367	493.16483	[M+Na]+	C22H30O11	Fatty acyl glycosides	---

1615	6-[(8a-carboxy-4,4,6a,6b,11,11,14b-heptamethyl-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicen-3-yl)oxy]-5-[3,5-dihydroxy-6-(hydroxymethyl)-4-(3,4,5-trihydroxy-6-methyloxan-2-yl)oxyoxan-2-yl]oxy-3,4-dihydroxoxane-2-6:3+6O fatty acyl hexoside	10.543	985.49634	[M-H]-	C48H76O18	Triterpene glycosides	---
1616	6,7-Dimethoxy-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid	6.21	353.07013	[M-H]-	C12H18O12	Fatty acyl hexosides	---
1617	6,10a-Dihydroxy-4-(hydroxymethyl)-4,7,11b-trimethyl-1,2,3,4a,5,6,6a,7,11,11a-decahydronaphtho[2,1-][1]benzouran-9-one	6.561	238.10651	[M+H]+	C12H15NO4	Tetrahydroisoquinolines	---
1618	6,10,14-Trimethyl-5,9,13-pentadecatrien-2-one	12.513	349.2027	[M-H]-	C20H30O5	Naphthofurans	---
1619	6-(4-Sulfophenyl)Nonanoic Acid	13.005	263.23529	[M+H]+	C18H30O	Prenol lipids	---
1620	5-phenyl-3-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}pentanoic acid	1.823	313.11206	[M-H]-	C15H22O5S	Benzenesulfonic acids and derivatives	---
1621	5-Pentyl-2-furanheptanoic acid	8.753	379.13431	[M+Na]+	C17H24O8	Fatty acyl glycosides	---
1622	5-Oxo-octadecanoic acid	11.445	265.17889	[M-H]-	C16H26O3	Fatty Acyls	---
1623	5-O-Methylvisammioside	12.324	297.24185	[M-H2O-H]-	C18H34O3	Fatty Acyls	---
1624	5-O-Methylvisammioside	10.772	475.15604	[M+Na]+	C22H28O10	Chromones	---
1625	5-O-Methylvisammioside	10.973	453.17383	[M+H]+	C22H28O10	Chromones	---
1626	5-octenoylglycine	9.047	198.11147	[M-H]-	C10H17NO3	Carboxylic acids and derivatives	---
1627	5-Nonyltetrahydro-2-oxo-3-furancarboxylic acid	11.575	255.15846	[M-H]-	C14H24O4	Lactones	---
1628	5-Methoxyindole-2-carboxylic acid	6.726	192.0649	[M+H]+	C10H9NO3	Indoles and derivatives	---
1629	5-Hydroxymethylcytosine	6.696	142.06451	[M+NH4]+	C5H7N3O2	Hydroxypyrimidines	---
1630	5-Hydroxymethylcytidine	9.396	272.09052	[M-H]-	C10H15N3O6		---
1631	5-Hydroxymaltol	1.656	143.03337	[M+H]+	C6H6O4	Pyrans	---
1632	5-Hydroxyhexadecanoic acid	12.143	271.22635	[M-H]-	C16H32O3	Fatty Acyls	---
1633	5-hydroxycalamenene	11.721	219.17328	[M+H]+	C15H22O	Prenol lipids	---
1634	5-hydroxy-8,8-dimethyl-6-(2-methylpropanoyl)-4-phenyl-2H,8H-pyrano[2,3-f]chromen-2-one	6.818	391.15591	[M+H]+	C24H22O5	Prenylated neoflavonoids	---

1635	5-Hydroxy-3-(hydroxymethyl)-6-isopropyl-2-oxo-3-cyclohexen-1-yl 3-methylpentanoate	6.88	316.21094	[M+H] ⁺	C16H26O5	Menthane monoterpenoids	---
1636	5-Hydroxy-3-(hydroxymethyl)-6-isopropyl-2-oxo-3-cyclohexen-1-yl 3-methylpentanoate	7.187	316.21085	[M+CH3OH+H] ⁺	C16H26O5	Menthane monoterpenoids	---
1637	5-Hydroxy-2-ethylhexyl diphenyl phosphate	6.428	379.16937	[M+H] ⁺	C20H27O5P	Aryl phosphates	---
1638	5-Heptyltetrahydro-2-oxo-3-furancarboxylic acid	10.799	227.12677	[M-H] ⁻	C12H20O4	Lactones	---
1639	5-Heptenoic acid, 2-[(4alpha,5alpha,6beta,8alpha,9beta,13alpha,14beta,16beta,17E)-16-(acetyloxy)-6-hydroxy-4,8,10,14-tetramethyl-3,7-dioxogon-1-en-17-ylidene]-6-methyl-, (2E)-	10.313	525.2879	[M-H] ⁻	C31H42O7	Steroid esters	---
1640	5-Cyclohexadecen-1-one	12.145	237.22038	[M+H] ⁺	C16H28O	Ketones	---
1641	5-Chlorodivaticatinic acid	6.818	243.04256	[M-H2O-H] ⁻	C11H13ClO4	Methoxybenzoic acids and derivatives	---
1642	5-chloro-3-[(E)-3,4-dihydroxy-3,5-dimethylhept-1-enyl]-7,8-dihydroxy-7-methyl-8,8a-dihydro-1H-isochromen-6-one	9.002	387.16061	[M+H] ⁺	C19H27ClO6	Azaphilones	---
1643	5-chloro-2,4-dihydroxy-3-[(E)-4-hydroxy-3-methyl-5-(1,2,6-trimethyl-3-oxocyclohexyl)pent-2-enyl]-6-methylbenzaldehyde	6.782	423.19446	[M+H] ⁺	C23H31ClO5	Aldehydes	---
1644	5-chloro-2,4-dihydroxy-3-[(E)-4-hydroxy-3-methyl-5-(1,2,6-trimethyl-3-oxocyclohexyl)pent-2-enyl]-6-methylbenzaldehyde	6.562	421.17996	[M-H] ⁻	C23H31ClO5	Aldehydes	---
1645	5-chloro-2,4-dihydroxy-3-[(E)-4-hydroxy-3-methyl-5-(1,2,6-trimethyl-3-oxocyclohexyl)pent-2-enyl]-6-methylbenzaldehyde	6.792	421.17996	[2M-H] ⁻	C23H31ClO5	Aldehydes	---
1646	5-amino-3-[(2E)-2-(3,5-dimethyl-2-oxocyclohexylidene)ethyl]-5-oxopentanoic acid	6.575	304.14963	[M+CH3OH+H] ⁺	C15H23NO4	Medium-chain fatty acids	---

1647	5-[5-Hydroxy-3-(hydroxymethyl)pentyl]-8a-(hydroxymethyl)-5,6-dimethyl-3,4,4a,6,7,8-hexahydronaphthalene-1-carboxylic acid	13.444	353.26697	[M-H]-	C20H34O5	Colensane and clerodane diterpenoids	---
1648	5-[3-methoxy-4-(phenylmethoxy)phenyl]-2,2-dimethyl-1,2,3,5,6-pentahydrobenzo[a]phenanthridin-4-one	7.035	490.23843	[M+H-H2O]+	C33H31NO3	Phenylquinolines	---
1649	5-[3-methoxy-4-(phenylmethoxy)phenyl]-2,2-dimethyl-1,2,3,5,6-pentahydrobenzo[a]phenanthridin-4-one	7.022	488.22217	[M-H]-	C33H31NO3	Phenylquinolines	---
1650	5-[3-[(E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxymethyl]-5-hydroxypentyl]-5,6,8a-trimethyl-3,4,4a,6,7,8-hexahydronaphthalene-1-carboxylic acid	8.163	501.28729	[M+2H]2+	C29H40O7	Colensane and clerodane diterpenoids	---
1651	5-[3-[(E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxymethyl]-5-hydroxypentyl]-5,6,8a-trimethyl-3,4,4a,6,7,8-hexahydronaphthalene-1-carboxylic acid	9.4	499.26639	[M-H]-	C29H40O7	Colensane and clerodane diterpenoids	---
1652	5-[(Z)-14-(3,5-dihydroxyphenyl)tetradec-10-enyl]benzene-1,3-diol	12.281	451.2272	[M+CH3OH+H]+	C26H36O4	Resorcinols	---
1653	5-[(6-bromo(2H-benzo[d]1,3-dioxolen-5-yl))methylene]-2-imino-3-[4-(trifluoromethoxy)phenyl]-1,3-thiazolidin-4-one	8.547	486.95782	[M+H]+	C18H10BrF3N2O4S	Benzodioxoles	---
1654	5,7-dinitro-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one	5.959	299.0408	[M+CH3OH+H]+	C11H8N4O5	Quinazolines	---
1655	5,7-dihydroxy-3,6-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one	5.217	299.04083	[M+H]+	C11H8N4O5	Quinazolines	---
1656	5,6-dihydroxy-9,12,13-trimethyl-14-(2-methylpropyl)-2H,5H,6H,7H,8H,13H,13aH,14H,15H,16H,16bH-oxacyclododeca[3,2-e]isindole-2,16-dione	10.795	405.11819	[M+Na]+	C20H20O9	6-O-methylated flavonoids	---
1657	5,6-Dihydroxy-2-methylaminotetralin	2.615	456.21564	[M+H]+	C24H35NO5	Aspochalasins	---
1658		6.242	194.11673	[M+H]+	C11H15NO2	Tetralins	---

1659	5,6-Bis(benzoyloxy)- 3,4a,10a-trihydroxy- 4,7,11b-trimethyl-9-oxo- 1,2,3,4,4a,5,6,6a,7,9,10a, 11,11a,11b- tetradecahydrophenanthr o[3,2-b]furan-4- carboxylic acid	9.304	619.21826	[M-H]-	C34H36O11	Steroid lactones	---
1660	5,5-Dimethyl-2(5H)- furanone	5.124	113.05971	[M+H]+	C6H8O2	Dihydrofurans	---
1661	5,5-bis(trifluoromethyl)- 1,3-dimethyl-7-benzyl- 1,3,5,8- tetrahydropyrimidino[4, 5-d]pyrimidine-2,4-dione	6.039	419.09302	[M-H]-	C17H14F6N4O2	Pyrimidones	---
1662	5-(hydroxymethyl)-6-(1- hydroxypropyl)-4- methoxyvovan-2-one	6.315	215.09048	[2M+H]+	C10H14O5	Pyranones and derivatives	---
1663	5-(hydroxymethyl)-3-(1- hydroxy-5- methylhexyl)oxolan-2- one	1.112	247.90219	[M+NH4]+	C12H22O4	Fatty alcohols	---
1664	5-(4-Acetyloxy-3- hydroxy-2,5,5,8a- tetramethyl-3,4,4a,6,7,8- hexahydronaphthalen-1- yl)-3-methylpentanoic acid	12.618	425.25491	[M-H]-	C22H36O5	Diterpenoids	---
1665	5-(4-Acetyloxy-3- hydroxy-2,5,5,8a- tetramethyl-3,4,4a,6,7,8- hexahydronaphthalen-1- yl)-3-methylpentanoic acid	9.267	381.26108	[M+H]+	C22H36O5	Diterpenoids	---
1666	5-(4-Acetyloxy-3- hydroxy-2,5,5,8a- tetramethyl-3,4,4a,6,7,8- hexahydronaphthalen-1- yl)-3-methylpentanoic acid	11.59	398.28647	[M+H- H2O]+	C22H36O5	Diterpenoids	---
1667	5-(3',4'- Dihydroxyphenyl)- gamma-valerolactone	11.078	207.06384	[M-H]-	C11H12O4	Phenols	---
1668	4-Methylphthalic anhydride	10.312	163.03842	[M+H]+	C9H6O3	Phthalic anhydrides	---
1669	4-methyl-6-(1,2,3,4- tetrahydroquinolyl)sulfon yl)hydroquinolin-2-one	8.341	353.09863	[M-H]-	C19H18N2O3S	Hydroquinolones	---
1670	4-methyl-3,4-dihydro- 1H-1,4-benzodiazepine- 2,5-dione	5.8	191.0804	[M+H]+	C10H10N2O2	1,4-benzodiazepines	---
1671	4-methyl-2-({[2,4,6- tris(methylethyl)phenyl]s ulfonyl}amino)pentanoic acid	12.601	398.23914	[M+H]+	C21H35NO4S	Amino acids and derivatives	---
1672	4-methyl-2-({[2,4,6- tris(methylethyl)phenyl]s ulfonyl}amino)pentanoic acid	12.335	398.23917	[M+Na]+	C21H35NO4S	Amino acids and derivatives	---

1673	4-methyl-1-(2-purin-6-ylthioethoxy)benzene 4-methoxy-1-[(7-methylindeno[3,2-b]pyridin-5-ylidene)methyl]benzene	2.546	309.07977	[M+CH ₃ OH+H] ⁺	C ₁₄ H ₁₄ N ₄ O ₅	6-thiopurines	---
1674		7.39	300.13998	[M+H] ⁺	C ₂₁ H ₁₇ NO	Anisoles	---
1675	Hydroxybenzoylcholine	6.135	224.12712	[M] ⁺	C ₁₂ H ₁₈ NO ₃	Benzoic acid esters	---
1676	4-Hydroxybenzotriazole	6.817	134.03499	[M-H] ⁻	C ₆ H ₅ N ₃ O	Benzotriazoles	---
1677	4-hydroxy-6-methoxy-3-benzylhydroquinolin-2-one	8.709	280.09631	[M-H] ⁻	C ₁₇ H ₁₅ NO ₃	Hydroxyquinolines	---
1678	4-hydroxy-5-(1,2,3-trihydroxy-3-phenylpropyl)oxolan-2-one	6.174	286.12726	[M+H] ⁺	C ₁₃ H ₁₆ O ₆	Gamma butyrolactones	---
1679	4-hydroxy-3-phenyl-6-(phenylmethoxy)hydroquinolin-2-one	6.747	366.1138	[M+Na] ⁺	C ₂₂ H ₁₇ NO ₃	Phenylquinolines	---
1680	4-hydroxy-3-phenyl-6-(phenylmethoxy)hydroquinolin-2-one	6.039	342.11002	[M-H] ⁻	C ₂₂ H ₁₇ NO ₃	Phenylquinolines	---
1681	4-hydroxy-3,3,5-trimethyl-4-[(1E)-3-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}but-1-en-1-yl]cyclohexan-1-one	8.363	406.24548	[M+2H] ²⁺	C ₁₉ H ₃₂ O ₈	Fatty acyl glycosides	---
1682	4-Hydroxy-2H-pyran-3-carboxaldehyde 4H-Cyclopenta[a]cyclopropa[f]cycloundecen-4-one, 4a,7,8-tris(acetyloxy)-	1.687	127.03864	[M+H] ⁺	C ₆ H ₆ O ₃	Pyrans	---
1683	1,1a,4a,5,6,7,7a,8,9,10,11,11a-dodecahydro-1,1,3,6-tetramethyl-9-methylene-, (1aR,2E,4aR,6S,7S,7aR,4H)-1-Benzopyran-4-one, 2,3-dihydro-5,7-dimethoxy-8-(3-methyl-2-butenyl)-2-phenyl-, (2S)-	2.293	499.20956	[M+H] ⁺	C ₂₆ H ₃₆ O ₇	Diterpenoids	---
1684		7.587	351.16373	[M-H] ⁻	C ₂₂ H ₂₄ O ₄	8-prenylated flavans	---
1685	4-Glucogallic acid	6.273	331.06503	[M-H ₂ O-H] ⁻	C ₁₃ H ₁₆ O ₁₀	Organooxygen compounds	---
1686	4-Deoxypyridoxine	5.299	154.08545	[M+H-H ₂ O] ⁺	C ₈ H ₁₁ NO ₂	Pyridines and derivatives	---
1687	4-Deoxyphloridzin	0.946	419.13797	[M-H] ⁻	C ₂₁ H ₂₄ O ₉	Flavonoid O-glycosides	---
1688	4-Deoxyerythronic acid	1.174	119.03254	[M-H] ⁻	C ₄ H ₈ O ₄	Organooxygen compounds	---
1689	4-chlorophenylthio 3,4,5-trimethoxyphenyl ketone	10.403	337.03333	[M-H] ⁻	C ₁₆ H ₁₅ ClO ₄ S	Benzoic acids and derivatives	---
1690	4-Chloro-N-methylaniline	0.231	142.03838	[M+NH ₄] ⁺	C ₇ H ₈ ClN	Aralkylamines	---
1691	4-Chloro-N-methylaniline	6.914	142.03835	[M+H] ⁺	C ₇ H ₈ ClN	Aralkylamines	---
1692	4-Chloro-N-methylaniline	1.11	142.03801	[M+Na] ²⁺	C ₇ H ₈ ClN	Aralkylamines	---
1693	4-Chloro-N-methylaniline	13.527	142.03799	[M+H] ²⁺	C ₇ H ₈ ClN	Aralkylamines	---
1694	4-Chlorohippuric acid	13.524	196.01622	[2M+H] ⁺	C ₉ H ₈ ClNO ₃	Benzamides	---

1695	4-Anilino-4-oxobutanoic acid	3.963	194.08008	[M+NH4] ⁺	C10H11NO3	Benzene and substituted derivatives	---
1696	4-Aminophenylacetic acid	8.43	152.07004	[M+H] ⁺	C8H9NO2	Benzene and substituted derivatives	---
1697	4-[5-(benzimidazol-2-ylmethylthio)(1,3,4-oxadiazol-2-yl)]-1,2-dimethoxybenzene	6.249	367.08551	[M-H] ⁻	C18H16N4O3S	Dimethoxybenzenes	---
1698	4-[5-(4-hydroxy-3,5-dimethoxyphenyl)-3,4-dimethyloxolan-2-yl]-2,6-dimethoxyphenol	11.107	427.17123	[M+Na] ⁺	C22H28O7	7,7'-epoxylignans	---
1699	4-[4-[(4-hydroxy-3-methoxyphenyl)methyl]-3-(hydroxymethyl)oxolan-2-yl]benzene-1,2-diol	8.394	391.13824	[M-H] ⁻	C19H22O6	7,9'-epoxylignans	---
1700	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	12.212	425.28497	[M+H] ⁺	C24H42O7	Colensane and clerodane diterpenoids	---
1701	4-[3-(Hydroxymethyl)-5-(3-hydroxypropyl)-7-methoxy-2,3-dihydro-1-benzofuran-2-yl]-2-methoxyphenyl 6-deoxy-alpha-D-mannopyranoside	6.502	529.20203	[M+H] ⁺	C26H34O10	2-arylbenzofuran flavonoids	---
1702	4-[2-[5,5-Dimethyl-8-(4-methylphenyl)-6H-naphthalen-2-yl]ethynyl]benzoic acid	6.842	393.18503	[M+H] ⁺	C28H24O2	Prenol lipids	---
1703	4-[2-[5,5-Dimethyl-8-(4-methylphenyl)-6H-naphthalen-2-yl]ethynyl]benzoic acid	6.465	393.18573	[M+Na]2 ⁺	C28H24O2	Prenol lipids	---
1704	4-[2-[[3S)-2,3-Dihydroxy-2-[(1S)-1-hydroxyethyl]butanoyl]oxymethyl]anilino]-4-oxobutanoic acid	6.904	352.13812	[M+CH3OH+H] ⁺	C17H23NO8	Benzyloxycarbonyls	---
1705	4-[2-[[3S)-2,3-Dihydroxy-2-[(1S)-1-hydroxyethyl]butanoyl]oxymethyl]anilino]-4-oxobutanoic acid	6.73	352.13806	[M+H-H2O] ⁺	C17H23NO8	Benzyloxycarbonyls	---
1706	4-[2-[(2-Ethyl-2,3-dihydroxybutanoyl)oxymethyl]anilino]-4-oxobutanoic acid	6.92	368.13196	[M-H] ⁻	C17H23NO8	Benzyloxycarbonyls	---
1707	4-[2-[(2-Ethyl-2,3-dihydroxybutanoyl)oxymethyl]anilino]-4-oxobutanoic acid	6.314	354.15381	[M+CH3OH+H] ⁺	C17H23NO7	Benzyloxycarbonyls	---
1708	4-[2-[(2-Ethyl-2,3-dihydroxybutanoyl)oxymethyl]anilino]-4-oxobutanoic acid	6.908	352.14276	[M+H] ⁺	C17H23NO7	Benzyloxycarbonyls	---

1709	4-[[2-(4-butyl-6-chloro-2-oxochromen-7-yl)oxypropanoylamino]methyl]cyclohexane-1-carboxylic acid	6.195	464.18619	[M+CH ₃ OH+H] ⁺	C ₂₄ H ₃₀ ClNO ₆	Coumarins and derivatives	---
1710	4-[(3-(2H-benzo[3,4-d]1,3-dioxolan-5-yl)-3-oxopropyl)amino]benzoic acid	10.169	312.08606	[M-H] ⁻	C ₁₇ H ₁₅ NO ₅	Aminobenzoic acids and derivatives	---
1711	4-[(2E)-3-(2,3,4-trimethoxyphenyl)prop-2-enoyl]phenyl thiodiphenyl-2-carboxylate	0.819	423.08853	[M-H] ⁻	C ₂₃ H ₂₀ O ₆ S	Retrochalcones	---
1712	dimethoxyphenoxy)methyl]hydroquinolin-2-one	8.762	312.12201	[M+H] ⁺	C ₁₈ H ₁₇ NO ₄	Hydroquinolones	---
1713	4,6-Dihydroxy-3-(3-hydroxy-2,5-dimethylphenoxy)-5-methoxy-2,5-dimethylcyclohex-2-en-1-one	3.206	321.16415	[M+H] ⁺	C ₁₇ H ₂₂ O ₆	Xylenols	---
1714	4,5-Dimethylloxazole	6.414	98.06032	[M+H] ⁺	C ₅ H ₇ NO	Azoles	---
1715	4,5-dihydroxy-3-propylcyclopent-2-en-1-one	7.824	174.11174	[M+H] ⁺	C ₈ H ₁₂ O ₃	Polyols	---
1716	4,5-dihydroxy-3-propylcyclopent-2-en-1-one	7.979	174.11166	[M+NH ₄] ⁺	C ₈ H ₁₂ O ₃	Polyols	---
1717	4,5-Diferuloylquinic Acid	6.4	543.15253	[2M-H] ⁻	C ₂₇ H ₂₈ O ₁₂	Cyclic alcohols and derivatives	---
1718	4,5,8-trihydroxy-5-(hydroxymethyl)-3-(3-methoxy-3-oxoprop-1-en-2-yl)-8a-methyldecahydronaphthalen-2-yl 3,4-dihydroxy-2-methylidenephutanoate	6.722	443.19025	[M-H] ⁻	C ₂₁ H ₃₂ O ₁₀	Eudesmane, isoeudesmane or cycloeudesmane sesquiterpenoids	---
1719	4,4-Bis(6,8-dihydroxy-3-methyl-1-oxoisochromen-7-yl)-2-methoxybutanoic acid	6.211	497.11197	[M-H ₂ O-H] ⁻	C ₂₅ H ₂₂ O ₁₁	Isocoumarins and derivatives	---
1720	4,4-Bis(6,8-dihydroxy-3-methyl-1-oxoisochromen-7-yl)-2-methoxybutanoic acid	6.776	497.11243	[M-H] ⁻	C ₂₅ H ₂₂ O ₁₁	Isocoumarins and derivatives	---
1721	4,4'-(3,5-Diacetoxyheptane-1,7-diyl)bispvocatechol	10.012	467.14908	[M-H] ⁻	C ₂₃ H ₂₈ O ₈	Linear diarylheptanoids	---
1722	4,15,26-trihydroxy-1-oxa-4,9,15,20,26,31-hexazacyclotritriacontane-5,8,16,19,27,30-hexone	11.361	603.33124	[M+H] ⁺	C ₂₆ H ₄₆ N ₆ O ₁₀	Macrolactams	---
1723	4,15,26-trihydroxy-1-oxa-4,9,15,20,26,31-hexazacyclotritriacontane-5,8,16,19,27,30-hexone	11.955	603.33093	[M+Na] ⁺	C ₂₆ H ₄₆ N ₆ O ₁₀	Macrolactams	---
1724	4-(Hydroxymethyl)-1-isopropyl-3-cyclohexen-1-yl beta-D-glucopyranoside	8.27	377.17984	[M-H] ⁻	C ₁₆ H ₂₈ O ₇	Terpene glycosides	---

1725	4-(beta-D-Glucopyranosyloxy)benzyl 3-(beta-D-glucopyranosyloxy)-2-[[[(2Z)-3-(4-hydroxyphenyl)-2-propenoyl]oxy}-3-methylbutanoate 4-(4-Sulfophenyl)heptanoic acid 4-(3-Hydroxybutyl)phenyl beta-D-glucopyranoside 4-(2-Furanyl)methylene)-3,4-dihydro-2H-pyrrole 4-((9S)-3,5,14-trihydroxy-10-((E)-((1-hydroxybutan-2-yl)imino)methyl)-13-methylhexadecahydro-1H-cyclopenta[a]phenanthren-17-yl)furan-2(5H)-one 3-Phenylacetylaminodione 2,6-piperidinedione 3-Oxotetradecanoic acid 3-Oxo-octadecanoic acid 3-Oxo-hexadecanoic acid 3-oxo-C9-HSL 3-oxo-3-[[[(2R,3S,4S,5R,6S)-3,4,5-trihydroxy-6-(4-hydroxy-5-methyl-2-propan-2-ylphenoxy)oxan-2-yl]methoxy]propanoic acid 3-O-p-hydroxybenzoyl ceanothic acid 3-Methylpimelic acid 3-methylmalate(2-) 3-Methylene-indolenine 3-Methylazelaic acid 3-methyl-5-(phenylmethoxy)indol-2-yl morpholin-4-yl ketone 3-methyl-2-(4-methyl-2-(4-oxo-4-(((5aS,6R,12S)-3,6,9-trimethyldecahydro-3H-3,12-epoxy[1,2]dioxepino[4,3-i]isochromen-10-yl)oxy)butanamido)pentamido)pentanoic acid 3-Methoxysalicylic acid	1.33	711.24878	[M+H] ⁺	C33H42O17	Glycosyl compounds	---
1726	4-(3-Hydroxybutyl)phenyl beta-D-glucopyranoside	1.009	285.0802	[M-H] ⁻	C13H18O5S	Benzenesulfonic acids and derivatives	---
1727	4-(2-Furanyl)methylene)-3,4-dihydro-2H-pyrrole	9.335	351.13922	[M+Na] ⁺	C16H24O7	Glycosyl compounds	---
1728	4-((9S)-3,5,14-trihydroxy-10-((E)-((1-hydroxybutan-2-yl)imino)methyl)-13-methylhexadecahydro-1H-cyclopenta[a]phenanthren-17-yl)furan-2(5H)-one	6.611	148.07495	[M+H] ⁺	C9H9NO	Heteroaromatic compounds	---
1729	3-Phenylacetylaminodione 2,6-piperidinedione	7.545	476.30487	[M+NH4] ⁺	C27H41NO6	Cardenolides and derivatives	---
1730	3-Oxotetradecanoic acid	6.256	247.10643	[M+H] ⁺	C13H14N2O3	Carboxylic acids and derivatives	---
1731	3-Oxo-octadecanoic acid	10.691	241.17911	[M-H] ⁻	C14H26O3	Fatty Acyls	---
1732	3-Oxo-hexadecanoic acid	11.421	297.24182	[M-H] ⁻	C18H34O3	Fatty Acyls	---
1733	3-oxo-C9-HSL	11.338	269.21057	[M-H] ⁻	C16H30O3	Fatty Acyls	---
1734	3-oxo-3-[[[(2R,3S,4S,5R,6S)-3,4,5-trihydroxy-6-(4-hydroxy-5-methyl-2-propan-2-ylphenoxy)oxan-2-yl]methoxy]propanoic acid	9.545	256.15311	[M+Na] ⁺	C13H21NO4	Amino acids and derivatives	---
1735	3-O-p-hydroxybenzoyl ceanothic acid	8.173	413.14185	[M-H] ⁻	C19H26O10	Terpene glycosides	---
1736	3-Methylpimelic acid	12.225	605.34912	[M-H] ⁻	C37H50O7	Triterpenoids	---
1737	3-methylmalate(2-)	8.172	173.07988	[M-H] ⁻	C8H14O4	Fatty Acyls	---
1738	3-Methylene-indolenine	1.998	147.02768	[M-H] ⁻	C5H8O5	Fatty Acyls	---
1739	3-Methylazelaic acid	6.696	130.06462	[M+CH3OH+H] ⁺	C9H7N	Indoles and derivatives	---
1740	3-methyl-5-(phenylmethoxy)indol-2-yl morpholin-4-yl ketone	9.369	201.1111	[M-H] ⁻	C10H18O4	Fatty Acyls	---
1741	3-methyl-2-(4-methyl-2-(4-oxo-4-(((5aS,6R,12S)-3,6,9-trimethyldecahydro-3H-3,12-epoxy[1,2]dioxepino[4,3-i]isochromen-10-yl)oxy)butanamido)pentamido)pentanoic acid	6.389	349.15939	[M-H] ⁻	C21H22N2O3	Indolecarboxamides and derivatives	---
1742	3-Methoxysalicylic acid	8.391	611.35431	[M+2H] ²⁺	C31H50N2O10	Peptides	---
1743	3-Methoxysalicylic acid	7.153	167.03265	[M-H] ⁻	C8H8O4	Benzene and substituted derivatives	---

1744	3-Methoxysalicyl alcohol	6.985	137.05927	[M+H-H ₂ O] ⁺	C ₈ H ₁₀ O ₃	Methoxyphenols	---
1745	3-methoxy-4-[2-methoxy-4-(1,2,3-trihydroxypropyl)phenoxyl]benzoic acid	10.362	347.11139	[M+H] ⁺	C ₁₈ H ₂₀ O ₈	Diphenylethers	---
1746	3-Methoxy-4,5-methylenedioxybenzoic acid	10.732	207.06436	[M+H] ⁺	C ₁₁ H ₁₀ O ₄	Benzodioxoles	---
1747	3-Methoxy-4,5-methylenedioxybenzoic acid	6.873	195.02783	[M-H] ⁻	C ₉ H ₈ O ₅	Benzene and substituted derivatives	---
1748	3-isobutyl-6-(1-hydroxy-2-methylpropyl)-2(1H)-pyrazinone	6.394	225.15858	[M+H] ⁺	C ₁₂ H ₂₀ N ₂ O ₂	Pyrazines	---
1749	Hydroxytetradecanedioic acid	8.716	273.16843	[M-H] ⁻	C ₁₄ H ₂₆ O ₅	Fatty Acyls	---
1750	3-Hydroxyoctadecanoic Acid	12.062	299.25702	[M-H] ⁻	C ₁₈ H ₃₆ O ₃	Fatty Acyls	---
1751	3-Hydroxymethylglutaric acid	3.664	161.04347	[M-H] ⁻	C ₆ H ₁₀ O ₅	Dicarboxy fatty acids	---
1752	3-Hydroxymethyl xylitol	0.894	181.06944	[M-H] ⁻	C ₆ H ₁₄ O ₆	Organooxygen compounds	---
1753	3-Hydroxyhexadecanoic acid	12.763	271.22617	[M-H] ⁻	C ₁₆ H ₃₂ O ₃	Fatty Acyls	---
1754	3-Hydroxyhexadecanoic acid	12.627	271.22626	[2M-H] ⁻	C ₁₆ H ₃₂ O ₃	Fatty Acyls	---
1755	3-Hydroxyhexadecanoic Acid	12.146	255.23019	[M+Na] ⁺	C ₁₆ H ₃₂ O ₃	Long-chain fatty acids	---
1756	3-Hydroxyglabrol	8.94	407.18954	[M-H] ⁻	C ₂₅ H ₂₈ O ₅	Prenylated flavanones	---
1757	3-Hydroxyglabrol	10.801	407.18948	[M-H ₂ O-H] ⁻	C ₂₅ H ₂₈ O ₅	Prenylated flavanones	---
1758	3-Hydroxydesloratadine	1.854	325.11166	[M-H] ⁻	C ₁₉ H ₁₉ ClN ₂ O	Benzocycloheptapyridines	---
1759	3-Hydroxydesloratadine	6.018	325.11182	[M-2H] ₂ ⁻	C ₁₉ H ₁₉ ClN ₂ O	Benzocycloheptapyridines	---
1760	3-Hydroxycolensoic acid	7.11	457.18948	[M-H] ⁻	C ₂₅ H ₃₀ O ₈	Depsides and depsidones	---
1761	3-Hydroxycolensoic acid	7.834	457.18958	[M-H ₂ O-H] ⁻	C ₂₅ H ₃₀ O ₈	Depsides and depsidones	---
1762	3-Hydroxycapric acid	10.568	187.13129	[M-H] ⁻	C ₁₀ H ₂₀ O ₃	Hydroxy acids and derivatives	---
1763	3-Hydroxyadipic acid 3,6-lactone	5.415	145.04915	[M+H] ⁺	C ₆ H ₈ O ₄	Lactones	---
1764	3-Hydroxyadipic acid 3,6-lactone	1.62	145.04913	[M+H-H ₂ O] ⁺	C ₆ H ₈ O ₄	Lactones	---
1765	3-hydroxy-6,6-dimethyl-2-(3,4,5-trimethoxyphenyl)-3,5,6,7-tetrahydrobenzimidazole	0.995	369.13892	[M+H] ⁺	C ₁₈ H ₂₂ N ₂ O ₅	Substituted imidazoles	---
1766	3-hydroxy-5-methoxy-3-methoxycarbonyl-5-oxopentanoic acid	1.299	238.0905	[M+H] ⁺	C ₈ H ₁₂ O ₇	Tricarboxylic acids and derivatives	---
1767	3-hydroxy-4-(2,6,7-trihydroxy-6-methylheptan-2-yl)benzoic acid	11.46	281.1373	[M+H-H ₂ O] ⁺	C ₁₅ H ₂₂ O ₆	Sesquiterpenoids	---
1768	3-Hydroxy-2-quinoxalinecarboxylic acid	1.111	213.02332	[M+Na] ⁺	C ₉ H ₆ N ₂ O ₃	Quinoxalines	---

1769	3-Hydroxy-2H-pyran-2-one	4.29	113.02323	[M+H] ⁺	C ₅ H ₄ O ₃	Pyrans	---
1770	3-Hydroxy-2H-pyran-2-one	10.132	111.00642	[M-H ₂ O-H] ⁻	C ₅ H ₄ O ₃	Pyrans	---
1771	3-Hydroxy-2H-pyran-2-one	8.04	111.00645	[M-H] ⁻	C ₅ H ₄ O ₃	Pyrans	---
1772	3h-Indole-3-propanoic acid,a-amino-	6.657	203.08043	[M-H] ⁻	C ₁₁ H ₁₂ N ₂ O ₂	Indoles and derivatives	---
1773	3-Hexenedioic acid	5.252	145.04913	[M+H] ⁺	C ₆ H ₈ O ₄	Medium-chain fatty acids	---
1774	3-Hexadecyl-4-methoxy-5-methyloxolan-2-one	12.311	372.34616	[M+H] ⁺	C ₂₂ H ₄₂ O ₃	Gamma butyrolactones	---
1775	3-Ethylphenylsulfate	1.496	307.09872	[M+H] ⁺	C ₁₆ H ₁₈ O ₄ S	Organic sulfuric acids and derivatives	---
1776	3-Buten-2-one, 4-[4-(beta-D-glucopyranosyloxy)-2-hydroxy-2,6,6-trimethylcyclohexylidene	7.415	409.18158	[M+Na] ⁺	C ₁₉ H ₃₀ O ₈	Terpene glycosides	---
1777	3-bromophenyl 1-(4-ethoxyphenyl)(1,2,3,4-tetrahydrobeta-carbolin-2-yl) ketone	6.262	473.08728	[M-H] ⁻	C ₂₆ H ₂₃ BrN ₂ O ₂	Harmala alkaloids	---
1778	3beta,6beta-Dihydroxynortropane	1.507	144.10152	[M+NH ₄] ⁺	C ₇ H ₁₃ NO ₂	Tropane alkaloids	---
1779	3-Azetidinecarboxylic acid	1.563	102.05489	[M+H] ⁺	C ₄ H ₇ NO ₂	Azetidines	---
1780	3-Anilinoalanine	7.548	181.09648	[M+H] ⁺	C ₉ H ₁₂ N ₂ O ₂	Carboxylic acids and derivatives	---
1781	3-Aminopicolinaldehyde	2.783	123.05506	[M+NH ₄] ⁺	C ₆ H ₆ N ₂ O	Pyridines and derivatives	---
1782	3-Aminopicolinaldehyde	13.595	123.05511	[M+H] ⁺	C ₆ H ₆ N ₂ O	Pyridines and derivatives	---
1783	3-Aminopicolinaldehyde	3.26	123.05505	[M+H-H ₂ O] ⁺	C ₆ H ₆ N ₂ O	Pyridines and derivatives	---
1784	3alpha,4,7,7alpha-Tetrahydro-4-hydroxy-1H-isoindole-1,3(2H)-dione	10.587	166.0486	[M-H] ⁻	C ₈ H ₉ NO ₃	Isoindoles and derivatives	---
1785	3-acetyl-1-[2-(4-chloro-2-methylphenoxy)ethyl]-5-hydroxy-2-methylindole	11.201	402.11176	[M-H] ⁻	C ₂₀ H ₂₀ ClNO ₃	N-alkylindoles	---
1786	3-Acetoxy-16alpha-Ethyl-Pregn-5-En-20-One	9.468	409.27188	[M+H-H ₂ O] ⁺	C ₂₅ H ₃₈ O ₃	Steroid esters	---
1787	3-{3-[(3-chloro-4-fluorophenyl)amino]propanovl}chromen-2-one	1.114	328.05417	[M+NH ₄] ⁺	C ₁₈ H ₁₃ ClFNO ₃	Coumarins and derivatives	---
1788	3-[[1-(tert-butyl)(1,2,3,4-tetraazol-5-yl)][4-benzylpiperazinyl]methyl]-6-ethoxyhydroquinolin-2-one	11.474	500.27554	[M-H] ⁻	C ₂₈ H ₃₅ N ₇ O ₂	Hydroquinolones	---

1789	3-[(4-ethylphenyl)(4-hydroxy-2-oxo-8-phenyl(3-hydroxy-5-oxo-2,5-dihydro-1H-pyrrol-2-yl)-2-hydroxy-2-phenylhydroquinolin-2-yl)methyl]-4-hydroxy-1-phenylhydroquinolin-2-yl]oxyoxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)-7-3-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-3-[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy-6-[[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxy-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-6-3,8-Dihydroxy-7,14-dimethoxy-17-methyl-12,16,21-trioxapentacyclo[15.3.1.0 ^{2,15} .0 ^{4,13} .0 ^{6,11}]henicosane-2(15),3,6(11),7,9,13-hexaen-5-one	11.469	446.2507	[M+H] ⁺	C ₂₅ H ₃₅ NO ₆	Sesquiterpenoids	---
1790	3-[(4-ethylphenyl)(4-hydroxy-2-oxo-8-phenyl(3-hydroxy-5-oxo-2,5-dihydro-1H-pyrrol-2-yl)-2-hydroxy-2-phenylhydroquinolin-2-yl)methyl]-4-hydroxy-1-phenylhydroquinolin-2-yl]oxyoxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)-7-3-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-3-[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy-6-[[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxy-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-6-3,8-Dihydroxy-7,14-dimethoxy-17-methyl-12,16,21-trioxapentacyclo[15.3.1.0 ^{2,15} .0 ^{4,13} .0 ^{6,11}]henicosane-2(15),3,6(11),7,9,13-hexaen-5-one	1.276	579.17468	[M-H] ⁻	C ₃₇ H ₂₅ FN ₂ O ₄	Phenylquinolines	---
1791	3-[(4-ethylphenyl)(4-hydroxy-2-oxo-8-phenyl(3-hydroxy-5-oxo-2,5-dihydro-1H-pyrrol-2-yl)-2-hydroxy-2-phenylhydroquinolin-2-yl)methyl]-4-hydroxy-1-phenylhydroquinolin-2-yl]oxyoxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)-7-3-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-3-[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy-6-[[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxy-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-6-3,8-Dihydroxy-7,14-dimethoxy-17-methyl-12,16,21-trioxapentacyclo[15.3.1.0 ^{2,15} .0 ^{4,13} .0 ^{6,11}]henicosane-2(15),3,6(11),7,9,13-hexaen-5-one	1.065	579.1748	[2M-H] ⁻	C ₃₇ H ₂₅ FN ₂ O ₄	Phenylquinolines	---
1792	3-[(4-ethylphenyl)indol-3-ylmethyl]indole-3-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)-7-3-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-3-[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy-6-[[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxy-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-6-3,8-Dihydroxy-7,14-dimethoxy-17-methyl-12,16,21-trioxapentacyclo[15.3.1.0 ^{2,15} .0 ^{4,13} .0 ^{6,11}]henicosane-2(15),3,6(11),7,9,13-hexaen-5-one	1.437	351.18573	[M+NH ₄] ⁺	C ₂₅ H ₂₂ N ₂	Aromatic monoterpenoids	---
1793	3-[(4-ethylphenyl)indol-3-ylmethyl]indole-3-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)-7-3-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-3-[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy-6-[[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxy-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-6-3,8-Dihydroxy-7,14-dimethoxy-17-methyl-12,16,21-trioxapentacyclo[15.3.1.0 ^{2,15} .0 ^{4,13} .0 ^{6,11}]henicosane-2(15),3,6(11),7,9,13-hexaen-5-one	7.332	623.15631	[M-H] ⁻	C ₂₈ H ₃₂ O ₁₆	Flavonoid O-glycosides	---
1794	3-[(4-ethylphenyl)indol-3-ylmethyl]indole-3-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)-7-3-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-3-[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy-6-[[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxy-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-6-3,8-Dihydroxy-7,14-dimethoxy-17-methyl-12,16,21-trioxapentacyclo[15.3.1.0 ^{2,15} .0 ^{4,13} .0 ^{6,11}]henicosane-2(15),3,6(11),7,9,13-hexaen-5-one	1.366	799.22839	[M-H] ⁻	C ₃₅ H ₄₄ O ₂₁	Flavonoid O-glycosides	---
1795	3,8-di((E)-but-2-en-1-yl)-1-methyl-7,8-dihydro-1H-imidazo[2,1-f]purine-2,4(3H,6H)-dione	7.972	399.12692	[M-H] ⁻	C ₂₁ H ₂₀ O ₈	Dibenzopyrans	---
1796	3,8-di((E)-but-2-en-1-yl)-1-methyl-7,8-dihydro-1H-imidazo[2,1-f]purine-2,4(3H,6H)-dione	7.899	338.16025	[M+Na] ⁺	C ₁₆ H ₂₁ N ₅ O ₂	Xanthines	---

1797	3,8-di((E)-but-2-en-1-yl)- 1-methyl-7,8-dihydro- 1H-imidazo[2,1-f]purine- 2,4(3H,6H)-dione	7.898	316.1788	[M+2H]2+	C16H21N5O2	Xanthines	---
1798	3,7-O-diacetyl-5-O- benzoyl-13,17-oxy-14- oxopremyrsinol 3,6-dibenzyl-9-[(2,3- diamino-1,2- dihydroindol-3- yl)methyl]-1,4,7- triazonane-2,5,8-trione	9.175	577.24414	[M+Na]+	C31H38O9	Bicyclic monoterpenoids	---
1799	3,6,9,12,15,18,21,24,27- Nonaoxanonacosane- 1,29-diol	8.905	530.28918	[M+H]+	C29H32N6O3	Peptides	---
1800	3,6,9,12,15,18,21,24,27- Nonaoxanonacosane- 1,29-diol	7.546	459.27829	[M+H]+	C20H42O11	Dialkyl ethers	---
1801	3,6,9,12,15,18,21,24,27- Nonaoxanonacosane- 1,29-diol	7.547	481.26019	[M+Na]+	C20H42O11	Dialkyl ethers	---
1802	3,6,9,12,15,18,21,24,27, 30- Decaoxadotriacontane- 1,32-diol	7.696	503.30255	[M+H]+	C22H46O12	Dialkyl ethers	---
1803	3,5- Dihydroxyphenylglycine	10.3	182.04353	[M-H]-	C8H9NO4	Carboxylic acids and derivatives	---
1804	3',5'-Dideoxythymidine 3,5-dicyano-4- (dibutylamino)-N- phenylbenzenesulfonami de	6.398	211.1071	[M+NH4]+	C10H14N2O3	Diazines	---
1805	3,5-Dichloro-4-hydroxy- 2-methoxy-6- methylbenzoic acid	6.743	409.16879	[M-H]-	C22H26N4O2S	Aminobenzenesulfon amides	---
1806	3,4-Methylenesebacic acid	12.635	248.97131	[M-H]-	C9H8Cl2O4	Benzene and substituted derivatives	---
1807	3,4-Methylenesebacic acid	8.93	225.11118	[M-H]-	C12H18O4	Fatty Acyls	---
1808	3,4-Methylenesebacic acid	11.112	225.11125	[M-H2O-H]-	C12H18O4	Fatty Acyls	---
1809	3',4'-Methylenedioxy- 5,7-dimethylepicatechin	10.921	329.10132	[M-H]-	C18H18O6	Flavonoids	---
1810	3,4-Dimethyl-5-propyl-2- furannonanoic acid	11.278	293.21057	[M-H]-	C18H30O3	Fatty Acyls	---
1811	3',4',7-Trihydroxyflavone	10.023	269.04407	[M-H]-	C15H10O5	Flavones	---
1812	3,4,5-Trimethoxy-N-3- pyridylbenzamide	7.809	311.10086	[M+NH4]+	C15H16N2O4	Benzamides	---
1813	3,4,5- Trimethoxyhydrocinnami c acid	4.23	258.1322	[M+H]+	C12H16O5	Phenylpropanoic acids	---
1814	3,4,5- Trimethoxyhydrocinnami c acid	3.243	258.13214	[M+H- H2O]+	C12H16O5	Phenylpropanoic acids	---
1815	3,4',5-Trihydroxy-3',7- dimethoxyflavanone	9.583	331.07925	[M-H2O-H]-	C17H16O7	Flavonoids	---
1816	3,3,3-Trifluoro-1- propanol	1.179	113.0221	[M-H]-	C3H5F3O	PFSA	---
1817	3,29-Dibenzoyl Rarounitriol	12.619	667.43616	[M+Na]+	C44H58O5	Benzoic acid esters	---
1818	3-(sec-butyl)-2-hydroxy- 3H- benzo[e][1,4]diazepin- 5(4H)-one	7.266	233.1272	[M+H]+	C13H16N2O2	1,4-benzodiazepines	---

1819	3-(6-hydroxy-2,5,7,8-tetramethyl-3,4-dihydro-2H-1-benzopyran-2-yl)propanoic acid	12.435	301.13986	[M+Na] ⁺	C16H22O4	1-benzopyrans	---
1820	3-(4-Hydroxy-2,2-dimethyl-1-oxo-3,3a-dihydroimidazo[1,2-a]indol-4-yl)-2-(4-oxoquinazolin-3-yl)propanoic acid	5.726	433.15204	[M-H] ⁻	C23H22N4O5	Quinazolines	---
1821	3-(4-Hydroxy-2,2-dimethyl-1-oxo-3,3a-dihydroimidazo[1,2-a]indol-4-yl)-2-(4-oxoquinazolin-3-yl)propanoic acid	0.947	479.1593	[M-H2O-H] ⁻	C23H22N4O5	Quinazolines	---
1822	3-(4-Hydroxy-2,2-dimethyl-1-oxo-3,3a-dihydroimidazo[1,2-a]indol-4-yl)-2-(4-oxoquinazolin-3-yl)propanoic acid	0.931	433.15427	[2M-H] ⁻	C23H22N4O5	Quinazolines	---
1823	3-(3-Methoxy-4,5-methylenedioxyphenyl)propanoic acid	6.403	245.01003	[M-H] ⁻	C9H10O6S	Phenylsulfates	---
1824	3-(3,4-dihydroxy-2,2-dimethyl-1-oxo-3aH-imidazo[1,2-a]indol-4-yl)-2-(4-oxoquinazolin-3-yl)propanoic acid	11.076	209.07967	[M+H] ⁺	C11H12O4	Benzodioxoles	---
1825	3-(3,4-dihydro-2H-benzo[b][1,4]dioxepin-7-yl)-7-ethoxy-2-methyl-4H-chromen-4-one	1.005	449.14777	[M-H] ⁻	C23H22N4O6	Quinazolines	---
1826	3-(2-Furanylmethyl)-1H-pyrrole	6.574	375.12463	[M+Na] ⁺	C21H20O5	Isoflavones	---
1827	3-(2-Furanyl)-2-propenal	6.284	148.075	[M+NH4] ⁺	C9H9NO	Pyrroles	---
1828	3-(2,5-dihydroxy-6-methyl-3-propan-2-ylphenyl)-2-methyl-5-propan-2-ylbenzene-1,4-diol	8.135	121.02715	[M-H] ⁻	C7H6O2	Heteroaromatic compounds	---
1829	3-(2-(2H,3H-benzo[3,4-e]1,4-dioxin-6-yl)-2-oxoethyl)-3-hydroquinazolin-4-one	11.616	375.18164	[M-H] ⁻	C20H26O4	Biphenols	---
1830	3-(1-Hydroxymethyl-1-propenyl)pentanedioic acid	10.692	345.08578	[M+Na] ⁺	C18H14N2O4	Quinazolines	---
1831	3-(1H-Imidazol-4-ylmethyl)-6-(1H-indol-3-ylmethyl)-2,5-piperazinedione	7.335	201.07446	[M-H] ⁻	C9H14O5	Fatty Acyls	---
1832	3-(1-Azatricyclo[7.3.1.0 ^{5,13}]trideca-5,7,9(13)-trien-7-yl)-2-cyanoprop-2-enoic acid	6.451	324.14331	[M+H] ⁺	C17H17N5O2	Amino acids and derivatives	---
1833	Azatricyclo[7.3.1.0 ^{5,13}]trideca-5,7,9(13)-trien-7-yl)-2-cyanoprop-2-enoic acid	7.3	269.12769	[M+NH4] ⁺	C16H16N2O2	Quinolines and derivatives	---

1834	3-({2-[(11-ethyl-8,9-dihydroxy-4,6,16,18-tetramethoxy-11-azahexacyclo[7.7.2.1,?.0,?.0,?.0,?])nonadecan-13-yl}methoxy)carbonyl}phenyl}carbamoyl)-3-methylpropanoic acid	11.434	701.36755	[M+Na] ⁺	C37H52N2O11	Aconitane-type diterpenoid alkaloids	---
1835	3-({2-[(11-ethyl-8,9-dihydroxy-4,6,16,18-tetramethoxy-11-azahexacyclo[7.7.2.1,?.0,?.0,?.0,?])nonadecan-13-yl}methoxy)carbonyl}phenyl}carbamoyl)-3-methylpropanoic acid	11.293	701.36755	[M+H] ⁺	C37H52N2O11	Aconitane-type diterpenoid alkaloids	---
1836	3-((Ethylphenylamino)methyl)benzenesulfonic acid	6.599	290.08582	[M-H ₂ O-H] ⁻	C15H17NO3S	Phenylbenzamines	---
1837	3-((Ethylphenylamino)methyl)benzenesulfonic acid	1.426	292.10153	[M+H] ⁺	C15H17NO3S	Phenylbenzamines	---
1838	2-Thiocytidine	1.289	260.07312	[M+H] ⁺	C9H13N3O4S	Pyrimidine nucleosides	---
1839	2-thiocyanatopupukeanane [C16H25NS]	10.054	286.16388	[M+H] ⁺	C16H25NS	Sesquiterpenoids	---
1840	2-Phenylethyl 6-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranoside	8.319	448.21741	[M+2H] ²⁺	C20H30O10	Glycosyl compounds	---
1841	2-Phenylbenzimidazole	7.802	195.09114	[M+H] ⁺	C13H10N2	Phenylbenzimidazole	---
1842	2-Phenethylmalonic Acid	10.545	207.06384	[M-H] ⁻	C11H12O4	Benzene and substituted derivatives	---
1843	2-oxo-Butanal	6.415	85.02724	[M-H] ⁻	C4H6O2	Organooxygen compounds	---
1844	2-oxo-Butanal	1.497	87.04436	[M+H] ⁺	C4H6O2	Organooxygen compounds	---
1845	2'-O-Methylribothymidine	10.794	273.10632	[M+H] ⁺	C11H16N2O6	Pyrimidine nucleosides	---
1846	2-O-Acetyl-20-hydroxyecdysone	11.985	545.30652	[M+H-H ₂ O] ⁺	C29H46O8	Pentahydroxy bile acids, alcohols and derivatives	---
1847	2-Methyltryptoline	10.514	187.12532	[M+CH ₃ OH+H] ⁺	C12H14N2	Beta carbolines	---
1848	2-methylidene-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxobutanoic acid	1.882	296.13312	[M+H-H ₂ O] ⁺	C11H18O8	Saccharolipids	---
1849	2-methylidene-3-(6-oxalooxyhexyl)butanedioic acid	6.288	320.13354	[2M+H] ⁺	C13H18O8	Tetracarboxylic acids and derivatives	---
1850	2-Methylglutarate	5.188	147.06407	[M-H] ⁻	C6H10O4	Methyl-branched fatty acids	---
1851	2-Methylaminobenzoyl 6-Deoxy- α -L-Talopyranoside	6.304	315.15378	[M+NH ₄] ⁺	C14H19NO6	Monosaccharides	---

1852	2-Methyl-4-pentenoic acid	7.026	113.05861	[M-H ₂ O-H]-	C ₆ H ₁₀ O ₂	Branched fatty acids	---
1853	2-Methyl-4-pentenoic acid	7.603	113.05855	[M-H]-	C ₆ H ₁₀ O ₂	Branched fatty acids	---
1854	2-Methyl-4-oxopentanedioic acid	9.337	159.02757	[M-H]-	C ₆ H ₈ O ₅	Keto acids and derivatives	---
1855	2-Methyl-4-oxopentanedioic acid	6.004	159.02745	[M-H ₂ O-H]-	C ₆ H ₈ O ₅	Keto acids and derivatives	---
1856	(methylthio)-2-morpholinopropiophenone	1.59	280.13733	[M+H-H ₂ O] ⁺	C ₁₅ H ₂₁ NO ₂ S	Ketones	---
1857	(methylthio)-2-morpholinopropiophenone	2.209	280.13736	[M+H] ⁺	C ₁₅ H ₂₁ NO ₂ S	Ketones	---
1858	2-methoxyethyl 5-hydroxy-2-methyl-1-(3-methylphenyl)benzo[g]indole-3-carboxylate	8.419	388.15839	[M-H]-	C ₂₄ H ₂₃ NO ₄	Indolecarboxylic acids and derivatives	---
1859	2-methoxyethyl 5-hydroxy-2-methyl-1-(2-naphthylethyl)benzo[g]indole-3-carboxylate	3.555	454.20093	[M+H-H ₂ O] ⁺	C ₂₉ H ₂₇ NO ₄	Indolecarboxylic acids and derivatives	---
1860	2-methoxy-6-methyl-5-(phenylmethoxy)-2H-3,4,5,6-tetrahydropyran-3,4-diol	5.709	291.11667	[M+H] ⁺	C ₁₄ H ₂₀ O ₅	Glycosyl compounds	---
1861	2-methoxy-6-[(triphenylmethoxy)methyl]-2H-3,4,5,6-tetrahydropyran-3,4,5-triol	11.464	437.19131	[M+H] ⁺	C ₂₆ H ₂₈ O ₆	Triphenyl compounds	---
1862	2-methoxy-3,5-dimethyl-6-[4-[(E)-2-methyl-3-(4-hydroxymethyl)-5-(3-hydroxypropyl)-7-hydroxybenzofuran-2-yl]phenyl]beta-D-glucopyranoside	0.984	523.1842	[M-H]-	C ₂₄ H ₃₀ O ₁₀	2-arylbenzofuran flavonoids	---
1863	2-methoxy-3,5-dimethyl-6-[4-[(E)-2-methyl-3-(4-nitrophenyl)prop-2-enylidene]oxolan-2-yl]pyran-4-one	1.436	396.14856	[M+NH ₄] ⁺	C ₂₂ H ₂₃ NO ₆	Nitrobenzenes	---
1864	2-imino-N-[2-(4-methoxyphenyl)ethyl]-5-oxo-1-(oxolan-2-yl)methylidene-1,2-dihydro-2H-pyrido[2,3-d]pyrimidin-6(1H)-one	3.131	474.21661	[M+H] ⁺	C ₂₆ H ₂₇ N ₅ O ₄	Pyrido[2,3-d]pyrimidines	---
1865	2-Hydroxyvaleric acid	6.598	117.05364	[M-H]-	C ₅ H ₁₀ O ₃	Fatty Acyls	---
1866	2-Hydroxypurine	6.366	137.04527	[M+H] ⁺	C ₅ H ₄ N ₄ O	Imidazopyrimidines	---
1867	2-Hydroxyphenazine-1-Carboxylic acid	6.681	239.04776	[M-H]-	C ₁₃ H ₈ N ₂ O ₃	Quinoxalines	---
1868	2-Hydroxymyristic acid	10.447	243.19443	[M-H]-	C ₁₄ H ₂₈ O ₃	Fatty Acyls	---
1869	2-Hydroxyenterolactone	11.708	313.1055	[M-H]-	C ₁₈ H ₁₈ O ₅	Furanoid lignans	---
1870	2-Hydroxydecanedioic acid	8.313	217.10588	[M-H]-	C ₁₀ H ₁₈ O ₅	Hydroxy acids and derivatives	---
1871	2-Hydroxy-4-oxopentanoic acid	6.363	131.03284	[M-H]-	C ₅ H ₈ O ₄	Keto acids and derivatives	---
1872	2-Hydroxy-4-imino-2,5-cyclohexadienone	6.687	124.03898	[M+H] ⁺	C ₆ H ₅ NO ₂	Organonitrogen compounds	---
1873	2-Hydroxy-4-imino-2,5-cyclohexadienone	6.512	122.0226	[M-H]-	C ₆ H ₅ NO ₂	Organonitrogen compounds	---

1874	2-Hydroxy-3-(2-hydroxyphenyl)propanoic acid	6.816	181.04828	[M-H]-	C9H10O4	Phenylpropanoic acids	---
1875	2-Hydroxy-2-(2-methoxy-2-oxoethyl)butanedioic acid	6.269	224.07701	[M+Na]+	C7H10O7	Tricarboxylic acids and derivatives	---
1876	2H-benzo[d][1,3-dioxolan-5-yl-N-(4,5-dimethyl(1,3-thiazol-2-yl))carboxamide	0.896	275.05225	[M-H]-	C13H12N2O3S	Benzodioxoles	---
1877	2-Ethyl-1,2,3,4-tetrahydro-isoquinoline-3-carboxylic acid	9.352	228.10051	[M+Na]+	C12H15NO2	Tetrahydroisoquinolines	---
1878	2-decyl-3-hydroxypentanedioic acid	9.131	311.18405	[M+H-H2O]+	C15H28O5	Long-chain fatty acids	---
1879	2-Cyclopenten-1-one	6.316	83.04939	[M+H]+	C5H6O	Organooxygen compounds	---
1880	2-Cyclohexen-1-one, 4-[(1E)-3-(beta-D-glucopyranosyloxy)-1-buten-1-yl]-4-hydroxy-5-(hydroxymethyl)-3,5-dimethyl-	10.774	425.181	[M+Na]+	C19H30O9	Fatty acyl glycosides	---
1881	2-Carboxy-4-dodecanolide	8.779	241.1427	[M-H]-	C13H22O4	Lactones	---
1882	2-Butenoic acid, 2-methyl-, 5-(acetyloxy)-8-(3-furanyl)hexadecahydro-1,1,5a,7a,10b-pentamethyl-7-(2-methyl-1-oxopropoxy)-3-oxooxireno[1',5']cyclonona[1',2'-butene-1,4-diol, 2-[(1S,8aR)-1,4,4a,5,6,7,8,8a-octahydro-2-(hydroxymethyl)-5,5,8a-trimethyl-1-naphthalenyl]ethyl]-, (1R,7R)-	8.42	655.34552	[M+2H]2+	C37H50O10	Limonoids	---
1883	2-Butanone, 4-[3-(beta-D-glucopyranosyloxy)-4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl]-	12.524	345.23615	[M+Na]+	C20H34O3	Diterpenoids	---
1884	2-Aminoethyl oleate	10.111	371.20236	[M+Na]+	C19H32O8	Terpene glycosides	---
1885	2-Aminoethyl oleate	13.113	326.30411	[M+CH3OH+H]+	C20H39NO2	Fatty Acyls	---
1886	2-Aminobicyclo[3.1.0]hexane-2,6-dicarboxylic acid	12.022	186.07556	[M+H]+	C8H11NO4	Carboxylic acids and derivatives	---
1887	2-Amino-7-hydroxy-4-phenyl-4H-chromene-3-carbonitrile	9.673	263.08032	[M-H2O-H]-	C16H12N2O2	Neoflavonoids	---
1888	2-amino-6-{[2-(furan-2-yl)-2-oxoethyl]amino}hexanoic acid	6.46	253.11726	[M-H]-	C12H18N2O4	Amino acids and derivatives	---

1889	2-amino-5-oxo-4-(3,4,5-trimethoxyphenyl)-4H-pyrano[3,2-c]chromene-3-carbonitrile	6.172	441.08487	[M-2H]2-	C22H18N2O6	Angular pyranocoumarins	---
1890	2-Amino-5-methylbenzenesulfonic acid	7.959	188.03667	[M+H]+	C7H9NO3S	Benzenesulfonic acids and derivatives	---
1891	2-amino-5-[2-[[[(3S)-2,3-dihydroxy-2-[(1S)-1-hydroxyethyl]butanoyl]oxymethyl]anilino]-5-oxopentanoic acid	9.795	397.16385	[M-H]-	C18H26N2O8	Amino acids and derivatives	---
1892	2-amino-4-hydroxy-5-[[1-(4-methoxy-6-oxopyran-2-yl)-3-methylbutyl]amino]-5-oxopentanoic acid	6.891	339.15338	[M+H]+	C16H24N2O7	Amino acids and derivatives	---
1893	2-amino-4-(3-chlorophenyl)-6-(hydroxymethyl)-8-oxo-4H-pyrano[3,2-b]pyran-3-carbonitrile	0.935	331.05133	[M+H]+	C16H11ClN2O4	Pyranones and derivatives	---
1894	2-amino-4-(2,5-dimethylphenyl)-6-(hydroxymethyl)-8-oxo-4H-pyrano[3,2-b]pyran-3-carbonitrile	7.976	323.10052	[M-H]-	C18H16N2O4	p-Xylenes	---
1895	2-amino-3-hydroxynonanoic acid	6.414	172.13232	[M+H-H2O]+	C9H19NO3	Amino acids and derivatives	---
1896	2-Acetylpyrrolidine	4.511	114.09116	[M+H-H2O]+	C6H11NO	Pyrrolidines	---
1897	2-Acetyl-amino-N-Furan-2-Ylmethyl-3-Phenyl-Acrylamide	12.666	283.1077	[M-H]-	C16H16N2O3	Amino acids and derivatives	---
1898	2-Acetyl-1,5,6,7-tetrahydro-6-hydroxy-7-(hydroxymethyl)-4H-azepine-4-one	1.408	200.091	[M+CH3OH+H]+	C9H13NO4	Azepines	---
1899	2-Acetamido-4-methylphenyl acetate	7.928	208.09595	[M+H]+	C11H13NO3	Phenol esters	---
1900	2-Acetamido-4-methylphenyl acetate	8.362	206.08047	[M-H]-	C11H13NO3	Phenol esters	---
1901	2,6,28-dimethoxy-5,11,17,23-tetrakis(tert-butyl)pentacyclo[19.3.1.1<3,7>.1<9,13>.1<15,19>]octacosane	10.019	699.43378	[M+H]+	C46H60O4	Anisoles	---
1902	24-Nor Ursodeoxycholic Acid	12.899	377.27005	[M-H]-	C23H38O4	Steroids and steroid derivatives	---
1903	22-Hydroxy-2-hopen-1-one	10.165	441.37134	[M+H]+	C30H48O2	Hopanoids	---
1904	2-{4-[4-{3,5-Dihydroxy-4-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]phenyl}-2,5-bis(4-hydroxyphenyl)oxolan-3-yl]-2,6-dihydroxyphenyl}-6-(hydroxymethyl)oxane-3,4,5-triol	6.28	814.29303	[M+Na]+	C40H44O17	Stilbene glycosides	---

1905	2-{4-[(6-ethyl-2-oxochromen-4-yl)methyl]piperazinyl}-N-(3-methylthiophenyl)acetamide	6.705	452.20117	[M+H-H ₂ O] ⁺	C ₂₅ H ₂₉ N ₃ O ₃ S	Amino acids and derivatives	---
1906	2-{2-oxo-4-[N-benzylcarbamoyl]hydroquinolinyl}-N-(2,4,6-trimethylphenyl)acetamide	7.59	452.20081	[M-H] ⁻	C ₂₈ H ₂₇ N ₃ O ₃	Quinoline carboxamides	---
1907	2-{1-[(4-chlorophenyl)carbonyl]-5-methoxy-2-methylindol-3-yl}-N-(2-methoxyethyl)acetamide	4.748	459.13315	[M-H] ⁻	C ₂₂ H ₂₃ ClN ₂ O ₄	Benzoylindoles	---
1908	2-[6-hydroxy-2-(3,4,5-trimethoxyphenyl)-3-azabicyclo[4.4.0]dec-3-yl]-N-(4-methoxyphenyl)acetamide	8.627	529.2522	[M-H] ⁻	C ₂₇ H ₃₆ N ₂ O ₆	Phenylpiperidines	---
1909	2-[5-[2-[2-[5-[2-[2-[5-[2-[2-[5-(2-Hydroxybutyl)oxolan-2-yl]propanoyloxy]propyl]oxolan-2-yl]propanoyloxy]propyl]oxolan-2-yl]propanoyloxy]propyl]oxolan-2-yl]propanoic acid	12.395	807.58063	[M+H] ⁺	C ₄₁ H ₆₈ O ₁₃	Tetracarboxylic acids and derivatives	---
1910	2-[5-[2-[2-[5-(2-Hydroxypropyl)oxolan-2-yl]propanoyloxy]propyl]oxolan-2-yl]propanoic acid	9.152	369.22302	[M+CH ₃ OH+H] ⁺	C ₂₀ H ₃₄ O ₇	Dicarboxylic acids and derivatives	---
1911	2-[5-[2-[2-[5-(2-Hydroxypropyl)oxolan-2-yl]propanoyloxy]propyl]oxolan-2-yl]propanoic acid	10.929	369.22287	[M+H-H ₂ O] ⁺	C ₂₀ H ₃₄ O ₇	Dicarboxylic acids and derivatives	---
1912	2-[5-[2-[2-[5-(2-Hydroxypropyl)oxolan-2-yl]propanoyloxy]propyl]oxolan-2-yl]propanoic acid	11.252	369.22281	[M+H] ⁺	C ₂₀ H ₃₄ O ₇	Dicarboxylic acids and derivatives	---
1913	2-[4-(2-furylcarbonyl)piperazinyl]-N-(6-methoxybenzothiazol-2-yl)acetamide	9.97	399.11197	[M-H] ⁻	C ₁₉ H ₂₀ N ₄ O ₄ S	Amino acids and derivatives	---
1914	2-[4-(2-furylcarbonyl)piperazinyl]-N-(6-methoxybenzothiazol-2-yl)acetamide	13.58	399.11169	[2M-H] ⁻	C ₁₉ H ₂₀ N ₄ O ₄ S	Amino acids and derivatives	---

1915	2-[3-[2-(1,3-Benzodioxol-5-yl)-7-methoxy-1-benzofuran-5-yl]-3-hydroxypropoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	11.394	487.15912	[M+Na] ⁺	C25H28O11	2-arylbenzofuran flavonoids	---
1916	2-[2-oxo-4-(piperidylcarbonyl)hydroquinolyl]-N-(2-nphenylethyl)acetamide	6.363	462.20679	[M-H] ⁻	C25H27N3O3	Quinoline carboxamides	---
1917	2-[2-oxo-4-(N-propylcarbonyl)hydroquinolyl]-N-(2,4,6-trimethylphenyl)acetamid	8.296	406.21484	[M+2H] ²⁺	C24H27N3O3	Quinoline carboxamides	---
1918	2-[2-amino-3-(1H-imidazol-5-yl)propanamido]-3-hydroxypropanoic acid	13.654	241.09131	[M-H] ⁻	C9H14N4O4	Peptides	---
1919	2-[1-[(2R,3R,4S,5R)-4-hydroxy-3,5-bis[[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]oxan-2-yl]indol-2-yl]acetic acid	9.312	649.24689	[M+H] ⁺	C27H37NO16	Indole-3-acetic acid derivatives	---
1920	2-[1-(4-methoxyphenyl)(1,2,3,4-tetrahydrobeta-carbolin-2-yl)]-N-naphthylacetamide	1.567	462.21689	[M+H] ⁺	C30H27N3O2	Harmala alkaloids	---
1921	2-[1-(4-hydroxy-3,5-dimethoxyphenyl)-3-(hydroxymethyl)-6,8-dimethoxy-1,2,3,4-tetrahydronaphthalen-2-yl]methoxy]-6-(hydroxymethyl)oxane-2,4,5-triol	12.223	581.26599	[M-H] ⁻	C28H38O13	Lignan glycosides	---
1922	2-[4-[4-(2,4-dimethoxy-6-methylbenzoyl)oxy-2-methyl-6-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybenzoyl]oxy-2-hydroxy-6-methylbenzoyl]amino]propanoic acid	3.983	730.23944	[M+H] ⁺	C35H39NO16	Hydrolyzable tannins	---
1923	2-[4-[4-(2,4-dimethoxy-6-methylbenzoyl)oxy-2-methyl-6-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybenzoyl]oxy-2-hydroxy-6-methylbenzoyl]amino]propanoic acid	5.874	730.23969	[M+2H] ²⁺	C35H39NO16	Hydrolyzable tannins	---

1924	2-[[4-(2,4-Dihydroxy-3,5,6-trimethylbenzoyl)oxy-2-hydroxy-6-methylbenzoyl]amino]-3-hydroxybutanoic acid	10.795	446.14545	[M+H] ⁺	C22H25NO9	Depsidates and depsidones	---
1925	2-[[2-(6-chloro-2-oxo-4-propylchromen-7-yl)oxyacetyl]amino]-3-(5-hydroxy-1H-indol-3-yl)propanoic acid	4.92	499.12811	[M+NH4] ⁺	C25H23ClN2O7	Serotonins	---
1926	2-[[2-(6-chloro-2-oxo-4-propylchromen-7-yl)oxyacetyl]amino]-3-(5-hydroxy-1H-indol-3-yl)propanoic acid	4.098	499.12817	[M+H] ⁺	C25H23ClN2O7	Serotonins	---
1927	2-[(E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enyl]oxybutanedioic acid	1.432	328.10471	[M+H] ⁺	C14H14O8	Coumaric acids and derivatives	---
1928	2-[(4-methoxy-3,5-dimethyl-2-pyridyl)methylthio]quinazolin-4-ol	9.214	326.10114	[M-H] ⁻	C17H17N3O2S	Quinazolines	---
1929	2-[(4-hydroxy-3-methoxyphenyl)methylene]cyclopenta[1,2-a]benzene-1,3-dione	6.256	279.06985	[M-H] ⁻	C17H12O4	Indanediones	---
1930	2-[(3,6-dimethyl-2,4-dioxo-1,3-dihydropyrimidinyl)methyl]benzoic acid	7.574	273.08615	[M-H] ⁻	C14H14N2O4	Benzoic acids	---
1931	2-[(2-phenylquinazolin-4-yl)amino]ethyl pyridine-3-carboxylate	3.496	405.11292	[M-H] ⁻	C22H18N4O2	Quinazolines	---
1932	2-[(2E,5E,7E,11E)-10-Hydroxy-3,7,9,11-tetramethyl-2,5,7,11-tridecatetraen-1-yl]-5,6-dimethoxy-3-methyl-4-pyridinyl 6-deoxy- α -D-mannopyranoside	8.267	562.34003	[M+2H] ²⁺	C31H47NO8	Sesquiterpenoids	---
1933	2-[(2E)-3-(3,4-dihydroxyphenyl)prop-2-enamido]-3-(4-hydroxyphenyl)propanoic acid	8.808	342.0965	[M-H2O-H] ⁻	C18H17NO6	Amino acids and derivatives	---
1934	2-[(2E)-3-(3,4-dihydroxyphenyl)prop-2-enamido]-3-(4-hydroxyphenyl)propanoic acid	9.154	342.09537	[M-H] ⁻	C18H17NO6	Amino acids and derivatives	---
1935	2,9-dimethyl-8-({5-methyl-2-[4-(methylethoxy)phenyl](1,3-oxazol-4-yl)}methylthio)hydropurin-6-one	6.14	426.15784	[M+NH4] ⁺	C21H23N5O3S	Phenyl-1,3-oxazoles	---
1936	2,9-dimethyl-8-({5-methyl-2-[4-(methylethoxy)phenyl](1,3-oxazol-4-yl)}methylthio)hydropurin-6-one	1.451	426.15775	[M+H] ⁺	C21H23N5O3S	Phenyl-1,3-oxazoles	---

1937	2,8-Dihydroxy-5,5,8-trimethyl-11-oxatetracyclo[7.3.1.0~1,9~.0~3,7~]tridecan-10-one	5.55	289.13776	[M+Na]+	C15H22O4	Diterpenoids	---
1938	2,6-Diaminopurine 2',3'-dideoxyriboside	10.854	249.10829	[M-H]-	C10H14N6O2	Purine nucleosides	---
1939	2,6-Diamino-9-(2-hydroxyethoxymethyl)purine	9.369	223.09319	[2M-H]-	C8H12N6O2	Imidazopyrimidines	---
1940	2,6-bis[(4-methoxyphenyl)methylene]-4-ethylcyclohexan-1-one	9.799	385.18146	[M+Na]+	C24H26O3	Linear diarylheptanoids	---
1941	2,6-bis[(4-methoxyphenyl)methylene]-4-ethylcyclohexan-1-one	9.797	363.19962	[M+H]+	C24H26O3	Linear diarylheptanoids	---
1942	2,6-Anhydro-5-O-[4-({6-O-[4-(beta-D-glucopyranosyloxy)-2-methylenebutanoyl]-beta-D-glucopyranosyl}oxy)-2-methylenebutanoyl]-1-O-(4-hydroxy-2-methylenebutanoyl)hexitol	5.16	827.27869	[M-H]-	C33H50O21	Saccharolipids	---
1943	2,6,10-Trimethyldodeca-6,11-Diene-2,3,10-Triol	9.824	279.19156	[M+Na]+	C15H28O3	Sesquiterpenoids	---
1944	2,5-Dihydroxybenzamide	10.221	152.03302	[M-H2O-H]-	C7H7NO3	Benzene and substituted derivatives	---
1945	2,5-Dihydro-2,4,5-trimethyloxazole	12.013	114.09113	[M+H]+	C6H11NO	Azolines	---
1946	2,5,9,10-Tetraacetoxy-14-(2-Methylbutanoyloxy)Taxa-4(20).11-Diene	13	643.29034	[M+H]+	C33H48O10	Taxanes and derivatives	---
1947	2,4-Dimethyl-1,3-oxazole-5-carboxylic acid	3.03	142.04926	[M+H]+	C6H7NO3	Azoles	---
1948	2,4-Dihydroxypyridine	7.357	112.03934	[M+H]+	C5H5NO2	Pyridines and derivatives	---
1949	2,4,18-Trihydroxy-15-(3-hydroxy-3-methylbutyl)-7,9,13-trioxapentacyclo[10.8.0.03,10.04,8.014,19]icosa-1,3(10),5,11,14,16,18-hentaen-20-one	13.498	411.11047	[M-H]-	C22H20O8	Dibenzopyrans	---
1950	2,3-O-Isopropylidene-1-O-Methyl-D-Ribosic Acid	6.519	263.07529	[2M-H]-	C9H14O6	Acetals	---
1951	2',3'-O-Isopropylidene uridine	8.518	329.09811	[M-H]-	C12H16N2O6	Pyrimidones	---
1952	2',3'-Epoxyindicolactone	6.411	381.10083	[M-H]-	C21H18O7	Psoralens	---
1953	2,3-Dimethyl-5-propylpyrazine	6.296	151.12256	[M+NH4]+	C9H14N2	Diazines	---
1954	2,3-dihydroxypropyl 3-hydroxytetradecanoate	7.727	336.27234	[M+H]+	C17H34O5	Fatty alcohols	---
1955	2,3-Dihydrobenzofuran	3.837	121.06448	[M+H]+	C8H8O	Coumarans	---

1956	2,3-Dihydro-6-methyl-1H-pyrrolizine-5-carboxaldehyde	8.868	150.09099	[M+H] ⁺	C9H11NO	Pyrrolizines	---
1957	2,3-Dihydro-6-methyl-1H-pyrrolizine-5-carboxaldehyde	6.396	150.09108	[M+H-H ₂ O] ⁺	C9H11NO	Pyrrolizines	---
1958	2,3-Dihydro-1H-pyrrolizine-5-carboxaldehyde	8.268	136.07506	[M+H-H ₂ O] ⁺	C8H9NO	Pyrrolizines	---
1959	2,3-Dihydro-1H-pyrrolizine-5-carboxaldehyde	7.028	136.07503	[M+H] ⁺	C8H9NO	Pyrrolizines	---
1960	2,3,4,6-tetrahydroxy-5-oxo-5h-benzo[7]annulene-8-carboxylic acid	6.693	219.04918	[M-H] ⁻	C12H8O7	Tropolones	---
1961	2,3,4,6-tetrahydroxy-5-oxo-5h-benzo[7]annulene-8-carboxylic acid	6.446	219.04926	[M-H ₂ O-H] ⁻	C12H8O7	Tropolones	---
1962	Pentahydroxyhexyl 2-[2-[2-(2-acetyloxy-3-methylbutanoyl)oxy-3-methylpentanoyl]oxy-3-methylpentanoyl]oxy-3-methylpentanoate	8.617	798.44641	[M+2H] ²⁺	C37H64O17	Hexacarboxylic acids and derivatives	---
1963	[(5xi,9xi,13xi,17xi,18xi,19xi)-Lup-20(29)-Ene-3,28-Diylbis(Oxycarbonyl)]Di benzoic Acid	8.501	739.42047	[M+H] ⁺	C46H58O8	Triterpenoids	---
1964	2,2,6,6-Tetramethylpiperidin-1-ol	11.037	158.15334	[M+H] ⁺	C9H19NO	Piperidines	---
1965	2,2',4,4',6,6'-hexamethoxy-1,1'-biphenyl	11.812	333.13281	[M-H] ⁻	C18H22O6	Biphenyls and derivatives	---
1966	2,2,2-trifluoro-N-[2-(5-methoxy-2-methylindol-3-yl)ethyl]acetamide	7.148	345.10666	[M-H] ⁻	C14H15F3N2O2	3-alkylindoles	---
1967	2,17-Dimethylspiro[15-oxa-2,10,17-triazatetracyclo[10.3.2.0.2,11.0.4,9]heptadeca-4,6,8,10-tetraene-14,4'-3,3a-dihydro-2H-imidazo[1,2-a]indole]-2,17alpha-Dimethyl-17beta-Hydroxymethyl-18-Nor-5alpha-Androsta-13-Ene-3-One	1.443	444.16837	[M+H-H ₂ O] ⁺	C24H21N5O4	Quinazolines	---
1968	2-(N-Morpholino)ethanesulfonic acid	10.073	281.22437	[M+H-H ₂ O] ⁺	C21H32O2	---	---
1969	2-(acetylamino)-3-indol-3-yl-N-[2-(2-phenylphenoxy)ethyl]propanamide	7.26	218.04741	[M+CH3OH+H] ⁺	C6H13NO4S	Morpholines	---
1970	2-(7-hydroxy-6-methyloctyl)-2H-furan-5-one	1.352	464.19559	[M+H-H ₂ O] ⁺	C27H27N3O3	Amino acids and derivatives	---
1971	2-(7-hydroxy-6-methyloctyl)-2H-furan-5-one	10.06	244.1899	[M+H] ⁺	C13H22O3	Fatty alcohols	---

1972	2-(7-Hydroxy-11-methyl-2,9-dioxo-12,15-dioxatetracyclo[8.4.1.01,10.03,8]pentadeca-3(8),4,6-trien-13-yl)acetic acid	6.372	336.1102	[M+Na] ⁺	C16H14O7	Naphthopyranones	---
1973	2-(6-Hydroxyhexyl)-3-methylenesuccinic acid	8.233	229.10619	[M-H] ⁻	C11H18O5	Medium-chain hydroxy acids and derivatives	---
1974	2-(5-methoxy-4,8,8-trimethyl-2-oxo-2,8,9,10-tetrahydropyrano[2,3-f]chromen-3-yl)-N-(pyridin-2-yl)acetamide	11.335	409.17389	[M+Na] ⁺	C23H24N2O5	Angular pyranocoumarins	---
1975	2-(4-oxoquinazolin-3(4H)-yl)ethyl isobutyrate	7.692	261.12158	[M+H] ⁺	C14H16N2O3	Quinazolines	---
1976	2-(4-hydroxy-5,7-dimethylpyridino[2,3-d]pyrimidin-2-ylthio)-N-(2-methoxyphenyl)acetamide	6.853	369.10181	[M-H] ⁻	C18H18N4O3S	Pyrido[2,3-d]pyrimidines	---
1977	2-(4-fluorophenyl)-3-hydroxy-7-methylchromen-4-one	8.408	271.07684	[M+H] ⁺	C16H11FO3	Flavonols	---
1978	2-(4-Ethenyl-2,5-Dimethylhexa-2,5-Dienoxy)-6-(Hydroxymethyl)Oxane-3,4,5-Triol	1.324	337.17007	[M+H] ⁺	C16H26O6	Fatty acyl glycosides	---
1979	2-(4-Ethenyl-2,5-Dimethylhexa-2,5-Dienoxy)-6-(Hydroxymethyl)Oxane-3,4,5-Triol	1.554	337.17023	[M+NH4] ⁺	C16H26O6	Fatty acyl glycosides	---
1980	2-(4-chloro-3-methylphenoxy)-N-[3-methyl-4-(2-oxochromen-3-yl)phenyl]acetamide	5.544	434.11658	[M+H] ⁺	C25H20ClNO4	Isoflav-3-enones	---
1981	2-(4-chloro-3-methylphenoxy)-N-[3-methyl-4-(2-oxochromen-3-yl)phenyl]acetamide	5.439	434.11658	[M+2H] ²⁺	C25H20ClNO4	Isoflav-3-enones	---
1982	2-(4a,9,10a-trihydroxy-1-methyl-5,10-dioxo-3,4-dihydro-1H-benzo[g]isochromen-3-yl)acetic acid	7.984	335.0777	[M-H] ⁻	C16H16O8	Naphthopyranones	---
1983	2-(3-carboxypropanoylamino)hexanoic acid	7.67	254.101	[M+H] ⁺	C10H17NO5	Amino acids and derivatives	---
1984	2-[2-(3,4-dihydroxyphenyl)ethoxy]-2-oxoethyl]-5-hydroxy-4a,5,7,7a-tetrahydro-4H-furo[3,4-b]pyran-3-carboxylate	6.264	515.15961	[2M-H] ⁻	C26H28O11	Tyrosols and derivatives	---
1985	2-(3,4-dihydroxyoxolan-2-yl)-2-hydroxyethyl octadecanoate	13.079	431.3356	[M+H] ⁺	C24H46O6	Fatty acid esters	---

1986	2-(3,4-dihydroxyoxolan-2-yl)-2-hydroxyethyl hexadecanoate	11.922	403.30319	[M+H-H ₂ O] ⁺	C ₂₂ H ₄₂ O ₆	Fatty acid esters	---
1987	2-(2-hydroxybut-3-en-2-yl)-3a,6,6,9a-tetramethyl-2,4,5,5a,7,8,9,9b-octahydro-1H-benzo[e][1]benzofuran-4,5-diol	12.367	361.23318	[M+Na] ⁺	C ₂₀ H ₃₄ O ₄	Naphthofurans	---
1988	2-(2-amino-3-carbamoylpropanamido)-3-phenylpropanoic acid	6.572	280.12836	[M+Na] ⁺	C ₁₃ H ₁₇ N ₃ O ₄	Peptides	---
1989	2-(2,4-difluorophenoxy)-N-[2-(2-methylindol-3-yl)ethyl]acetamide	9.147	389.12842	[2M-H] ⁻	C ₁₉ H ₁₈ F ₂ N ₂ O ₂	3-alkylindoles	---
1990	2-(2,4-difluorophenoxy)-N-[2-(2-methylindol-3-yl)ethyl]acetamide	10.266	389.12833	[M-H] ⁻	C ₁₉ H ₁₈ F ₂ N ₂ O ₂	3-alkylindoles	---
1991	2-(2-(2-Methylphenoxy)methyl)-phenyl-2-(methoxyimido)acetic acid	8.329	298.10663	[M-H] ⁻	C ₁₇ H ₁₇ NO ₄	Phenol ethers	---
1992	2-(2-(2-Methylphenoxy)methyl)-phenyl-2-(methoxyimido)acetic acid	8.784	298.10651	[M-H ₂ O-H] ⁻	C ₁₇ H ₁₇ NO ₄	Phenol ethers	---
1993	2-(1-hydroxy-1-methoxy-3-methylbutyl)-6-methyl-5H-[1,3]dioxolo[4,5-c]pyridin-4-one	6.488	292.11703	[M+Na] ⁺	C ₁₃ H ₁₉ NO ₅	Pyridinones	---
1994	2-(1-hydroxy-1-methoxy-3-methylbutyl)-6-methyl-5H-[1,3]dioxolo[4,5-c]pyridin-4-one	6.754	270.13226	[M+H] ⁺	C ₁₃ H ₁₉ NO ₅	Pyridinones	---
1995	2-(1H)-Azulenone, 6-(beta-D-glucopyranosyloxy)-4,5,6,7,8,8a-hexahydro-5-hydroxy-5-(1-hydroxy-1-methylethyl)-3,8-dimethyl-	7.372	453.20819	[M+Na] ⁺	C ₂₁ H ₃₄ O ₉	Terpene glycosides	---
1996	benzo[de]isoquinolin-2(3H)-yl)-4-methylpentanoic acid	8.465	310.10602	[M-H ₂ O-H] ⁻	C ₁₈ H ₁₇ NO ₄	Amino acids and derivatives	---
1997	benzo[de]isoquinolin-2(3H)-yl)-4-methylpentanoic acid	7.919	310.10596	[M-H] ⁻	C ₁₈ H ₁₇ NO ₄	Amino acids and derivatives	---
1998	2-(1-(/acetamido-1,2,3-trimethoxy-9-oxo-5,6,7,9-tetrahydrobenzo[a]heptalen-10-yl)amino)-N-(3-isopropyl-1H-1,2,4-triazol-5-yl)-4-(methylthio)butanamide	7.771	625.2793	[M+H] ⁺	C ₃₁ H ₄₀ N ₆ O ₆ S	Amino acids and derivatives	---

1999	2-((10R,11S,13S,17R)-11,17-dihydroxy-10,13-dimethyl-3-oxo-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl)-2-oxoethyl 4-((2-(4-(4-methoxyphenyl)-1,2,5-trimethylpiperidin-4-yl)ethyl)amino)-4,4-dimethyl-2-((tert-butoxycarbonyl)amino)methyl-6-ethyl-3-(4-methylthiazol-2-yl)-4-oxo-4H-chromen-7-yl 2-((tert-butoxycarbonyl)amino)acetate	8.571	743.427	[M+2H] ²⁺	C ₄₂ H ₆₀ N ₂ O ₈	Glucocorticoids, progestogens and derivatives	---
2000	2-((tert-butoxycarbonyl)amino)acetate	2.492	574.21729	[M+2H] ²⁺	C ₂₈ H ₃₅ N ₃ O ₈ S	Amino acids and derivatives	---
2001	Pyrrolidinecarboxaldehyde	6.469	100.07575	[M+H-H ₂ O] ⁺	C ₅ H ₉ NO	Pyrrolidines	---
2002	Pyrrolidinecarboxaldehyde	1.426	100.07574	[M+H] ⁺	C ₅ H ₉ NO	Pyrrolidines	---
2003	Piperidinecarboxaldehyde	7.133	114.09112	[M+H] ⁺	C ₆ H ₁₁ NO	Piperidines	---
2004	1-O-Sinapoylglucose	7.051	387.1268	[M-H] ⁻	C ₁₇ H ₂₂ O ₁₀	Hydroxycinnamic acid esters	---
2005	1-Oleoyl-2-acetylgllycerol	11.838	381.298	[M+H-H ₂ O] ⁺	C ₂₃ H ₄₂ O ₅	Diacylglycerols	---
2006	1-Methylpseudouridine	4.127	257.07593	[M-H] ⁻	C ₁₀ H ₁₄ N ₂ O ₆	Nucleoside and nucleotide analogues	---
2007	1-Methyl-2-pyrrolecarboxaldehyde	6.56	108.04328	[M-H] ⁻	C ₆ H ₇ NO	Organooxygen compounds	---
2008	1-Hydroxymethylpyrene	1.841	231.08487	[M+H] ⁺	C ₁₇ H ₁₂ O	Pyrenes	---
2009	1-Hydroxymethylpyrene	4.111	231.08563	[M+H-H ₂ O] ⁺	C ₁₇ H ₁₂ O	Pyrenes	---
2010	1-Hydroxyibuprofen	10.671	221.11617	[M-H] ⁻	C ₁₃ H ₁₈ O ₃	Phenylpropanoic acids	---
2011	1-Hydroxy-2,2,5,5-tetramethylpyrrolidine-3-carboxylic acid	5.612	188.12714	[M+H] ⁺	C ₉ H ₁₇ NO ₃	Pyrrolidines	---
2012	1H-Pyrrole-2-carboxaldehyde	7.123	94.0276	[M-H] ⁻	C ₅ H ₅ NO	Organooxygen compounds	---
2013	1H-Indene-4-carboxylic acid, octahydro-3a-hydroxy-3-(hydroxymethyl)-1,1,3,5-tetramethyl-	10.895	253.17592	[M+H] ⁺	C ₁₅ H ₂₆ O ₄	Iridoids and derivatives	---
2014	1H-Imidazole-4-carboxamide tri-1H-imidazo[1,2-a]indole-9-propanoic acid, 2,3,9,9a-tetrahydro-	2.253	112.05037	[M+H] ⁺	C ₄ H ₅ N ₃ O	Carboxylic acids and derivatives	---
2015	9-hydroxy-2-(2-methylpropyl)-3-oxo-α-(4-oxo-3(4H)-quinazolinyl)-, methyl ester	7.831	475.19992	[M-H] ⁻	C ₂₆ H ₂₈ N ₄ O ₅	Amino acids and derivatives	---

2016	1H-imidazo[1,2-a]indole-9-propanoic acid, 2,3,9,9a-tetrahydro-9-hydroxy-2-(2-methylpropyl)-3-oxo-alpha-(4-oxo-3(4H)-quinazolinyl)-, methyl ester	10.812	521.20624	[M-H ₂ O-H]-	C ₂₆ H ₂₈ N ₄ O ₅	Amino acids and derivatives	---
2017	Methanocyclopent[c]oxocin-4-carboxylic acid, octahydro-4-hydroxy-7-(2-hydroxy-1-methylethylidene)-, (7E)-	10.886	281.14069	[M-H]-	C ₁₅ H ₂₂ O ₅	Alpha hydroxy acids and derivatives	---
2018	1H,5H-Imidazo[1',2'	7.705	412.22061	[M+CH ₃ OH+H] ⁺	C ₂₃ H ₂₉ N ₃ O ₄	Pyridoindolones	---
2019	1-Dodecyl-2-pyrrolidinone	10.464	254.24602	[M+H] ⁺	C ₁₆ H ₃₁ NO	N-alkylpyrrolidines	---
2020	1-Cyclopropyl-6,7-difluoro-8-methoxy-1,4-dihydro-4-oxoquinoline-3-carboxylic acid	0.901	294.08093	[M-H]-	C ₁₄ H ₁₁ F ₂ NO ₄	Quinoline carboxylic acids	---
2021	Carboxyethylphenylalanine	8.418	236.09073	[M-H]-	C ₁₂ H ₁₅ NO ₄	Carboxylic acids and derivatives	---
2022	1beta-Methylcarbapenem	6.408	124.07542	[M+H] ⁺	C ₇ H ₉ NO	Lactams	---
2023	1-Aminocyclopentane-1,3-Dicarboxylic Acid	6.218	174.07701	[M+Na] ⁺	C ₇ H ₁₁ NO ₄	Carboxylic acids and derivatives	---
2024	1-acyl-PAF	10.421	538.34784	[M+H] ⁺	C ₂₆ H ₅₂ NO ₈ P	Glycerophospholipids	---
2025	1-acetyl-4-[(4-chlorophenyl)methoxy]-3-methoxybenzene	3.438	289.06564	[M-H]-	C ₁₆ H ₁₅ ClO ₃	Ketones	---
2026	19-hydroxy-18-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxicosanoic acid	13.08	505.33612	[M-H]-	C ₂₆ H ₅₀ O ₉	Saccharolipids	---
2027	18-Aminoabieta-8,11,13-Triene Sulfate	10.445	401.24857	[M+Na] ⁺	C ₂₀ H ₃₃ NO ₄ S	Diterpenoids	---
2028	18-Aminoabieta-8,11,13-Triene Sulfate	11.231	401.2486	[M+2H] ²⁺	C ₂₀ H ₃₃ NO ₄ S	Diterpenoids	---
2029	17-Hydroxypregnenolone sulfate	7.111	411.18381	[M-H]-	C ₂₁ H ₃₂ O ₆ S	Steroids and steroid derivatives	---
2030	17-(3-Furyl)-4,4,8-Trimethyl-3,16-Dioxoandrosta-1,14-Dien-7-Yl Acetate	12.306	489.33838	[M+Na] ⁺	C ₂₈ H ₃₄ O ₅	Limonoids	---
2031	16-Hydroxy-10-oxohexadecanoic acid	11.011	285.2059	[M-H]-	C ₁₆ H ₃₀ O ₄	Fatty Acyls	---
2032	15-Oxospirosolan-3-yl 2-O-(6-deoxy-alpha-L-mannopyranosyl)-beta-D-glucopyranoside	8.545	738.44421	[M+2H] ²⁺	C ₃₉ H ₆₃ NO ₁₂	Steroidal saponins	---
2033	15-Hydroxyspirosolan-3-yl 2-O-(6-deoxy-alpha-L-mannopyranosyl)-beta-D-glucopyranoside	8.227	740.46124	[M+NH ₄] ⁺	C ₃₉ H ₆₅ NO ₁₂	Steroidal saponins	---
2034	15-Acetyldeoxynivalenol	11.207	361.12598	[M+H] ⁺	C ₁₇ H ₂₂ O ₇	Trichothecenes	---

2035	15,17-Dihydroxy-9-methyl-4,10-dioxatricyclo[11.4.0.03,5]heptadeca-1(13),14,16-triene-2,11-dione	6.337	324.14331	[M+H] ⁺	C16H18O6	Ketones	---
2036	15,16-DiHODE	11.164	311.22116	[M-H2O-H] ⁻	C18H32O4	Fatty Acyls	---
2037	15,16-DiHODE	10.604	313.23499	[M+CH3OH+H] ⁺	C18H32O4	Lineolic acids and derivatives	---
2038	15,16-DiHODE	9.95	313.23499	[M+H] ⁺	C18H32O4	Lineolic acids and derivatives	---
2039	15,16-DiHODE	12.354	313.23355	[M+Na] ⁺	C18H32O4	Lineolic acids and derivatives	---
2040	1,3-dihydroxy-6-(1-hydroxyethyl)-12,14-dimethyl-3-methylidene-15-nonyl-9-propan-2-yl-1-oxa-4,7,10-triazacyclopentadecane-2,5,8,11-tetrone	9.811	584.35236	[M-H] ⁻	C28H49N3O7	Cyclic depsipeptides	---
2041	12-Oxo-20-trihydroxy-leukotriene B4	7.246	381.18918	[M-H] ⁻	C20H30O7	Fatty Acyls	---
2042	12-Hydroxyjasmonic Acid	9.779	227.12677	[M+H] ⁺	C12H18O4	Oxidized fatty acids	---
2043	12,16-dimethoxy-21-methyl-4,6-dioxa-21-azapentacyclo[10.9.0.02,10.03,7.013,18]henicos-2(10),3(7),8,13,15,17-hexaen-15-ol	11.336	387.19135	[M+H] ⁺	C21H23NO5	Benzazepines	---
2044	12(13)Ep-9-KODE	11.102	293.20908	[M+H-H2O] ⁺	C18H30O4	Long-chain fatty acids	---
2045	11-Hydroxytephrosin 11-{3-chloro-4-[(2-fluorophenyl)methoxy]phenyl}-3,3-dimethyl-	1.291	425.12817	[M-H] ⁻	C23H22O8	Rotenones	---
2046	2,3,4-trihydro-5H,10H,11H-benzo[b]benzo[2,1-f]1,4-diazepin-1-one	9.477	475.15817	[M-H] ⁻	C28H26ClFN2O ₂	Benzodiazepines	---
2047	Dimethoxydihydrokawaiin 11-(2-bromo-3,6-dimethoxyphenyl)-3,3-dimethyl-2,3,4-trihydro-5H,10H,11H-benzo[b]benzo[2,1-f]1,4-diazepin-1-one	11.077	315.12054	[M+Na] ⁺	C16H20O5	Kavalactones	---
2048	11-(2-bromo-3,6-dimethoxyphenyl)-3,3-dimethyl-2,3,4-trihydro-5H,10H,11H-benzo[b]benzo[2,1-f]1,4-diazepin-1-one	1.203	455.09894	[M-H] ⁻	C23H25BrN2O3	Benzodiazepines	---
2049	11-(2-bromo-3,6-dimethoxyphenyl)-3,3-dimethyl-2,3,4-trihydro-5H,10H,11H-benzo[b]benzo[2,1-f]1,4-diazepin-1-one	6.283	455.10168	[M-H2O-H] ⁻	C23H25BrN2O3	Benzodiazepines	---
2050	10-Oxo-13-hydroxy-11-octadecenoic acid	11.636	311.2211	[M-H] ⁻	C18H32O4	Fatty Acyls	---
2051	10-Oxo-13-hydroxy-11-octadecenoic acid	11.881	311.22134	[M-H2O-H] ⁻	C18H32O4	Fatty Acyls	---
2052	10-ethyl-14-methyl-12-oxa-4-azatetracyclo[7.6.1.0?,?.0?]hexadecan-13-one	11.767	278.21063	[M+H] ⁺	C17H27NO2	Stenine-type alkaloids	---

2053	1-{2-[(4-fluorophenyl)methyl](1,2,3,4-tetrahydrobeta-carbolinyl)}-4-methoxyphenylene	6.415	387.186	[M+H] ⁺	C25H23FN2O	Harmala alkaloids	---
2054	1-{2-[(4-fluorophenyl)methyl](1,2,3,4-tetrahydrobeta-carbolinyl)}-4-methoxyphenylene	6.282	387.18591	[M+CH3OH+H] ⁺	C25H23FN2O	Harmala alkaloids	---
2055	1-{2-[(2-chlorophenyl)methyl](1,2,3,4-tetrahydrobeta-carbolinyl)}-4-methoxyphenylene	7.56	403.15567	[M+Na] ⁺	C25H23ClN2O	Harmala alkaloids	---
2056	1-[benzyloxycarbonyl]pyrrolidine-2-carboxylic acid	6.339	250.10646	[M+CH3OH+H] ⁺	C13H15NO4	Amino acids and derivatives	---
2057	1-[8-[6-[[3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxymethyl]-3,4,5-trihydroxyoxan-2-yl]oxy-7-hydroxy-1-[(4-hydroxyphenyl)methyl]-3,4-dihydro-1H-isoquinolin-2-yl]-1-[4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-5-(trifluoromethyl)-1,3-dihydropyrimidine-2,4-dione	0.961	606.22229	[M-H] ⁻	C29H37NO13	Benzylisoquinolines	---
2058	1-[4,5-Dihydroxy-6-(Hydroxymethyl)-3-[(E)-3-(4-Hydroxyphenyl)Prop-2-Enyl]Oxyoxan-2-Yl]Oxy-6-Hydroxy-7-Methylidene-4a,5,6,7a-Tetrahydro-1H-Cyclopenta[C]Pyran-4-yl]-1-[4,5-Bis(hydroxymethyl)-3-methoxy-2-methylphenoxy]-3-methylbutane-2,3-diol	2.548	295.05713	[M-H] ⁻	C10H11F3N2O5	Pyrimidine 2'-deoxyribonucleosides	---
2059	1-[4,5-Bis(hydroxymethyl)-3-methoxy-2-methylphenoxy]-3-methylbutane-2,3-diol	3.45	519.15234	[M+H] ⁺	C25H28O12	Hydroxycinnamic acid esters	---
2060	1-[4,5-Bis(hydroxymethyl)-3-methoxy-2-methylphenoxy]-3-methylbutane-2,3-diol	9.253	323.14514	[M+Na] ⁺	C15H24O6	Benzyl alcohols	---
2061	1-[4,5-Bis(hydroxymethyl)-3-methoxy-2-methylphenoxy]-3-methylbutane-2,3-diol	8.051	318.19473	[M+2H] ²⁺	C15H24O6	Benzyl alcohols	---
2062	1,6-Dimethoxy-9H-carbazole-3-carboxaldehyde	7.073	256.09579	[M+H] ⁺	C15H13NO3	Indoles and derivatives	---
2063	1,3-dimethyl-7-(3-methylbut-2-en-1-yl)-3,7-dihydro-1H-purine-2,6-dione	6.967	249.13196	[M+H-H2O] ⁺	C12H16N4O2	Xanthines	---

2064	1,3,7-Trimethyl-9-Hydroxy-9H-Purine-2,6,8(1H,3H,7H)-Trione	6.042	225.05989	[M-H]-	C8H10N4O4	Xanthines	---
2065	1,3,5-Hexatriene	0.949	81.07022	[M+H]+	C6H8	Unsaturated hydrocarbons	---
2066	1,3,4-trimethoxy-5-[(E)-3-[2-(4-hydroxy-3-methoxyphenyl)-3-(hydroxymethyl)-7-methoxy-2,3-dihydro-1-benzofuran-5-yl]prop-2-enoyl]oxycyclohexane-1-carboxylic acid	1.452	545.16833	[M-H]-	C27H30O12	2-arylbenzofuran flavonoids	---
2067	1,2-seco-tryptacidin	10.101	345.09589	[M-H]-	C18H18O7	Benzophenones	---
2068	1,2-O-Dilinoleoyl-3-O-beta-D-galactopyranosylracglycerol	13.439	801.54712	[M+H]+	C45H78O10	1,2-diacyl-3-O-beta-D-galactosyl-sn-glycerols	---
2069	1,2-O-Dilinoleoyl-3-O-beta-D-galactopyranosylracglycerol	13.124	779.56201	[M+2H]2+	C45H78O10	1,2-diacyl-3-O-beta-D-galactosyl-sn-glycerols	---
2070	1,2-dihydroxyheptadec-16-en-4-yl acetate	13.391	327.25171	[M-H]-	C19H36O4	Long-chain fatty alcohols	---
2071	1,2-Dihydroquinoline	6.696	132.08017	[M+NH4]+	C9H9N	Quinolines and derivatives	---
2072	1,2-Dihydroisoquinoline	8.556	130.0638	[M-H]-	C9H9N	Organonitrogen compounds	---
2073	1,2:3,4-Di-O-isopropylidene-D-galactopyranose	8.959	283.11359	[M+Na]+	C12H20O6	Dioxolopyrans	---
2074	1,2,3,4-Tetrahydroquinoline	6.694	134.0961	[M+NH4]+	C9H11N	Quinolines and derivatives	---
2075	1,2,3,4-Tetrahydroisoquinoline-3-carboxylic acid	6.37	178.08531	[M+H]+	C10H11NO2	Tetrahydroisoquinolines	---
2076	1,2,3,4-Tetrahydro-1,5,7-trimethylnapthalene	10.844	175.14751	[M+H]+	C13H18	Tetralins	---
2077	1,2,3,4,5,6,7,8,9,10-decahydrobenzo[a][12]annulen-12-yl-N-[6-(1,2,3,4,5,6,7,8,9,10-decahydrobenzo[a][12]annulen-12-ylcarbonylamino)hexyl]carbamate	8.05	617.30798	[M+2H]2+	C32H44N2O10	Alkyl aryl ethers	---
2078	1-(9-hydroxy-2-isopropyl-10-(2,3,4-trimethoxyphenyl)pyrrolol[3',4']-1-(5-methoxy-1H-indol-3-yl)-2-piperidin-1-yllethane-1,2-dione	6.585	476.22098	[M+H]+	C27H29N3O5	Benzazepines	---
2079	1-(5-methoxy-1H-indol-3-yl)-2-piperidin-1-yllethane-1,2-dione	7.3	287.13736	[2M+H]+	C16H18N2O3	Indoles	---
2080	1-(5,10-Dioxohexahydro-1H,5H-dipyrrolo[1,2-a:1',2'-d]pyrazin-5a(6H)-yl)-2-propanyl carbamate	6.372	318.09958	[M+Na]+	C14H21N3O4	Amino acids and derivatives	---

2081	1-(4-Hydroxy-3-methoxyphenyl)-3-(hydroxymethyl)-7-hydroxy-6-methoxy-1,2,3,4-tetrahydronaphthalene-2-ylmethyl beta-D-glucopyranoside	7.995	567.20538	[M-H]-	C26H34O11	Lignan glycosides	---
2082	1-(4-Acetamidobenzene-1-sulfonyl)proline	6.315	357.07764	[M-H]-	C13H16N2O5S	Amino acids and derivatives	---
2083	1-(3-carboxypropyl)-3,7-dimethylxanthine	2.653	267.10626	[M+H]+	C11H14N4O4	Xanthines	---
2084	1-(2-oxo-2-(2-1,2,3,4-tetrahydroisoquinolyl)ethyl)benzo[d]azolidine-2,3-dione	1.11	343.10767	[M+H]+	C19H16N2O3	Tetrahydroisoquinolines	---
2085	1-(2H-benzo[3,4-d]1,3-dioxolen-5-yl)-3-[(3-fluorophenyl)amino]propan-1-one	1.509	288.10645	[M+CH3OH+H]+	C16H14FNO3	Benzodioxoles	---
2086	1-(2H-benzo[3,4-d]1,3-dioxolen-5-yl)-3-[(3-fluorophenyl)amino]propan-1-one	2.8	288.10654	[M+H]+	C16H14FNO3	Benzodioxoles	---
2087	1-(1-hydroxybutyl)-1,3,4,5,6,7-hexahydro-2-benzofuran-4,5,6,7-tetrol	10.541	283.11572	[M+Na]+	C12H20O6	Isobenzofurans	---
2088	1-(1-hydroxybutyl)-1,3,4,5,6,7-hexahydro-2-benzofuran-4,5,6,7-tetrol	7.411	283.11584	[M+H-H2O]+	C12H20O6	Isobenzofurans	---
2089	{[2-(2,5-dimethylindol-3-yl)ethyl]amino}-N-(4-chlorophenyl)carboxamide	1.29	364.11871	[M+Na]+	C19H20ClN3O	N-phenylureas	---
2090	{[2-(2,5-dimethylindol-3-yl)ethyl]amino}-N-(4-chlorophenyl)carboxamide	2.491	342.13748	[M+H]+	C19H20ClN3O	N-phenylureas	---
2091	{[2-(2,5-dimethylindol-3-yl)ethyl]amino}-N-(4-chlorophenyl)carboxamide	2.809	342.13763	[M+NH4]+	C19H20ClN3O	N-phenylureas	---
2092	{[2-(2,5-dimethylindol-3-yl)ethyl]amino}-N-(4-chlorophenyl)carboxamide	0.879	340.12317	[M-H]-	C19H20ClN3O	N-phenylureas	---
2093	{[1,4a-dimethyl-1-(methylethyl)(1,2,3,4,9,10,10a,4a-octahydrophenanthryl)methyl]amino}-N-(4-methoxy-3-methylphenyl)sulfonylamine	8.43	470.26944	[2M+H]2+	C28H39NO3S	Diterpenoids	---

2094	[7-(acetyloxymethyl)-4- [[4,5-dihydroxy-6- (hydroxymethyl)-3-[(E)- 3-(4- hydroxyphenyl)prop-2- enyl]oxyoxan-2- yl]oxymethyl]-7- hydroxy-4a,5,6,7a- tetrahydro-1H- cyclopenta[c]pyran-1-yl] [5-(1,3,4-trihydroxy- 2,5- bis(hydroxymethyl)oxola n-2-yl]oxy-3,4,5- trihydroxyoxan-2- yl]methoxy]-3,4,5- trihydroxyoxan-2- yl]methyl (E)-2- [5-(1,3,4-trihydroxy- 2,5- bis(hydroxymethyl)oxola n-2-yl]oxy-3,4,5- trihydroxyoxan-2- yl]methoxy]-3,4,5- trihydroxyoxan-2- yl]methyl (E)-2- methylbut-2-enoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-6- (hydroxymethyl)-4-(2- methylpropanoyloxy)oxa n-3-yl] decanoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-4-(2- methylpropanoyloxy)-6- (2- methylpropanoyloxymeth yl)oxan-3-yl] decanoate [5-Acetyloxy-3- (hydroxymethyl)-2-oxo- 6-propan-2-ylcyclohex-3- en-1-yl] 3- methylbutanoate [5-(Benzoyloxy)-3- chloro-4,6-dihydroxy-1- cyclohexen-1-yl]methyl benzoate [4-(3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2- yl]oxyphenyl]methyl 3- acetyloxy-2-hydroxy-2- [(4- hydroxyphenyl)methyl]b utanoate	6.554	695.25885	[M-H]-	C32H42O14	Terpene glycosides	---
2095	trihydroxyoxan-2- yl]methoxy]-3,4,5- trihydroxyoxan-2- yl]methyl (E)-2- [5-(1,3,4-trihydroxy- 2,5- bis(hydroxymethyl)oxola n-2-yl]oxy-3,4,5- trihydroxyoxan-2- yl]methoxy]-3,4,5- trihydroxyoxan-2- yl]methyl (E)-2- methylbut-2-enoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-6- (hydroxymethyl)-4-(2- methylpropanoyloxy)oxa n-3-yl] decanoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-4-(2- methylpropanoyloxy)-6- (2- methylpropanoyloxymeth yl)oxan-3-yl] decanoate [5-Acetyloxy-3- (hydroxymethyl)-2-oxo- 6-propan-2-ylcyclohex-3- en-1-yl] 3- methylbutanoate [5-(Benzoyloxy)-3- chloro-4,6-dihydroxy-1- cyclohexen-1-yl]methyl benzoate [4-(3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2- yl]oxyphenyl]methyl 3- acetyloxy-2-hydroxy-2- [(4- hydroxyphenyl)methyl]b utanoate	4.486	604.24231	[M+H]+	C23H38O17	Saccharolipids	---
2096	trihydroxyoxan-2- yl]methoxy]-3,4,5- trihydroxyoxan-2- yl]methyl (E)-2- methylbut-2-enoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-6- (hydroxymethyl)-4-(2- methylpropanoyloxy)oxa n-3-yl] decanoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-4-(2- methylpropanoyloxy)-6- (2- methylpropanoyloxymeth yl)oxan-3-yl] decanoate [5-Acetyloxy-3- (hydroxymethyl)-2-oxo- 6-propan-2-ylcyclohex-3- en-1-yl] 3- methylbutanoate [5-(Benzoyloxy)-3- chloro-4,6-dihydroxy-1- cyclohexen-1-yl]methyl benzoate [4-(3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2- yl]oxyphenyl]methyl 3- acetyloxy-2-hydroxy-2- [(4- hydroxyphenyl)methyl]b utanoate	6.148	604.24194	[2M+H]+	C23H38O17	Saccharolipids	---
2097	trihydroxyoxan-2- yl]methoxy]-3,4,5- trihydroxyoxan-2- yl]methyl (E)-2- methylbut-2-enoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-6- (hydroxymethyl)-4-(2- methylpropanoyloxy)oxa n-3-yl] decanoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-4-(2- methylpropanoyloxy)-6- (2- methylpropanoyloxymeth yl)oxan-3-yl] decanoate [5-Acetyloxy-3- (hydroxymethyl)-2-oxo- 6-propan-2-ylcyclohex-3- en-1-yl] 3- methylbutanoate [5-(Benzoyloxy)-3- chloro-4,6-dihydroxy-1- cyclohexen-1-yl]methyl benzoate [4-(3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2- yl]oxyphenyl]methyl 3- acetyloxy-2-hydroxy-2- [(4- hydroxyphenyl)methyl]b utanoate	8.792	654.37219	[M+2H]2+	C30H52O14	Saccharolipids	---
2098	trihydroxyoxan-2- yl]methoxy]-3,4,5- trihydroxyoxan-2- yl]methyl (E)-2- methylbut-2-enoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-6- (hydroxymethyl)-4-(2- methylpropanoyloxy)oxa n-3-yl] decanoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-4-(2- methylpropanoyloxy)-6- (2- methylpropanoyloxymeth yl)oxan-3-yl] decanoate [5-Acetyloxy-3- (hydroxymethyl)-2-oxo- 6-propan-2-ylcyclohex-3- en-1-yl] 3- methylbutanoate [5-(Benzoyloxy)-3- chloro-4,6-dihydroxy-1- cyclohexen-1-yl]methyl benzoate [4-(3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2- yl]oxyphenyl]methyl 3- acetyloxy-2-hydroxy-2- [(4- hydroxyphenyl)methyl]b utanoate	9.844	751.37231	[2M-H]-	C34H58O15	Saccharolipids	---
2099	trihydroxyoxan-2- yl]methoxy]-3,4,5- trihydroxyoxan-2- yl]methyl (E)-2- methylbut-2-enoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-6- (hydroxymethyl)-4-(2- methylpropanoyloxy)oxa n-3-yl] decanoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-4-(2- methylpropanoyloxy)-6- (2- methylpropanoyloxymeth yl)oxan-3-yl] decanoate [5-Acetyloxy-3- (hydroxymethyl)-2-oxo- 6-propan-2-ylcyclohex-3- en-1-yl] 3- methylbutanoate [5-(Benzoyloxy)-3- chloro-4,6-dihydroxy-1- cyclohexen-1-yl]methyl benzoate [4-(3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2- yl]oxyphenyl]methyl 3- acetyloxy-2-hydroxy-2- [(4- hydroxyphenyl)methyl]b utanoate	11.058	325.16324	[M-H]-	C17H26O6	Menthane monoterpenoids	---
2100	trihydroxyoxan-2- yl]methoxy]-3,4,5- trihydroxyoxan-2- yl]methyl (E)-2- methylbut-2-enoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-6- (hydroxymethyl)-4-(2- methylpropanoyloxy)oxa n-3-yl] decanoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-4-(2- methylpropanoyloxy)-6- (2- methylpropanoyloxymeth yl)oxan-3-yl] decanoate [5-Acetyloxy-3- (hydroxymethyl)-2-oxo- 6-propan-2-ylcyclohex-3- en-1-yl] 3- methylbutanoate [5-(Benzoyloxy)-3- chloro-4,6-dihydroxy-1- cyclohexen-1-yl]methyl benzoate [4-(3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2- yl]oxyphenyl]methyl 3- acetyloxy-2-hydroxy-2- [(4- hydroxyphenyl)methyl]b utanoate	10.647	425.24969	[M+CH3OH +H]+	C21H19ClO6	Benzoic acid esters	---
2101	trihydroxyoxan-2- yl]methoxy]-3,4,5- trihydroxyoxan-2- yl]methyl (E)-2- methylbut-2-enoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-6- (hydroxymethyl)-4-(2- methylpropanoyloxy)oxa n-3-yl] decanoate [5-hydroxy-2-[4- hydroxy-2,5- bis(hydroxymethyl)-3-(2- methylpropanoyloxy)oxo lan-2-yl]oxy-4-(2- methylpropanoyloxy)-6- (2- methylpropanoyloxymeth yl)oxan-3-yl] decanoate [5-Acetyloxy-3- (hydroxymethyl)-2-oxo- 6-propan-2-ylcyclohex-3- en-1-yl] 3- methylbutanoate [5-(Benzoyloxy)-3- chloro-4,6-dihydroxy-1- cyclohexen-1-yl]methyl benzoate [4-(3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2- yl]oxyphenyl]methyl 3- acetyloxy-2-hydroxy-2- [(4- hydroxyphenyl)methyl]b utanoate	8.024	535.17957	[M-H]-	C26H32O12	Glycosyl compounds	---

2102	[4,5-dihydroxy-3,4-bis(hydroxymethyl)-4a,8,8-trimethyl-5,6,7,8a-tetrahydro-1H-naphthalen-1-yl] octanoate	12.418	395.27505	[M+Na] ⁺	C23H40O6	Fatty acid esters	---
2103	[4,5-dihydroxy-3,4-bis(hydroxymethyl)-4a,8,8-trimethyl-5,6,7,8a-tetrahydro-1H-naphthalen-1-yl]	12.223	457.27728	[M-H] ⁻	C23H40O6	Fatty acid esters	---
2104	1,3-bis(methyl-1-oxo-1-(2,3,4,5,6-pentahydroxyhexoxy)pentan-2-yl)oxy-1-oxopentan-2-yl] 2-acetyloxy-3-methylpentanoate	8.851	698.39575	[M+H] ⁺	C32H56O15	Depsipeptides	---
2105	1,3-bis(methyl-1-oxo-1-(2,3,4,5,6-pentahydroxyhexoxy)pentan-2-yl)oxy-1-oxopentan-2-yl] 2-acetyloxy-3-methylpentanoate	7.322	360.16104	[M+Na] ⁺	C32H56O15	Depsipeptides	---
2106	[3-Methyl-1-[3-methyl-1-[3-methyl-1-oxo-1-(2,3,4,5,6-pentahydroxyhexoxy)pentan-2-yl]oxy-1-oxopentan-2-yl]oxy-1-oxopentan-2-yl] 2-hydroxy-3-methylpentanoate	11.517	787.39294	[M-H] ⁻	C36H64O16	Depsipeptides	---
2107	1,3-bis(methyl-1-oxo-1-(2,3,4,5,6-pentahydroxyhexoxy)pentan-2-yl)oxy-1-oxopentan-2-yl]oxy-1-oxopentan-2-yl] 2-acetyloxy-3-methylpentanoate	6.261	417.19672	[M+H] ⁺	C38H66O17	Hexacarboxylic acids and derivatives	---
2108	[3-Hydroxy-1-oxo-1-(2,3,4,5,6-pentahydroxyhexoxy)decan-5-yl] 3,5-dihydroxydecanoate	11.057	577.31641	[M+Na] ⁺	C26H50O12	Fatty alcohols	---
2109	[3-Hydroxy-1-oxo-1-(2,3,4,5,6-pentahydroxyhexoxy)decan-5-yl] 3,5-dihydroxydecanoate	12.015	535.30835	[M-H] ⁻	C26H50O12	Fatty alcohols	---

2110	[3-Hydroxy-1-[3-hydroxy-1-oxo-1-(2,3,4,5,6-pentahydroxyhexoxy)dec-5-yl]oxy-1-oxodecan-5-yl] 3,5-dihydroxydecanoate	13.326	723.45148	[M+H] ⁺	C36H68O15	Tricarboxylic acids and derivatives	---
2111	[3,8-Dihydroxy-6,9-bis(methylene)-2-oxododecahydroazulenol[4,5-b]furan-3-yl]methyl acetate	8.051	340.17603	[M+CH3OH+H] ²⁺	C17H22O6	Sesquiterpene lactones	---
2112	[3,4-dihydroxy-6-[5-hydroxy-2-(4-hydroxyphenyl)-4-oxo-7-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-3-yl]oxy-5-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]methyl acetate	8.172	843.21442	[M-H] ⁻	C35H42O21	Flavonoid O-glycosides	---
2113	[3,4,5-Trihydroxy-6-(hydroxymethyl)oxan-2-yl] 3-hydroxy-4,5-dimethoxybenzoate	1.329	383.09314	[M+H] ⁺	C15H20O10	Hydrolyzable tannins	---
2114	[3,4,5-Trihydroxy-6-(hydroxymethyl)oxan-2-yl] 3-hydroxy-4,5-dimethoxybenzoate	4.707	383.09299	[M+NH4] ⁺	C15H20O10	Hydrolyzable tannins	---
2115	[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl] 2-prop-1-en-2-yl-2,3-dihydro-1-benzofuran-5-carboxylate	10.428	367.13928	[M+H] ⁺	C18H22O8	Monosaccharides	---
2116	[2-(5-fluoro-2-methylindol-3-yl)ethyl][(2-methoxy-4,5-dimethylphenyl)sulfonyl]amine	7.257	391.14853	[M+H] ⁺	C20H23FN2O3S	Benzenesulfonamides	---
2117	[2-(5-fluoro-2-methylindol-3-yl)ethyl][(2-methoxy-4,5-dimethylphenyl)sulfonyl]amine	0.952	389.13544	[M-H] ⁻	C20H23FN2O3S	Benzenesulfonamides	---
2118	[2-(2,5-dimethylindol-3-yl)ethyl][(4-methoxynaphthyl)sulfonyl]amine	7.261	409.15808	[M+H] ⁺	C23H24N2O3S	1-naphthalene sulfonic acids and derivatives	---
2119	[1-(1-hydroxy-2,4,6,8-Tetramethyl-4,4a,5,6,7,8a,9,10-Octahydro-3H-Phenanthren-2-yl)-2-[3,4,5-Trihydroxy-6-(Hydroxymethyl)Oxan-2-yl]oxyethyl] Acetate	7.804	565.27948	[M+H] ⁺	C28H46O9	Diterpene glycosides	---

2120	[(3aR,4S,6R,11aR)-6,9-dihydroxy-6,10-dimethyl-3-methylidene-2,7-dioxo-3a,4,5,8,9,11a-hexahydrocycloclodeca[b]furan-4-yl] 2-methylprop-2-enoate	8.098	382.18591	[M+2H] ²⁺	C19H24O7	Sesquiterpene lactones	---
2121	[(2S,3R,4S,5R,6S)-4,5-dihydroxy-6-[5-hydroxy-2-(4-hydroxyphenyl)-4-oxo-7-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxychromen-3-yl]oxy-2-methyloxan-3-yl] [(2S,3R,4S,5R,6S)-4,5-dihydroxy-6-[5-hydroxy-2-(4-hydroxyphenyl)-4-oxo-7-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxychromen-3-yl]oxy-2-methyloxan-3-yl] [(2R,3S,4S,5R,6S)-6-[4-[6-[4-[(2S,3R,4S,5S,6R)-6-(acetyloxymethyl)-3,4,5-trihydroxyoxan-2-yl]oxy-3-methoxyphenyl]-1,3,3a,4,6,6a-hexahydrofuro[3,4-c]furan-3-yl]-2-methoxyphenoxy]-3,4,5-trihydroxyoxan-2-yl]methyl acetate [(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 [(2R,3S,4S,5R,6R)-6-[1,7-bis(4-hydroxyphenyl)-5-oxoheptan-3-yl]oxy-3,4,5-trihydroxyoxan-2-yl]methyl (E)-3-(4-hydroxyphenyl)prop-2-enoate [(2R,3S,4S,5R,6R)-3,4,5-trihydroxy-6-[2-(4-hydroxyphenyl)ethoxy]oxan-2-yl]methyl 2-(2-oxo-1,3-dihydroindol-3-yl)acetate	4.967	619.16693	[M-H] ⁻	C29H32O15	Flavonoid O-glycosides	---
2122	[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxychromen-3-yl]oxy-2-methyloxan-3-yl] [(2R,3S,4S,5R,6S)-6-[4-[6-[4-[(2S,3R,4S,5S,6R)-6-(acetyloxymethyl)-3,4,5-trihydroxyoxan-2-yl]oxy-3-methoxyphenyl]-1,3,3a,4,6,6a-hexahydrofuro[3,4-c]furan-3-yl]-2-methoxyphenoxy]-3,4,5-trihydroxyoxan-2-yl]methyl acetate [(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 [(2R,3S,4S,5R,6R)-6-[1,7-bis(4-hydroxyphenyl)-5-oxoheptan-3-yl]oxy-3,4,5-trihydroxyoxan-2-yl]methyl (E)-3-(4-hydroxyphenyl)prop-2-enoate [(2R,3S,4S,5R,6R)-3,4,5-trihydroxy-6-[2-(4-hydroxyphenyl)ethoxy]oxan-2-yl]methyl 2-(2-oxo-1,3-dihydroindol-3-yl)acetate	6.182	619.16949	[2M-H] ⁻	C29H32O15	Flavonoid O-glycosides	---
2123	methoxyphenyl]-1,3,3a,4,6,6a-hexahydrofuro[3,4-c]furan-3-yl]-2-methoxyphenoxy]-3,4,5-trihydroxyoxan-2-yl]methyl acetate [(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 [(2R,3S,4S,5R,6R)-6-[1,7-bis(4-hydroxyphenyl)-5-oxoheptan-3-yl]oxy-3,4,5-trihydroxyoxan-2-yl]methyl (E)-3-(4-hydroxyphenyl)prop-2-enoate [(2R,3S,4S,5R,6R)-3,4,5-trihydroxy-6-[2-(4-hydroxyphenyl)ethoxy]oxan-2-yl]methyl 2-(2-oxo-1,3-dihydroindol-3-yl)acetate	1.84	784.30548	[M+H] ⁺	C36H46O18	Lignan glycosides	---
2124	methoxyphenyl]-1,3,3a,4,6,6a-hexahydrofuro[3,4-c]furan-3-yl]-2-methoxyphenoxy]-3,4,5-trihydroxyoxan-2-yl]methyl acetate [(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 [(2R,3S,4S,5R,6R)-6-[1,7-bis(4-hydroxyphenyl)-5-oxoheptan-3-yl]oxy-3,4,5-trihydroxyoxan-2-yl]methyl (E)-3-(4-hydroxyphenyl)prop-2-enoate [(2R,3S,4S,5R,6R)-3,4,5-trihydroxy-6-[2-(4-hydroxyphenyl)ethoxy]oxan-2-yl]methyl 2-(2-oxo-1,3-dihydroindol-3-yl)acetate	9.105	519.23944	[M+H] ⁺	C22H40O12	Saccharolipids	---
2125	methoxyphenyl]-1,3,3a,4,6,6a-hexahydrofuro[3,4-c]furan-3-yl]-2-methoxyphenoxy]-3,4,5-trihydroxyoxan-2-yl]methyl acetate [(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 [(2R,3S,4S,5R,6R)-6-[1,7-bis(4-hydroxyphenyl)-5-oxoheptan-3-yl]oxy-3,4,5-trihydroxyoxan-2-yl]methyl (E)-3-(4-hydroxyphenyl)prop-2-enoate [(2R,3S,4S,5R,6R)-3,4,5-trihydroxy-6-[2-(4-hydroxyphenyl)ethoxy]oxan-2-yl]methyl 2-(2-oxo-1,3-dihydroindol-3-yl)acetate	9.177	621.23291	[M-H] ⁻	C34H38O11	Curcuminoids	---
2126	methoxyphenyl]-1,3,3a,4,6,6a-hexahydrofuro[3,4-c]furan-3-yl]-2-methoxyphenoxy]-3,4,5-trihydroxyoxan-2-yl]methyl acetate [(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 [(2R,3S,4S,5R,6R)-6-[1,7-bis(4-hydroxyphenyl)-5-oxoheptan-3-yl]oxy-3,4,5-trihydroxyoxan-2-yl]methyl (E)-3-(4-hydroxyphenyl)prop-2-enoate [(2R,3S,4S,5R,6R)-3,4,5-trihydroxy-6-[2-(4-hydroxyphenyl)ethoxy]oxan-2-yl]methyl 2-(2-oxo-1,3-dihydroindol-3-yl)acetate	2.354	472.1637	[M-H] ⁻	C24H27NO9	Saccharolipids	---

2127	[(2R,3R,4S,5S,6R)-3-acetyloxy-2-(acetyloxymethyl)-5-hexanoyloxy-6-[(2S,3R)-2,3,4-trihydroxybutoxy]oxan-4-yl] tetradecanoate	8.519	699.40326	[M+2H] ²⁺	C34H60O13	Saccharolipids	---
2128	[(2R,3R,4S,5S,6R)-3-acetyloxy-2-(acetyloxymethyl)-5-butanoyloxy-6-[(2S,3R)-2,3,4-trihydroxybutoxy]oxan-4-yl] 14-hydroxytetradecanoate	10.003	663.3559	[2M-H] ⁻	C32H56O14	Saccharolipids	---
2129	[(2R,3R,4S,5S,6R)-3,5-diacetyloxy-2-(acetyloxymethyl)-6-[(2S,3R)-2,3,4-trihydroxybutoxy]oxan-4-yl] dodecanoate	11.188	575.30267	[M+Na] ⁺	C28H48O13	Saccharolipids	---
2130	[(2R,3R,4S,5R,6R)-6-[2-(3,4-dihydroxyphenyl)ethoxy]-3,5-dihydroxy-4-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]methyl (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-[(2R,3R,4S,5R,6R)-6-[2-(3,4-dihydroxyphenyl)ethoxy]-3,5-dihydroxy-4-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]methyl (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-[(2R,3R,4S,5R,6R)-6-[2-(3,4-dihydroxyphenyl)ethoxy]-3,5-dihydroxy-4-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]methyl (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-[(2E,6Z,10Z)-7,11-bis(acetyloxymethyl)-3,15-dimethylhexadeca-2,6,10,14-tetraenyl] acetate	1.041	683.21936	[2M-H] ⁻	C30H38O15	Coumaric acids and derivatives	---
2131	[(2R,3R,4S,5R,6R)-6-[2-(3,4-dihydroxyphenyl)ethoxy]-3,5-dihydroxy-4-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]methyl (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-[(2R,3R,4S,5R,6R)-6-[2-(3,4-dihydroxyphenyl)ethoxy]-3,5-dihydroxy-4-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]methyl (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-[(2R,3R,4S,5R,6R)-6-[2-(3,4-dihydroxyphenyl)ethoxy]-3,5-dihydroxy-4-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]methyl (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-[(2E,6Z,10Z)-7,11-bis(acetyloxymethyl)-3,15-dimethylhexadeca-2,6,10,14-tetraenyl] acetate	9.078	639.22955	[M+NH ₄] ⁺	C30H38O15	Coumaric acids and derivatives	---
2132	[(2R,3R,4S,5R,6R)-6-[2-(3,4-dihydroxyphenyl)ethoxy]-3,5-dihydroxy-4-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]methyl (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-[(2E,6Z,10Z)-7,11-bis(acetyloxymethyl)-3,15-dimethylhexadeca-2,6,10,14-tetraenyl] acetate	8.921	637.21106	[M-H] ⁻	C30H38O15	Coumaric acids and derivatives	---
2133	[(2E,6E)-1-Oxo-8-hydroxy-2,6-dimethylocta-2,6-dien-1-yl]beta-D-glucopyranoside	12.352	449.28568	[M+Na] ⁺	C26H40O6	Acyclic diterpenoids	---
2134	[(2E,6E)-1-Oxo-8-hydroxy-2,6-dimethylocta-2,6-dien-1-yl]beta-D-glucopyranoside	8.675	345.15222	[M-H] ⁻	C16H26O8	Terpene glycosides	---

2135	[(1R,2S,11S,14R,15R,18S,20R)-1,7,11,15,19,19-hexamethyl-5-oxo-8,10-dioxapentacyclo[12.8.0.0 2,11.04,9.015,20]docosa-4(9),6-dien-18-yl] acetate	8.104	479.27368	[M+2H] ²⁺	C28H40O5	Naphthopyrans	---
2136	(Z)-9,12,13-trihydroxyoctadec-15-enoic acid	10.485	353.22778	[M+Na] ⁺	C18H34O5	Long-chain fatty acids	---
2137	(Z)-5-[(2R,3S,4S)-4-Hydroxy-2-[(E)-3-hydroxyoct-1-enyl]oxan-3-yl]pent-3-enoic acid	10.932	325.19949	[M-H] ⁻	C18H30O5	Hydroxy acids and derivatives	---
2138	(Z)-5,8,11-trihydroxyoctadec-9-enoic acid	9.953	348.27222	[M+NH4] ⁺	C18H34O5	Long-chain fatty acids	---
2139	(Z)-2,6-dimethyl-7-(4-methyl-5-oxooxolan-2-yl)-3-[[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]hept-5-enoic acid	11.815	445.2081	[M-H] ⁻	C21H34O10	Saccharolipids	---
2140	(Z)-13-Oxo-9-octadecenoic acid	12.162	295.22549	[M-H] ⁻	C18H32O3	Fatty Acyls	---
2141	(S)-2-(3-(4-fluorophenyl)-7-hydroxy-4-oxo-4H-chromene-2-carboxamido)-5-guanidinopentanoic acid	8.888	457.14383	[M+H] ⁺	C22H21FN4O6	Isoflavones	---
2142	(R)-3-Hydroxydodecanoic acid	11.515	215.1628	[M-H] ⁻	C12H24O3	Hydroxy acids and derivatives	---
2143	(R)-2-Hydroxycaprylic acid	9.755	159.10066	[M-H2O-H] ⁻	C8H16O3	Medium-chain fatty acids	---
2144	(Methoxymethyl)triphenylphosphonium	3.885	308.13239	[M+H] ⁺	C20H20OP	Phenylphosphines and derivatives	---
2145	(E)-Resveratrolside	8.077	405.22162	[2M-H] ⁻	C20H22O9	Stilbene glycosides	---
2146	(E)-5-(3,4,5,6-Tetrahydro-3-pyridylidenemethyl)-2-furanmethanol	6.428	192.10152	[M+H] ⁺	C11H13NO2	Pyridines and derivatives	---
2147	(E)-4-hydroxy-4-[4-hydroxy-2-[(E)-6-oxohept-1-enyl]cyclopentyl]but-2-enoic acid	9.998	297.16766	[M+H-H2O] ⁺	C16H24O5	Fatty Acyls	---
2148	(E)-3-(acetyloxymethyl)-5-(2-formyl-4-hydroxy-5,5,8a-trimethyl-1,4,4a,6,7,8-hexahydronaphthalen-1-yl)pent-2-enoic acid	12.184	415.20926	[M+H] ⁺	C22H32O6	Diterpenoids	---
2149	(E)-3-(acetyloxymethyl)-5-(2-formyl-4-hydroxy-5,5,8a-trimethyl-1,4,4a,6,7,8-hexahydronaphthalen-1-yl)pent-2-enoic acid	10.052	415.2095	[M+NH4] ⁺	C22H32O6	Diterpenoids	---

2150	(E)-3-(4-Methoxyphenyl)-N-Phenylacrylamide (alpha-keto-dimethyl-	0.892	298.11218	[M-H ₂ O-H]-	C ₁₆ H ₁₅ NO ₂	Cinnamic acid amides	---
2151	delta-N,N-Dimethylguanidynol) valeric acid (9R,10S,12Z)-9,10-	6.386	202.11816	[M+NH ₄] ⁺	C ₈ H ₁₅ N ₃ O ₃	Short-chain keto acids and derivatives	---
2152	Dihydroxy-8-Oxo-12-Octadecenoic Acid (7S,9E,11S,12R,13S,14S,15S,16R,17S,18S,19E,21Z)-13-(acetyloxy)-15,17-dihydroxy-11-methoxy-	10.141	327.21536	[M-H]-	C ₁₈ H ₃₂ O ₅	Fatty Acyls	---
2153	3,7,12,14,16,18,22-heptamethyl-6,23,27,29-tetraoxo-26-(piperidin-1-yl)-8,30-dioxa-24-azatetracyclo[23.3.1.1 ⁴ {4,7}.0 ⁵ {5,28}]triaconta-1,3,5(28),9,19,21,25-heptaen... (6-methyl-6-	12.865	977.43243	[M+2H] ²⁺	C ₅₃ H ₆₆ N ₂ O ₁₄	Macrolactams	---
2154	azabicyclo[4.4.0]dec-2-yl)methyl 2,2-dimethylpropanoate, (6E,10E,14E,18E)-2,6,10,15,19,23-	9.539	268.22351	[M] ⁺	C ₁₆ H ₃₀ NO ₂ ⁺	Lupinine-type alkaloids	---
2155	hexamethyltetracosahexaene-1,2,3,22,23-pentol (4R,6S)-p-Menth-1-ene-4,6-diol 4-glucoside (5S,6R,9S,12R,15S,18R)-3-[(2R)-2-Butanyl]-6-isobutyl-9,12,15,18-	12.289	533.36249	[M+H] ⁺	C ₃₀ H ₅₄ O ₅	Triterpenoids	---
2156	tetraisopropyl-4,10,16-trimethyl-1,7,13-trioxa-4,10,16-triazacyclooctadecane-2,5,8,11,14,17-hexaene (3R)-N-cyclohexyl-6,7-dimethoxy-5-oxo-3,9b-dihydro-2H-[1,3]thiazolo[2,3-a]isoindole-3-carboxamide (3E,5Z)-1,3,5-Heptatriene (3-chloro-4-methylphenyl)[2-(ethylpropyl)quinazolin-4-yl]amine (3-bromophenyl)-N-{2-[2-methyl-5-(phenylmethoxy)indol-3-yl]ethyl}carboxamide	10.004	331.17358	[M-H]-	C ₁₆ H ₂₈ O ₇	Prenol lipids	---
2157		13.395	668.44299	[M+2H] ²⁺	C ₃₅ H ₆₁ N ₃ O ₉	Cyclic depsipeptides	---
2158		6.239	377.1539	[M+H] ⁺	C ₁₉ H ₂₄ N ₂ O ₄ S	Isoindolones	---
2159		10.838	95.08578	[M+H] ⁺	C ₇ H ₁₀	Unsaturated hydrocarbons	---
2160		10.061	374.11731	[M-H]-	C ₂₀ H ₂₂ ClN ₃	Quinazolines	---
2161		6.606	461.08752	[M-H]-	C ₂₅ H ₂₃ BrN ₂ O ₂	3-alkylindoles	---

	(3beta,5xi,9xi,18xi,22beta)-22,25-Dihydroxyolean-12-en-3-yl 6-deoxy-alpha-L-mannopyranosyl-(1->2)-beta-D-xylopyranosyl-(1->2)-beta-D-glucopyranosiduronic acid	10.378	935.49023	[M+Na] ⁺	C47H76O17	Triterpene glycosides	---
2162	(3beta,5xi,9xi,18xi,22beta)-22,25-Dihydroxyolean-12-en-3-yl 6-deoxy-alpha-L-mannopyranosyl-(1->2)-beta-D-xylopyranosyl-(1->2)-beta-D-glucopyranosiduronic acid	10.15	911.49683	[M-H] ⁻	C47H76O17	Triterpene glycosides	---
2163	(3beta,5xi,9xi,18xi,22beta)-22,25-Dihydroxyolean-12-en-3-yl 6-deoxy-alpha-L-mannopyranosyl-(1->2)-beta-D-xylopyranosyl-(1->2)-beta-D-glucopyranosiduronic acid	10.736	339.1395	[M-H] ⁻	C19H21ClN4	Quinazolines	---
2164	(3-{[2-(4-chlorophenyl)quinazolin-4-yl]amino}propyl)dimethylamine (3,5-dimethoxyphenyl)-N-[5-(2,2-dimethylpropyl)(1,3,4-thiadiazol-2-yl)]carboxamide	11.196	334.12543	[M-H] ⁻	C16H21N3O3S	Dimethoxybenzenes	---
2165	(3,5-dimethoxyphenyl)-N-(2-furylmethyl)carboxamide (3,4-dimethoxyphenyl)-N-[4-(5-chloro-3-methylpyrazolyl)phenyl]carboxamide	9.514	284.0874	[M+Na] ⁺	C14H15NO4	Dimethoxybenzenes	---
2166	(3,4-dimethoxyphenyl)-N-[3-(4-pyridylcarbonyl)phenyl]carboxamide (3,4-dimethoxyphenyl)-N-[2-(7-chloro-2-methylindol-3-yl)ethyl]carboxamide	2.357	372.11136	[M+H] ⁺	C19H18ClN3O3	Aromatic anilides	---
2167	(3,4-dimethoxyphenyl)-N-[3-(4-pyridylcarbonyl)phenyl]carboxamide (3,4-dimethoxyphenyl)-N-[2-(7-chloro-2-methylindol-3-yl)ethyl]carboxamide	6.225	397.09647	[M-H] ⁻	C21H18N2O4	Aromatic anilides	---
2168	(3,4-dimethoxyphenyl)-N-[2-(7-chloro-2-methylindol-3-yl)ethyl]carboxamide (3,4-dimethoxyphenyl)-N-[2-(7-chloro-2-methylindol-3-yl)ethyl]carboxamide	6.073	371.11734	[M-H] ⁻	C20H21ClN2O3	Dimethoxybenzenes	---
2169	(3,4-dimethoxyphenyl)-N-[2-(7-chloro-2-methylindol-3-yl)ethyl]carboxamide (3,4-dimethoxyphenyl)-N-[2-(7-chloro-2-methylindol-3-yl)ethyl]carboxamide	6.436	371.11752	[M-H2O-H] ⁻	C20H21ClN2O3	Dimethoxybenzenes	---
2170	(3,4-dimethoxyphenyl)-N-(1-ethyl-1-methylprop-2-ynyl)carboxamide (3,4,5-trimethoxyphenyl)-N-{2-[(3,4,5-trimethoxyphenyl)carbonylamino]phenyl}carboxamide	6.224	284.12277	[M+Na] ⁺	C15H19NO3	Dimethoxybenzenes	---
2171	(3,4,5-trimethoxyphenyl)-N-{2-[(3,4,5-trimethoxyphenyl)carbonylamino]phenyl}carboxamide (2Z)-2-benzoxazol-2-yl-3-(4-hydroxy-3-methoxyphenyl)-1-(4-methylphenyl)prop-2-en-1-one	3.068	531.15356	[M-H] ⁻	C26H28N2O8	Aromatic anilides	---
2172	(2Z)-2-benzoxazol-2-yl-3-(4-hydroxy-3-methoxyphenyl)-1-(4-methylphenyl)prop-2-en-1-one	6.363	384.12827	[M-H] ⁻	C24H19NO4	Retrochalcones	---
2173							

2174	(2Z)-2-(Acetylamino)-N-(2,5-Dimethylphenyl)-3-Phenylprop-2-Enamide	7.16	343.12198	[M-H]-	C19H20N2O2	Amino acids and derivatives	---
2175	(2S,3S,4S,5R,6S)-5-[(2S,3R,4R,5S,6S)-4-acetyloxy-3,5-dihydroxy-6-methyloxan-2-yl]oxy-6-[2-(3,4-dihydroxyphenyl)-5-hydroxy-4-oxochromen-7-yl]oxy-3,4-dihydroxyoxane-2-carboxylic acid (2S,3R,4S,5S,6R)-2-[4,6-dihydroxy-2-nonyl-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenoxy]-6-(hydroxymethyl)oxane-2-carboxylic acid	6.207	631.13293	[M-H]-	C29H30O17	Flavonoid O-glycosides	---
2176	(2S,3R)-2-(1-((S)-2-(tert-butoxycarbonyl)-1,2,3,4-tetrahydroisoquinoline-3-carbonyl)-4-phenylpiperidine-4-carboxamido)-3-methylpentanoic acid	11.675	637.27222	[M-H]-	C27H44O14	Glycosyl compounds	---
2177	(2S,3R)-2-(((S)-7-acetamido-1,2,3-trimethoxy-9-oxo-5,6,7,9-tetrahydrobenzo[a]heptalen-10-yl)amino)-N-(3-methoxypropyl)-3-methyl-N-(((1S,9aR)-octahydro-1H-quinolizin-1-yl)methyl)pentanamide	8.316	578.31769	[M+2H]2+	C33H43N3O6	Hybrid peptides	---
2178	(2S)-N-((1,3-benzodioxol-5-yl)-1-(4,5-dimethoxy-3-oxo-1H-2-benzofuran-1-yl)-5-oxopyrrolidine-2-carboxamide)-1-[(2S)-2-[(5-chloro-1-methylindole-2-carbonyl)amino]-3-methylpentanoyl]pyrrolidine-2-carboxylic acid	8.57	743.43213	[M+2H]2+	C41H60N4O7	Amino acids and derivatives	---
2179	(2S)-N-((1,3-benzodioxol-5-yl)-1-(4-methylphenyl)sulfonyl)pyrrolidine-2-carboxamide	9.134	429.2832	[M+H]+	C24H36N4O3	Hybrid peptides	---
2180	(2S)-1-[(2S)-2-[(5-chloro-1-methylindole-2-carbonyl)amino]-3-methylpentanoyl]pyrrolidine-2-carboxylic acid	10.537	441.1297	[M+CH3OH+H]+	C22H20N2O8	Amino acids and derivatives	---
2181	(2S)-1-[(2S)-2-[(5-chloro-1-methylindole-2-carbonyl)amino]-3-methylpentanoyl]pyrrolidine-2-carboxylic acid	1.338	420.16867	[M+NH4]+	C21H26ClN3O4	Peptides	---

2182	(2R,3S,4S,5R,6R)-2- [[[(2S,3R,4R)-3,4- dihydroxy-4- (hydroxymethyl)oxolan- 2-yl]oxymethyl]-6-[3- hydroxy-3- (hydroxymethyl)-4- methylpentoxy]oxane- (2R,3S,4S,5R,6R)-2- [[[(2R,3R,4R)-3,4- dihydroxy-4- (hydroxymethyl)oxolan- 2-yl]oxymethyl]-6-oct-1- en-3-yloxyoxane-3,4,5- (2R,3R,4S,5S,6R)-2- (((2aR,5aS,7S,11aR,12a S)-9-(((2S,3R,4S,5R)- 4,5-dihydroxy-3- (((2S,3R,4S,5S)-3,4,5- trihydroxytetrahydro-2H- pyran-2- yl)oxy)tetrahydro-2H- pyran-2-yl)oxy)-3-((2R)- 5,6-dihydroxy-6- methylheptan-2-yl)-7- hydroxy-2a,5a,8,8- tetramethylhexadecahydr ocyclopenta[a]cycloprop a[e]phenanthren-4- yl)oxy)-6- (hydroxymethyl)tetrahyd (2R,3R,4S,5R,7S,8R,9S, 13R,15R)-3,5,7,9,14,15- Hexaacetoxy-8-hydroxy- 14-oxojatropha- 6(17),11E- diene/jatropha ester isolated from Euphorbia amygdaloides ssp semiperfoliata (2R)-2-[[[(2S)-2-(1,2- dihydroimidazo[1,2- a]benzimidazole-3- carbonylamino)-4- methylsulfanylbutanoyl]a mino]-2-phenylacetic (2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E)-N-Isobutyl-6-(2- thienyl)hexa-2,4- dienamide	6.491	465.19504	[M+Na] ⁺	C18H34O12	Fatty acyl glycosides	---
2183	(2R,3R,4S,5S,6R)-2- (((2aR,5aS,7S,11aR,12a S)-9-(((2S,3R,4S,5R)- 4,5-dihydroxy-3- (((2S,3R,4S,5S)-3,4,5- trihydroxytetrahydro-2H- pyran-2- yl)oxy)tetrahydro-2H- pyran-2-yl)oxy)-3-((2R)- 5,6-dihydroxy-6- methylheptan-2-yl)-7- hydroxy-2a,5a,8,8- tetramethylhexadecahydr ocyclopenta[a]cycloprop a[e]phenanthren-4- yl)oxy)-6- (hydroxymethyl)tetrahyd (2R,3R,4S,5R,7S,8R,9S, 13R,15R)-3,5,7,9,14,15- Hexaacetoxy-8-hydroxy- 14-oxojatropha- 6(17),11E- diene/jatropha ester isolated from Euphorbia amygdaloides ssp semiperfoliata (2R)-2-[[[(2S)-2-(1,2- dihydroimidazo[1,2- a]benzimidazole-3- carbonylamino)-4- methylsulfanylbutanoyl]a mino]-2-phenylacetic (2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E)-N-Isobutyl-6-(2- thienyl)hexa-2,4- dienamide	6.644	440.24826	[M+H] ⁺	C19H34O10	Fatty acyl glycosides	---
2184	(2R,3R,4S,5R,7S,8R,9S, 13R,15R)-3,5,7,9,14,15- Hexaacetoxy-8-hydroxy- 14-oxojatropha- 6(17),11E- diene/jatropha ester isolated from Euphorbia amygdaloides ssp semiperfoliata (2R)-2-[[[(2S)-2-(1,2- dihydroimidazo[1,2- a]benzimidazole-3- carbonylamino)-4- methylsulfanylbutanoyl]a mino]-2-phenylacetic (2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E)-N-Isobutyl-6-(2- thienyl)hexa-2,4- dienamide	10.049	941.50366	[M+H] ⁺	C46H78O18	Steroidal saponins	---
2185	(2R,3R,4S,5R,7S,8R,9S, 13R,15R)-3,5,7,9,14,15- Hexaacetoxy-8-hydroxy- 14-oxojatropha- 6(17),11E- diene/jatropha ester isolated from Euphorbia amygdaloides ssp semiperfoliata (2R)-2-[[[(2S)-2-(1,2- dihydroimidazo[1,2- a]benzimidazole-3- carbonylamino)-4- methylsulfanylbutanoyl]a mino]-2-phenylacetic (2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E)-N-Isobutyl-6-(2- thienyl)hexa-2,4- dienamide	12.864	675.25916	[M+H] ⁺	C32H44O14	Jatropha and cyclojatropha diterpenoids	---
2186	(2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E)-N-Isobutyl-6-(2- thienyl)hexa-2,4- dienamide	6.385	468.16907	[M+H] ⁺	C23H25N5O4S	Peptides	---
2187	(2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E)-N-Isobutyl-6-(2- thienyl)hexa-2,4- dienamide	12.188	376.31705	[M+NH4] ⁺	C24H43NO3	N-acyl amines	---
2188	(2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E)-N-Isobutyl-6-(2- thienyl)hexa-2,4- dienamide	13.096	376.31635	[M+H] ⁺	C24H43NO3	N-acyl amines	---
2189	(2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E,14E)-13- hydroperoxy-N-(2- methylpropyl)icosa- 2,4,14-trienamide (2E,4E)-N-Isobutyl-6-(2- thienyl)hexa-2,4- dienamide	1.43	248.11159	[M+CH3OH +H] ⁺	C14H19NOS	N-acyl amines	---

2190	(2E)-3-{1-[2-(2,5-dimethylphenoxy)ethyl]indol-3-yl}-2-(2-1,2,3,4-tetrahydroisoquinolylcarbonyl)prop-2-enenitrile	2.98	476.23138	[M+H] ⁺	C31H29N3O2	Tetrahydroisoquinolines	---
2191	(2E)-3-(4-Acetoxy-2,3-dihydroxy-2,5,5,8a-tetramethyldecahydro-1-naphthalenyl)acrylic acid	12.324	353.19781	[M-H] ⁻	C19H30O6	Dicarboxylic acids and derivatives	---
2192	(2E)-3-(4-Acetoxy-2,3-dihydroxy-2,5,5,8a-tetramethyldecahydro-1-naphthalenyl)acrylic acid	6.943	377.18997	[M+Na] ⁺	C19H30O6	Dicarboxylic acids and derivatives	---
2193	(2E)-3-(3,4-dimethoxyphenyl)-N-naphthylprop-2-enamide	6.287	378.13156	[M-H] ⁻	C21H19NO3	Cinnamic acid amides	---
2194	(2E)-3-(2H-benzo[d][1,3-dioxolen-5-yl)-N-[N-(2-furylmethyl)carbamoyl]-N-phenylprop-2-enamide	6.213	425.09076	[M-2H] ²⁻	C22H18N2O5	N-phenylureas	---
2195	(2E)-1-{4-[(2E)-3-(3,4,5-trimethoxyphenyl)prop-2-enoyl]phenyl}-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one	8.138	541.18713	[M+Na] ⁺	C30H30O8	Retrochalcones	---
2196	(2E)-1-{4-[(2E)-3-(3,4,5-trimethoxyphenyl)prop-2-enoyl]phenyl}-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one	6.539	563.19385	[M-H] ⁻	C30H30O8	Retrochalcones	---
2197	(23R,24R)-3beta-(Beta-D-Xylopyranosyloxy)-9beta,19-Cyclo-16beta,23:16,24-Diepoxy-5alpha-Lanosta-7-Ene-15alpha,25-Diol (22Z,24E)-3-Oxocycloarta-22,24-Diene-26-Oic Acid (2-{4,5-Dimethoxy-2-[2-(4-methoxy-phenyl)-vinyl]-phenyl}-ethyl)-trimethylammonium (2,6-difluorophenyl)-N-[2-(2-methylindol-3-yl)ethyl]carboxamide	7.946	636.4137	[M+H] ⁺	C35H54O9	Cycloartanols and derivatives	---
2198	(22Z,24E)-3-Oxocycloarta-22,24-Diene-26-Oic Acid (2-{4,5-Dimethoxy-2-[2-(4-methoxy-phenyl)-vinyl]-phenyl}-ethyl)-trimethylammonium (2,6-difluorophenyl)-N-[2-(2-methylindol-3-yl)ethyl]carboxamide	11.835	435.32883	[M+H] ⁺	C30H44O3	Cycloartanols and derivatives	---
2199	(2,6-difluorophenyl)-N-[2-(2-methylindol-3-yl)ethyl]carboxamide	8.145	357.23279	[M+2H] ²⁺	C22H30NO3	Stilbenes	---
2200	(2,6-difluorophenyl)-N-[2-(2-methylindol-3-yl)ethyl]carboxamide	6.379	337.1113	[M+H-H2O] ⁺	C18H16F2N2O	3-alkylindoles	---

	(1S,3S,12S,14R,27S)-12-Hydroxy-1,3-dimethyl-2,5,15,23,25-pentaazaheptacyclo[12.1						
2201	0.2.1~2,5~.0~6,11~.0~12,27~.0~15,24~.0~17,22~]heptacos-6,8,10,17,19,21,23-heptaene-4,16,26-trione (19E)-4-Ethyl-2,16-	0.977	442.15427	[M-H ₂ O-H]-	C ₂₄ H ₂₁ N ₅ O ₄	Quinazolines	---
2202	Didehydrocur-19-En-4-Ium-17-Al (13R,14R)-8-Labdene-13,14,15-triol (11R,12S,13S)-Epoxy-	7.118	355.15903	[M-H]-	C ₂₁ H ₂₅ N ₂ O ⁺	Strychnos alkaloids	---
2203	hydroxyoctadeca-cis-9-cis-15-dien-1-oic acid (10betaH,11xi)-11-	12.653	323.25732	[M-H]-	C ₂₀ H ₃₆ O ₃	Prenol lipids	---
2204	Hydroxy-13-nor-6-eremophilen-8-one (+/-)-Vesamicol hydrochloride	11.097	309.20532	[M-H]-	C ₁₈ H ₃₀ O ₄	Fatty Acyls	---
2205	(-)-Erythro-Anethole Glycol 2-Glucoside	11.09	221.15279	[M-H]-	C ₁₄ H ₂₂ O ₂	Prenol lipids	---
2206	O-Methylsinapic Acid	7.948	296.18121	[M+H] ²⁺	C ₁₇ H ₂₆ ClNO	Phenylpiperidines	---
2207	O-Methylsinapic Acid	7.963	345.15088	[M+Na] ⁺	C ₁₆ H ₂₄ O ₈	Glycosyl compounds	---
2208		7.196	256.11627	[M+NH ₄] ⁺	C ₁₂ H ₁₄ O ₅	Coumaric acids and derivatives	---
2209		7.78	256.11627	[M+H] ⁺	C ₁₂ H ₁₄ O ₅	Coumaric acids and derivatives	---