

PE site		Compound category	Name	formula	Ion mode	RT	Response	Theoretical value	Measured value	MS/MS
1	15	phenylpropanoid	(E)-p-coumaric acid	C9H8O3	+	7.52	4.51E+06	165.0546	165.0538	147.04334,119.04449,93.03310
2	15	phenylpropanoid	Evodiamine	C19H16O4	+	7.42	6.47E+06	170.0320	170.0320	131.03813,135.04262
3	11	phenylpropanoid	IN00458	C9H6O3	+	8.86	1.63E+06	163.0390	163.0381	135.04334,105.03292,77.03817
4	12	phenylpropanoid	Umbelliferone	C9H6O3	+	12.89	3.58E+07	163.0390	163.0381	135.04327
5	513	phenylpropanoid	Coumarin	C9H6O2	+	9.85	1.10E+07	147.0441	147.0432	119.04485,105.05367
6	725	phenylpropanoid	3-Phenyl-1-propanol	C9H10O	+	7.23	2E+07	137.0494	137.0494	119.04493,93.06043,91.05378,79.05384,77.03822
7	799	phenylpropanoid	3-Phenylpropanoic acid	C9H10O2	+	8.85	5.01E+06	151.0746	151.0746	133.06416,105.06029,84.95926,79.05381,77.03818,57.03319,55.01753
8	8205	phenylpropanoid	onnamyl isolate	C14H16O2	+	10.48	2.75E+06	217.1223	217.1214	135.07971,107.0693,105.0693,91.05338,79.0538
9	1319	phenylpropanoid	3-Phenyl-1-propanol	C9H10O	+	7.23	2E+07	137.0494	137.0494	119.04493,93.06043,91.05378,79.05384,77.03818,57.03319,55.01753
10	2391	phenylpropanoid	Bergapten	C12H8O4	+	9.71	7.06E+07	217.0495	217.0487	173.0588,171.0434,147.0433
11	112496	phenylpropanoid	Asarone	C12H16O3	+	10.60	6.39E+07	209.1272	209.1163	194.0928,163.0745,131.0745,131.0746,121.0641,106.0643,95.0487,79.0539
12	12552	phenylpropanoid	6,7,8-trimethoxy-2H-chromen-2-one	C12H12O5	+	7.97	1.76E+07	237.0758	237.0747	205.0489,162.0615,162.0303,137.0589,107.0485
13	1719	phenylpropanoid	4-Methoxy-4-(prop-2-en-1-yl)-2H-1,3-benzodioxole	C12H14O3	+	10.52	1.32E+06	183.0868	183.0868	150.089,135.0435
14	1728	phenylpropanoid	Ethyl onnamate	C11H12O2	+	6.42	3.52E+06	177.0910	177.0900	149.0589,103.0579,91.0537,77.0382
15	1749	phenylpropanoid	Scopoletin	C11H10O4	+	7.37	1.83E+07	207.0652	207.0644	179.0693,163.0746,148.0511,119.0485
16	1755	phenylpropanoid	Fraxetin	C10H8O5	+	4.62	7.4E+07	209.0444	209.0433	191.0331,177.0173,165.0571,149.0589,135.0538,139.0383,109.0278
17	1761	phenylpropanoid	Scopoletin	C10H8O4	+	9.36	3.67E+06	193.0495	193.0486	165.1365,150.0303,135.0435,123.0591,107.0486,95.0487
18	18263	phenylpropanoid	Herniarin	C10H8O3	+	9.84	1.80E+07	177.0546	177.0537	149.0589,145.0277,131.0485,103.0537,77.0381
19	1887	phenylpropanoid	Isoscutellin	C10H12O2	+	14.99	9.72E+06	165.0591	165.0580	147.0797,137.0520,135.0747,123.0433,107.0486,93.0329,77.0382
20	2086	phenylpropanoid	6,2-Di-Methoxyvinaminaldehyde	C10H10O2	+	12.11	1.33E+06	163.0744	163.0744	135.0483,107.0485,105.0328,79.0538,77.0382
21	21507	phenylpropanoid	1256801	C17H20O4	+	11.90	3.56E+06	289.1420	289.1420	145.0640,177.1264,133.0641
22	22175	phenylpropanoid	Hexyl onnamaldehyde	C15H20O	+	14.40	4.20E+07	217.1587	217.1578	175.1108,147.0797,133.1005,105.0693,91.0538
23	23088	phenylpropanoid	AKOS R8-2919	C19H14O	+	9.46	3.21E+06	193.1117	193.1110	175.0380,172.0953,147.0433
24	439	terpene	Isoprene	C5H8	+	9.46	3.21E+06	193.1117	193.1110	97.10066,97.06427,83.04871,81.06947,67.05386,55.05393
25	2980	terpene	(Gbeta)-28-Hydroxyulcin-20(9)-en-3-yl (2E)-3,4-dihydro-2H-pyran-2-yl	C39H56O4	+	16.00	1.01E+08	589.4251	589.4253	121.0638,109.1005,81.0694,79.0538,69.0696,67.0539,55.0540
26	2983	terpene	Euphorbiolipifolene	C36H44O11	+	24.44	8.89E+07	653.2946	653.2946	92.0694,69.0696,67.0538,55.0540,53.0537
27	319	terpene	3-Acetoxy-12-en-23-oic acid	C20H32O5	+	19.70	1.93E+07	409.2375	409.2375	123.1162,109.1005,85.0850,81.0695,67.0539,57.0696,55.0540
28	352	terpene	Betulinal	C30H50O	+	29.71	2.00E+07	443.3884	443.3857	121.1006,109.1006,81.0695,69.0695,67.0539
29	355	terpene	1916451	C30H50O	+	19.81	3.43E+06	427.3934	427.3914	111.1163,109.1007,105.0694,81.0695,69.0696,67.0539
30	360	terpene	Asiatic acid	C30H48O3	+	12.25	2.27E+06	469.3515	469.3553	90.0747,97.1007,95.0850,89.0593,85.1008,83.0851,69.0696,67.0539,57.0696,55.0539
31	365	terpene	NP-00880	C23H36O4	+	7.95	1.30E+06	389.2484	389.2484	109.1006,93.0694,81.0695,79.0538,70.0648,67.0539,55.0539
32	9167	terpene	(4aS,5R,6S,8aS)-5-[(3E)-5-methoxy-3-methyl-5-oxopent-1-en-1-yl]-2,3-dimethyl-2,3-dihydro-1H-indene	C21H32O4	+	17.47	2.98E+08	349.2373	331.2225	149.0954,95.0850,80.0851,81.0694,69.0695,67.0539,57.0696,55.0539
33	10733	terpene	NP-006817	C21H32O3	+	17.17	9.96E+07	332.2424	332.2421	83.0851,81.0694,69.0695,67.0539,55.0539
34	1085	terpene	NP-006817	C20H36O	+	15.42	1.56E+06	243.2754	243.2754	117.0540,105.0693,97.1007,81.0695,67.0539,57.0696,55.0539
35	12181	terpene	7-Hydroxy-4a,6a,7-trimethyl-2,3-dihydro-1H-indene	C19H30O3	+	16.35	1.11E+07	307.2268	307.2254	139.0746,123.1162,97.1007,95.0850,69.0695,55.0540
36	131648	terpene	1-(5S,6S)-Tetramethyl-5,6,7,8-tetrahydro-2-naphthalene	C16H22O	+	10.48	1.46E+07	231.1743	231.1733	175.0643,133.0643,103.0330
37	14715	terpene	NP-001717	C15H26O3	+	14.68	2.53E+07	255.1955	255.1942	219.1734,97.1006,83.0851,71.0488,69.0695,55.0539,55.0176
38	1543	terpene	2-Ethyl-2-methyl-2-butanol	C15H22O	+	19.72	1.36E+06	223.0764	223.0764	187.1473,85.0644
39	16002	terpene	DEHYDROCOCTUS LACTONE	C15H18O2	+	10.80	3.15E+07	231.1380	231.1369	175.0747,159.1159,131.0849
40	17237	terpene	2-[1E]-1-Buten-3-yn-1-yl-1,3,3-trimethyl-2,3-dihydro-1H-indene	C15H18O	+	11.45	3.71E+07	175.1481	175.1472	175.1472
41	1791	terpene	Neopterin	C10H18O	+	12.04	4.47E+06	155.1472	155.1472	117.0799,83.0487,69.0332
42	19787	terpene	Pulegone	C10H18O	+	8.46	3.96E+06	153.1279	153.1266	109.0642,95.0550,81.0694,69.0695
43	20816	terpene	2-borneone	C10H18O	+	18.02	2.78E+06	137.1325	137.1319	137.1319
44	21657	terpene	1-carboxy-3-hydroxyadamantane	C11H16O3	+	7.08	7.44E+07	197.1172	197.1163	179.1057,161.0952,151.1110,133.1005,79.0538,77.0382
45	2222	terpene	C13H24O3	+	19.70	1.02E+06	229.1786	229.1786	123.1162,109.1006,81.0695,69.0695,67.0539,57.0696,55.0540	
46	231217	terpene	1,1,4,4-Tetramethyltetralin	C14H20O	+	14.50	1.87E+07	189.1830	189.1830	147.1160,133.1004,77.0382
47	241823	terpene	C1-Carvophyllene oxide	C15H24O	+	11.98	3E+08	221.1899	221.1891	175.1472,161.1316,147.1160,133.1162,121.1005,109.1006
48	1801	terpene	Hydroxy-2,10,10-trimethyl-2,3-dihydro-1H-indene	C15H24O	+	16.42	2.35E+06	243.2754	243.2754	208.1578,161.1473,137.1137,109.1006,95.0850
49	630	terpene	4-15-(7-Hydroxy-5,5,8-trimethyl-2-methylene)-dec-2-ene	C24H40O5	+	19.16	2.36E+07	409.2945	409.2932	181.0850,169.0850,154.0617,109.1006,95.0851,83.0851,81.0695,69.0695,57.0696,55.0539
50	27191	terpene	(Gbeta)-3-(3,3-Dimethylbutyryloxy)ulcin-20-en-28-oic acid	C36H58O4	+	17.63	1.24E+06	555.4048	555.4383	555.4383
51	28255	terpene	Lup-20(9)-ene-3,28-diol (2E,3E,8S,3-phenylacetyl)	C38H62O4	+	18.62	3.89E+07	703.4721	703.4714	81.0695,79.0539,69.0695,67.0539,55.0539
52	1472	terpene	NP-0154	C17H24O	+	14.43	2.02E+06	283.1786	283.1786	149.0953,119.0484,107.0486,95.0850,81.0694,81.0695
53	3012	terpene	ditranan-2-ol	C33H44O	+	19.76	7.80E+07	457.3465	457.3472	121.1006,109.1006,107.0486,95.0850,81.0695
54	31294	terpene	2595	C13H20O	+	9.01	1.12E+07	193.1587	193.1577	165.1266,151.1109,109.0642,83.0487,69.0331
55	1441	terpene	3,5-Dimethyladamantan-1-ol	C15H24O	+	14.10	1.05E+06	231.1777	231.1777	133.1285,119.0547,83.0332
56	33407	terpene	camodierol A	C30H44O2	+	16.67	5.96E+06	437.3414	437.3392	123.1162,109.1006,95.0850,83.0851,81.0695,71.0486,69.0695,67.0539,57.0696,55.0539
57	106821	steroid	NP-005821	C30H46O2	+	11.96	2.78E+07	455.3200	455.3495	135.1162,123.1162,107.0486,95.0850,81.0695,69.0695,67.0539,55.0540
58	420	steroid	Stigmasterol	C29H48O	+	19.76	1.87E+08	413.3778	413.3757	123.0798,109.0643,95.0851,83.0487,81.0695
59	442	steroid	Cholesterol	C27H46O	+	19.76	1.87E+08	413.3778	413.3757	123.0798,109.0643,95.0851,83.0487,81.0695
60	443	steroid	(28:38,9E,17Z,22E)-2,3,14,20,22-Pentahydroxysterol-7	C28H46O6	+	12.77	5.68E+06	479.367	479.336	109.1006,109.0729,95.0850,83.0851,81.0695,69.0695,67.0539
61	4502	steroid	(Galpha)5alpha-(21-4)-Methylphenylpropan-20-yn-3-ol	C28H38O	+	20.05	2.03E+06	391.2995	391.2979	157.1003,23.1160,105.0693,97.1007,93.0694,91.0538,79.0538
62	459	steroid	(Gbeta)5alpha-(21-4)-Methylphenylpropan-20-yn-3-ol	C28H38O	+	22.02	2.26E+06	467.3367	467.3363	121.1006,109.1006,107.0486,95.0850,81.0695,69.0695,67.0539,55.0540
63	464	steroid	Cholesterol-4-ene-3-one	C27H44O	+	18.93	2.22E+06	383.2499	383.2499	139.0798,109.0643,95.0850,83.0487,81.0695,71.0486,69.0695,67.0539,55.0540
64	8331	steroid	3alpha,7alpha-Dihydroxylcholesterol	C24H40O4	+	15.93	3.22E+06	393.2999	393.2999	109.1006,97.0643,95.0850,83.0487,69.0695,67.0539,57.0696,55.0540
65	954	steroid	17beta,23-Methoxy-17-tetrahydro-2H-zran-2-ylol	C24H34O3	+	16.99	1.64E+06	371.2581	371.2568	109.0592,83.0488,71.0486,95.0850,81.0695,69.0695,67.0539,55.0540
66	1012	steroid	Neopterin	C10H18O	+	12.04	4.47E+06	155.1472	155.1472	117.0799,83.0487,69.0332
67	11113	steroid	17beta,23-Methoxy-17-tetrahydro-2H-zran-2-ylol	C20H24O2	+	15.13	3.88E+06	297.1845	297.1835	131.0849,125.0955,121.1109,108.0497,100.0746,83.0487,81.0695,67.0539,55.0540
68	12115	steroid	Boldione	C19H24O2	+	14.90	1.20E+07	285.1849	285.1839	187.1112,149.1316
69	13187	steroid	Farnesol	C18H24O2	+	11.80	1.43E+07	288.1786	288.1765	173.0652,147.0796,109.0642,107.0485,97.0643,95.0850,81.0694,55.0539
70	1401	steroid	18-Norandrostenedione	C18H24O2	+	12.81	1.43E+07	288.1786	288.1765	125.1108,123.1116,107.0485,95.0850,83.0694,81.0695,79.0539,55.0539
71	15143	steroid	2-Hydroxysterone	C18H24O2	+	12.22	7.71E+05	287.1842	287.1829	193.1213,189.0901,123.0434
72	16120	steroid	3-Dioxysterone	C18H22O	+	11.54	1.55E+07	255.1743	255.1733	165.1266,151.1109,109.0642,83.0487,81.0695
73	187	flavonoid	Neopterin	C12H16O5	+	6.08	2.92E+06	255.1427	255.1427	91.0487,89.0592,57.0332
74	212	flavonoid	Phloretin	C15H14O5	+	11.22	1.50E+08	273.0767	273.0740	273.0740
75	3490	flavonoid	Genistein	C15H10O5	+	6.22	5.11E+04	269.0455	269.0456	269.0456
76	4157	flavonoid	5,6,7-Dihydroxy-3-methoxy-4-oxo-4H-chromen-2-one	C21H20O11	+	8.06	3.62E+07	447.0833	447.0817	447.0817
77	459	quinone	2-Hydroxy-5-methoxy-3-(10-pentadecylbenzo)-3-one	C22H32O4	+	2.30	2.51E+06	382.2514	382.2514	279.0903,165.0537,133.0538,125.0953,123.0434,107.0486
78	21479	quinone	Embelin	C17H26O4	+	14.26	1.71E+07	295.1004	295.1003	295.1003,195.1370,167.1421,155.0332

169	88	2192	phenolic acids, carl	1-Ethynyl-4-hexylbenzene	C14 H18	+	11.70	8.61E+06	187.1481	187.1472	145.1005,119.0849,91.0538,79.0539
170	89	2215	phenolic acids, carl	4-Methylbenzophenone	C14 H12 O	+	11.65	2.47E+06	197.0961	197.0953	166.0767,105.0330,77.0381
171	90	2224	phenolic acids, carl	VO2978400	C13 H24 O2	+	9.24	1.46E+06	213.1849	213.1841	153.1267,69.0696
172	91	2244	phenolic acids, carl	3408	C13 H22 O3	+	12.85	1.01E+07	227.1627	227.1632	181.1213,153.1266,83.0851,57.0696
173	92	2246	phenolic acids, carl	12-Tridecynoic acid	C13 H22 O2	+	10.20	1.35E+07	211.1693	211.1683	123.1162,109.1006,95.0850,81.0695,67.0539
174	93	2250	phenolic acids, carl	081804500	C13 H22 O	+	10.81	1.47E+06	195.1743	195.1734	111.0799,83.0852,69.0696
175	94	2288	phenolic acids, carl	645341	C13 H20 O3	+	8.79	8.34E+06	225.1485	225.1475	167.1058,149.0954,123.0799,109.0643
176	95	2293	phenolic acids, carl	Spherophoriol	C13 H20 O2	+	12.52	4.21E+07	209.1536	209.1527	137.0589,135.0797,125.0590,111.0433,107.0485,95.0486
177	96	2302	phenolic acids, carl	Hectylbenzene	C13 H20	+	19.39	1.46E+07	177.1638	177.1628	135.1162,121.1005,93.0694,79.0538
178	97	2322	phenolic acids, carl	p-Hydroxybenzoic Acid	C13 H10 O3	+	11.29	3.04E+07	223.1328	223.1319	197.0628,109.0643,95.0487,77.0381
179	98	2326	phenolic acids, carl	Heptanophenone	C13 H18 O	+	8.89	1.05E+08	191.1430	191.1421	149.0953,135.0797,117.0692,91.0537
180	99	2360	phenolic acids, carl	1-[4-hydroxy-3-(3-methylbut-2-en-1-yl)phenyl]ethan	C13 H16 O2	+	10.41	2.37E+07	205.1223	205.1215	173.0951,145.1004,91.0538
181	100	2366	phenolic acids, carl	Cyclohexyl phenyl ketone	C13 H16 O	+	9.50	1.44E+07	189.1274	189.1264	111.0798,105.0329,83.0851,79.0538
182	101	2373	phenolic acids, carl	4-Pentylphenylacetylene	C13 H16	+	11.57	1.24E+07	173.1325	173.1315	157.1003,143.0848,117.0693,91.0538,77.0382
183	102	2382	phenolic acids, carl	4-hex-1-ynylBenzaldehyde	C13 H14 O	+	10.56	1.17E+06	187.1117	187.1108	159.1160,103.0538,91.0538,77.0381
184	103	2407	phenolic acids, carl	NP-004036	C12 H22 O4	+	10.56	8.52E+06	231.1591	231.1582	117.0693,97.1007
185	104	2438	phenolic acids, carl	acetic acid, ceranyl ester	C12 H20 O2	+	10.75	8.92E+06	197.1536	197.1527	179.1058,125.0591,111.0435
186	105	2451	phenolic acids, carl	3-(3-methoxypropoxy)-4-methoxyphenylmethanol	C12 H18 O4	+	10.70	3.79E+06	227.1278	227.1267	135.0799,121.0643,109.0643,79.0539,77.0383
187	106	2459	phenolic acids, carl	Sedanolid	C12 H18 O2	+	12.02	4.27E+07	195.1380	195.1373	125.0590,111.0434,71.0852
188	107	2476	phenolic acids, carl	Propofol	C12 H18 O	+	13.64	8.25E+07	179.1430	179.1421	161.1318,147.1160,133.1004,119.0849
189	108	2481	phenolic acids, carl	1-(1-butyl-4-ethyl)benzene	C12 H18	+	11.45	1.06E+07	163.1481	163.1472	155.1161,57.0696,55.0539
190	109	2497	phenolic acids, carl	6-Phenylhexanoic acid	C12 H16 O2	+	14.07	1.27E+08	193.1223	193.1217	165.1265,147.1160,133.1005,119.0849,105.0693,91.0537,77.0382
191	110	2504	phenolic acids, carl	4-tert-Butylacetophenone	C12 H16 O	+	10.70	1.14E+07	177.1274	177.1267	133.1004,119.0849,91.0538
192	111	2511	phenolic acids, carl	C21330000	C12 H16	+	11.45	2.15E+07	161.1325	161.1316	159.1161,145.1008,119.0849,105.0693,91.0538
193	112	2544	phenolic acids, carl	Butylthiathalide	C12 H14 O2	+	8.88	8.63E+06	191.1067	191.1058	145.1004,91.0537
194	113	2545	phenolic acids, carl	4-Phenylcyclohexanone	C12 H14 O	+	9.86	4.33E+06	175.1117	175.1109	147.1160,133.1004,119.0849,91.0537
195	114	2572	phenolic acids, carl	(3S,4R)-3-(1-(4-hydroxyhexyl)-4-(hydroxymethyl)oxolan-2-yl)butanoic acid	C11 H20 O4	+	10.56	1.91E+07	217.1434	217.1425	181.1214,155.0697,111.0435
196	115	2605	phenolic acids, carl	Ethyl 3-cyclohexyl-3-oxopropionate	C11 H18 O5	+	10.24	2.27E+07	199.1328	199.1319	159.0747,111.0797
197	116	2619	phenolic acids, carl	3422	C11 H18 O	+	13.99	2.55E+06	167.1430	167.1424	121.0641,95.0486,67.0538
198	117	2663	phenolic acids, carl	5-Pentylresorcinol	C11 H16 O2	+	9.30	5.20E+08	181.1223	181.1220	163.1108,125.0590,111.0799,107.0486,95.0486
199	118	2669	phenolic acids, carl	SM675000	C11 H16 O	+	10.81	8.32E+06	165.1274	165.1267	147.1161,91.0538,77.0382
200	119	2684	phenolic acids, carl	Butylparaben	C11 H14 O3	+	9.60	1.07E+08	195.1016	195.1007	177.0901,149.0954,95.0487,79.0538
201	120	2686	phenolic acids, carl	2-Isopropyl-5-methylbenzoic acid	C11 H14 O2	+	14.08	3.96E+07	179.1067	179.1059	161.0952,137.0589,133.1004,105.0693,91.0537,77.0381
202	121	2687	phenolic acids, carl	Butyl benzoate	C11 H14 O2	+	9.00	2.51E+07	179.1067	179.1057	133.1004,105.0693
203	122	2698	phenolic acids, carl	1-Phenyl-2-nentanone	C11 H14 O	+	10.24	1.37E+07	163.1117	163.1109	135.0797,105.0330,77.0381
204	123	2708	phenolic acids, carl	6-METHYLTETRALIN	C11 H14	+	11.44	2.16E+07	147.1168	147.1160	145.1004,119.0849,105.0693,91.0537
205	124	2736	phenolic acids, carl	4-Methyl-1-Tetralone	C11 H12 O	+	12.28	4.75E+06	161.0961	161.0952	133.1004,119.0849,91.0537,77.0382
206	125	2773	phenolic acids, carl	Sedacac acid	C10 H18 O4	+	9.69	8.95E+06	203.1218	203.1209	121.0006,95.0851,81.0695,67.0539
207	126	2800	phenolic acids, carl	Ethyl 2-oxocycloheptanecarboxylate	C10 H16 O3	+	10.56	1.44E+07	185.1172	185.1163	139.0746,111.0798,85.0643,57.0696
208	127	2801	phenolic acids, carl	Mossao lactone	C10 H16 O2	+	8.30	2.28E+07	169.1223	169.1215	151.1110,123.1162,69.0696
209	128	2827	phenolic acids, carl	Guaiifenesin	C10 H14 O4	+	8.41	2.69E+06	199.0965	199.0957	184.0720,168.0772,153.0538,125.0590,95.0487,79.0538
210	129	2836	phenolic acids, carl	6-Pentyl-2H-pyran-2-one	C10 H14 O2	+	8.84	3.43E+06	167.1067	167.1058	149.0953,138.0542,121.1006,107.0850,95.0487
211	130	2856	phenolic acids, carl	p-cymene	C10 H14	+	9.31	8.45E+06	135.1168	135.1161	93.0694
212	131	2879	phenolic acids, carl	3,4'-Dimethylacetophenone	C10 H12 O3	+	9.55	6.25E+07	181.0859	181.0852	135.0433,133.0640,123.0433,95.0486,79.0538
213	132	2880	phenolic acids, carl	4-Phenylbutyric acid	C10 H12 O2	+	14.89	1.00E+07	165.0910	165.0901	137.0954,122.0730,119.0849,107.0486,91.0537,77.0381
214	133	2884	phenolic acids, carl	Butyrophenone	C10 H12 O	+	8.88	4.73E+06	149.10	149.10	105.0694,103.0536,95.0487,91.0538
215	134	2895	phenolic acids, carl	2-ISOPROPENYL TOLUENE	C10 H12	+	9.09	4.57E+07	133.1012	133.1004	131.0848,117.0692,105.0693,91.0537,77.0382

EA site	Compound card Name	formular	Ion model	RT	Response	theoretical value	Measured value	MS/MS
1	16	1	phenylpropanoic acid, 4-Coumaric acid	C9 H8 O3	+ 5.97	7.66E+06	165.0546	165.0538
2	18	2	phenylpropanoic acid, Cinnamic acid	C9 H8 O2	+ 9.83	1.52E+06	149.0591	149.0591
3	21	3	phenylpropanoic acid, trans-Cinnamaldehyde	C9 H8 O	+ 7.74	1.93E+06	133.0648	133.0642
4	25	4	phenylpropanoic acid, 3,5,7-Trihydroxy-4H-chromen-4-one	C9 H6 O5	+ 3.66	8.26E+06	195.0288	195.0279
5	30	5	phenylpropanoic acid, 5-Hydroxy-1-benzofuran-2-carboxylic acid	C9 H6 O4	+ 3.45	5.01E+07	179.0339	179.0330
6	32	6	phenylpropanoic acid, H2O458	C9 H6 O3	+ 12.91	4.38E+07	163.0390	163.0381
7	36	7	Coumarin	C9 H6 O2	+ 6.29	1.47E+07	147.0441	147.0436
8	92	8	phenylpropanoic acid, 3-Phenyl-1-propanol	C9 H12 O	+ 9.09	2.90E+07	137.0961	137.0954
9	1907	9	phenylpropanoic acid, isopentyl citrate	C14 H18 O2	+ 9.22	9.48E+06	219.1380	219.1371
10	1931	10	phenylpropanoic acid, cinnamyl tiglate	C14 H16 O2	+ 8.40	9.10E+06	217.1223	217.1215
11	1935	11	phenylpropanoic acid, 2,3-Di-2-hydroxypropyl-2-yl-2H-3H-7-furo[3,2-b]pyran-3-ol	C18 H24 O5	+ 18.65	2.75E+07	381.1655	381.1647
12	1946	12	phenylpropanoic acid, 8,8-dimethyl-2H-B-pyrano[3,2-g]chromen-2-one	C14 H12 O3	+ 10.80	2.64E+07	229.0859	229.0851
13	2114	13	phenylpropanoic acid, 5,6,7,8-Tetramethoxycoumarin	C14 H16 O4	+ 4.62	1.60E+06	267.0863	267.0855
14	2133	14	phenylpropanoic acid, (6-Oxo-6H-1-[3,1]oxolol[4,5-g]chromen-8-yl)acetate	C12 H8 O6	+ 3.66	8.99E+06	249.0394	249.0381
15	2134	15	phenylpropanoic acid, Berigapten	C12 H8 O4	+ 7.71	2.71E+07	217.0495	217.0489
16	2254	16	phenylpropanoic acid, Asarone	C12 H16 O3	+ 9.07	3.62E+07	209.1172	209.1164
17	2318	17	phenylpropanoic acid, 6,7,8-trimethoxy-2H-chromen-2-one	C12 H12 O5	+ 7.97	1.85E+07	237.0758	237.0747
18	2338	18	phenylpropanoic acid, 6,7-Dihydrocoumarin-4-acetic acid	C11 H8 O6	+ 3.66	1.63E+07	237.0394	237.0383
19	2456	19	phenylpropanoic acid, NP-014891	C11 H14 O3	+ 6.45	7.77E+07	195.1018	195.1006
20	2505	20	phenylpropanoic acid, Ethyl cinnamate	C11 H12 O2	+ 6.45	8.04E+06	177.0910	177.0902
21	2517	21	phenylpropanoic acid, Scoparone	C11 H10 O4	+ 7.35	8.41E+07	207.0652	207.0644
22	2528	22	phenylpropanoic acid, Fraxetin	C10 H8 O5	+ 4.59	8.61E+07	209.0444	209.0437
23	2534	23	phenylpropanoic acid, Scopoletin	C10 H8 O4	+ 8.26	5.14E+06	193.0495	193.0486
24	2684	24	phenylpropanoic acid, Isoeugenol	C10 H12 O2	+ 7.00	1.32E+07	165.0910	165.0902
25	2744	25	phenylpropanoic acid, Begenin	C14 H16 O5	+ 10.45	2.47E+06	227.0728	227.0718
26	2120	26	phenylpropanoic acid, CHEMBRDG-86.6484841	C13 H14 O2	+ 8.78	7.52E+06	203.1067	203.1059
27	2330	27	phenylpropanoic acid, (5,7-Dihydroxy-4-methyl-2-oxo-2H-chromen-3-yl)acetic acid	C13 H10 O6	+ 4.59	1.53E+08	251.0550	251.0539
28	2342	28	phenylpropanoic acid, 5-Methoxy-4-oxo-4H-chromene-2-carboxylic acid	C13 H8 O5	+ 4.34	1.32E+07	221.0444	221.0436
29	2488	29	phenylpropanoic acid, 4,5-Di-O-methyl-8-methylene-4-methoxyphenyl-5-methyl-2H-pyran-3-ol	C13 H16 O5	+ 23.79	3.18E+07	231.1380	231.1371
30	843	30	phenylpropanoic acid, Ethyl-3-(7-12-(alkoxy)-2-oxoethoxy)-4,8-dimethyl-2H-pyran-3-ol	C21 H24 O7	+ 7.41	1.88E+07	389.1595	389.1578
31	844	31	phenylpropanoic acid, (3R,4R)-4-[(3,4-dimethoxyphenyl)methyl]-3,4-dihydro-2H-pyran-3-ol	C21 H24 O6	+ 9.20	3.90E+07	373.1646	373.1578
32	1053	32	phenylpropanoic acid, Mataresinol	C20 H22 O6	+ 8.56	5.80E+06	359.1489	359.1474
33	1797	33	phenylpropanoic acid, Luwangtin	C15 H14 O4	+ 11.31	2.22E+08	259.0965	259.0954
34	1897	34	phenylpropanoic acid, 3-allyl-4-methoxyphenyl-5-methyl-2H-pyran-3-ol	C14 H20 O3	+ 8.85	2.46E+06	265.1597	265.1579
35	1904	35	phenylpropanoic acid, Trolox	C14 H18 O4	+ 8.63	1.75E+06	251.1278	251.1200
36	2401	36	phenylpropanoic acid, threo-Syringylglycerol	C11 H16 O6	+ 4.51	1.45E+07	245.1020	245.1012
37	2623	37	phenylpropanoic acid, Hydrocinnamyl Alcohol	C10 H14 O3	+ 7.04	1.17E+07	183.1018	183.1008
38	2638	38	phenylpropanoic acid, 4-Methoxybenzylidenehydrate	C10 H8 O3	+ 6.35	8.98E+06	159.0431	159.0423
39	2679	39	phenylpropanoic acid, 4-Methoxyhydrocinnamic acid	C10 H12 O3	+ 4.53	8.63E+06	181.0859	181.0850
40	5	40	phenylpropanoic acid, NP-021030	C9 H8 O4	+ 5.69	5.57E+06	181.0495	181.0486
41	429	1	terpene, Lup-20(29)-ene-3,28-diyol (2E,2'Ebis(3-phenylallyl)-3,28-dihydro-1,2,3,4-tetrahydronaphthalene-12-ene)	C48 H62 O4	+ 18.84	3.76E+07	703.4721	703.4720
42	451	2	terpene, Cheta-3, beta-D-Xylopranosylxylan-12-ene	C48 H58 O7	+ 18.90	6.35E+07	705.4003	705.4002
43	500	3	terpene, Triolollic acid	C40 H48 O3	+ 21.34	3.68E+06	457.36702	457.36504
44	513	4	terpene, NP-022711	C30 H48 O2	+ 22.98	1.03E+07	441.3708	441.3708
45	516	5	terpene, (1R,2S,5S,8R,10R,14R)-20-hydroxy-1,2,14,18-pentacyclic-1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100,101,102,103,104,105,106,107,108,109,110,111,112,113,114,115,116,117,118,119,120,121,122,123,124,125,126,127,128,129,130,131,132,133,134,135,136,137,138,139,140,141,142,143,144,145,146,147,148,149,150,151,152,153,154,155,156,157,158,159,160,161,162,163,164,165,166,167,168,169,170,171,172,173,174,175,176,177,178,179,180,181,182,183,184,185,186,187,188,189,190,191,192,193,194,195,196,197,198,199,200,201,202,203,204,205,206,207,208,209,210,211,212,213,214,215,216,217,218,219,220,221,222,223,224,225,226,227,228,229,230,231,232,233,234,235,236,237,238,239,240,241,242,243,244,245,246,247,248,249,250,251,252,253,254,255,256,257,258,259,260,261,262,263,264,265,266,267,268,269,270,271,272,273,274,275,276,277,278,279,280,281,282,283,284,285,286,287,288,289,290,291,292,293,294,295,296,297,298,299,300,301,302,303,304,305,306,307,308,309,310,311,312,313,314,315,316,317,318,319,320,321,322,323,324,325,326,327,328,329,330,331,332,333,334,335,336,337,338,339,340,341,342,343,344,345,346,347,348,349,350,351,352,353,354,355,356,357,358,359,360,361,362,363,364,365,366,367,368,369,370,371,372,373,374,375,376,377,378,379,380,381,382,383,384,385,386,387,388,389,390,391,392,393,394,395,396,397,398,399,400,401,402,403,404,405,406,407,408,409,410,411,412,413,414,415,416,417,418,419,420,421,422,423,424,425,426,427,428,429,430,431,432,433,434,435,436,437,438,439,440,441,442,443,444,445,446,447,448,449,450,451,452,453,454,455,456,457,458,459,460,461,462,463,464,465,466,467,468,469,470,471,472,473,474,475,476,477,478,479,480,481,482,483,484,485,486,487,488,489,490,491,492,493,494,495,496,497,498,499,500,501,502,503,504,505,506,507,508,509,510,511,512,513,514,515,516,517,518,519,520,521,522,523,524,525,526,527,528,529,530,531,532,533,534,535,536,537,538,539,540,541,542,543,544,545,546,547,548,549,550,551,552,553,554,555,556,557,558,559,560,561,562,563,564,565,566,567,568,569,570,571,572,573,574,575,576,577,578,579,580,581,582,583,584,585,586,587,588,589,590,591,592,593,594,595,596,597,598,599,600,601,602,603,604,605,606,607,608,609,610,611,612,613,614,615,616,617,618,619,620,621,622,623,624,625,626,627,628,629,630,631,632,633,634,635,636,637,638,639,640,641,642,643,644,645,646,647,648,649,650,651,652,653,654,655,656,657,658,659,660,661,662,663,664,665,666,667,668,669,670,671,672,673,674,675,676,677,678,679,680,681,682,683,684,685,686,687,688,689,690,691,692,693,694,695,696,697,698,699,700,701,702,703,704,705,706,707,708,709,710,711,712,713,714,715,716,717,718,719,720,721,722,723,724,725,726,727,728,729,730,731,732,733,734,735,736,737,738,739,740,741,742,743,744,745,746,747,748,749,750,751,752,753,754,755,756,757,758,759,760,761,762,763,764,765,766,767,768,769,770,771,772,773,774,775,776,777,778,779,780,781,782,783,784,785,786,787,788,789,790,791,792,793,794,795,796,797,798,799,800,801,802,803,804,805,806,807,808,809,810,811,812,813,814,815,816,817,818,819,820,821,822,823,824,825,826,827,828,829,830,831,832,833,834,835,836,837,838,839,840,841,842,843,844,845,846,847,848,849,850,851,852,853,854,855,856,857,858,859,860,861,862,863,864,865,866,867,868,869,870,871,872,873,874,875,876,877,878,879,880,881,882,883,884,885,886,887,888,889,890,891,892,893,894,895,896,897,898,899,900,901,902,903,904,905,906,907,908,909,910,911,912,913,914,915,916,917,918,919,920,921,922,923,924,925,926,927,928,929,930,931,932,933,934,935,936,937,938,939,940,941,942,943,944,945,946,947,948,949,950,951,952,953,954,955,956,957,958,959,960,961,962,963,964,965,966,967,968,969,970,971,972,973,974,975,976,977,978,979,980,981,982,983,984,985,986,987,988,989,990,991,992,993,994,995,996,997,998,999,1000,1001,1002,1003,1004,1005,1006,1007,1008,1009,1010,1011,1012,1013,1014,1015,1016,1017,1018,1019,1020,1021,1022,1023,1024,1025,1026,1027,1028,1029,1030,1031,1032,1033,1034,1035,1036,1037,1038,1039,1040,1041,1042,1043,1044,1045,1046,1047,1048,1049,1050,1051,1052,1053,1054,1055,1056,1057,1058,1059,1060,1061,1062,1063,1064,1065,1066,1067,1068,1069,1070,1071,1072,1073,1074,1075,1076,1077,1078,1079,1080,1081,1082,1083,1084,1085,1086,1087,1088,1089,1090,1091,1092,1093,1094,1095,1096,1097,1098,1099,1100,1101,1102,1103,1104,1105,1106,1107,1108,1109,1110,1111,1112,1113,1114,1115,1116,1117,1118,1119,1120,1121,1122,1123,1124,1125,1126,1127,1128,1129,1130,1131,1132,1133,1134,1135,1136,1137,1138,1139,1140,1141,1142,1143,1144,1145,1146,1147,1148,1149,1150,1151,1152,1153,1154,1155,1156,1157,1158,1159,1160,1161,1162,1163,1164,1165,1166,1167,1168,1169,1170,1171,1172,1173,1174,1175,1176,1177,1178,1179,1180,1181,1182,1183,1184,1185,1186,1187,1188,1189,1190,1191,1192,1193,1194,1195,1196,1197,1198,1199,1200,1201,1202,1203,1204,1205,1206,1207,1208,1209,1210,1211,1212,1213,1214,1215,1216,1217,1218,1219,1220,1221,1222,1223,1224,1225,1226,1227,1228,1229,1230,1231,1232,1233,1234,1235,1236,1237,1238,1239,1240,1241,1242,1243,1244,1245,1246,1247,1248,1249,1250,1251,1252,1253,1254,1255,1256,1257,1258,1259,1260,1261,1262,1263,1264,1265,1266,1267,1268,1269,1270,1271,1272,1273,1274,1275,1276,1277,1278,1279,1280,1281,1282,1283,1284,1285,1286,1287,1288,1289,1290,1291,1292,1293,1294,1295,1296,1297,1298,1299,1300,1301,1302,1303,1304,1305,1306,1307,1308,1309,1310,1311,1312,1313,1314,1315,1316,1317,1318,1319,1320,1321,1322,1323,1324,1325,1326,1327,1328,1329,1330,1331,1332,1333,1334,1335,1336,1337,1338,1339,1340,1341,1342,1343,1344,1345,1346,1347,1348,1349,1350,1351,1352,1353,1354,1355,1356,1357,1358,1359,1360,1361,1362,1363,1364,1365,1366,1367,1368,1369,1370,1371,1372,1373,1374,1375,1376,1377,1378,1379,1380,1381,1382,1383,1384,1385,1386,1387,1388,1389,1390,1391,1392,1393,1394,1395,1396,1397,1398,1399,1400,1401,1402,1403,1404,1405,1406,1407,1408,1409,1410,1411,1412,1413,1414,1415,1416,1417,1418,1419,1420,1421,1422,1423,1424,1425,1426,1427,1428,1429,1430,1431,1432,1433,1434,1435,1436,1437,1438,1439,1440,1441,1442,1443,1444,1445,1446,1447,1448,1449,1450,1451,1452,1453,1454,1455,1456,1457,1458,1459,1460,1461,1462,1463,1464,1465,1466,1467,1468,1469,1470,1471,1472,1473,1474,1475,1476,1477,1478,1479,1480,1481,1482,1483,1484,1485,1486,1487,1488,1489,1490,1491,1492,1493,1494,1495,1496,1497,1498,1499,1500,1501,1502,1503,1504,1505,1506,1507,1508,1509,1510,1511,1512,1513,1514,1515,1516,1517,1518,1519,1520,1521,1522,1523,1524,1525,1526,1527,1528,1529,1530,1531,1532,1533,1534,1535,1536,1537,1538,1539,1540,1541,1542,1543,1544,1545,1546,1547,1548,1549,1550,1551,1552,1553,1554,1555,1556,1557,1558,1559,1560,1561,1562,1563,1564,1565,1566,1567,1568,1569,1570,1571,1572,1573,1574,1575,1576,1577,1578,1579,1580,1581,1582,1583,1584,1585,1586,1587,1588,1589,1590,1591,1592,1593,1594,1595,1596,1597,1598,1599,1600,1601,1602,1603,1604,1605,1606,1607,1608,1609,1610,1611,1612,1613,1614,1615,1616,1617,1618,1619,1620,1621,1622,1623,1624,1625,1626,1627,1628,1629,1630,1631,1632,1633,1634,1635,1636,1637,1638,1639,1640,1641,1642,1643,1644,1645,1646,1647,1648,1649,1650,1651,1652,1653,1654,1655,1656,1657,1658,1659,1660,1661,1					



160	310 C36	phenolic acids, Benzoic acid	C7 H6 O2	+ 6.23	8.00E+06	123.0441	123.0434	95.0487,79.0538,77.0382,65.0383,51.0227
161	313 C37	phenolic acids, 5,6-Dioxo-1,3-cyclohexadiene-1-carboxylic acid	C7 H4 O4	+ 7.57	1.38E+07	153.0182	153.0175	125.027,97.0279,83.0123
162	315 C38	phenolic acids, 5-Hydroxy-1,3-benzodioxol-2-one	C7 H4 O6	+ 6.34	8.75E+06	153.0177	153.0177	92.0254,81.0332,1.0277
163	320 C39	phenolic acids, D-pinol	C7 H14 O6	+ 1.14	4.35E+06	159.0683	159.0685	159.0645,148.051,120.0802,69.0332
164	326 C40	phenolic acids, butyl acrylate	C7 H12 O2	+ 6.05	9.22E+05	129.0910	129.0541	111.0435,73.0281,69.0696
165	330 C41	phenolic acids, Succinylacetone	C7 H10 O4	+ 4.00	4.96E+06	159.0652	159.0645	141.0540,132.1337,113.0592,85.0281,57.0332
166	331 C42	phenolic acids, dimethyl itaconate	C7 H10 O4	+ 21.29	4.27E+06	159.0652	159.0644	119.0849,115.0536,99.0436,71.0488,55.0540
167	341 C43	phenolic acids, 3,6-Dimethyl-2-methylene-5-butyrolactone	C7 H12 O4	+ 6.17	7.6E+06	162.0456	162.0447	99.0436,85.0281,83.0525,55.0540
168	347 C44	phenolic acids, 5-Hydroxy-4-methoxy-2-hydroxy-2H-pyran-2-one	C6 H8 O4	+ 3.10	2.01E+07	145.0495	145.0489	127.0385,99.0437,85.0281,71.0486
169	355 C45	phenolic acids, 2,5-Bis(hydroxymethyl)furan	C6 H8 O3	+ 22.61	5.07E+08	129.0546	129.0539	111.0435
170	356 C46	phenolic acids, 3,5-Dihydroxy-2-hydroxymethyl-4H-pyran-4-one	C6 H8 O5	+ 2.44	1.63E+06	159.0288	159.0281	141.0716,113.0228,85.0283,67.0175,55.0176
171	359 C47	phenolic acids, Knic acid	C6 H8 O4	+ 4.34	3.37E+07	143.0339	143.0332	125.0277,115.0384,87.0436,83.0488,63.0320
172	365 C48	phenolic acids, 5-Hydroxymethyl-2-furaldehyde	C6 H8 O3	+ 6.35	2.90E+07	127.0390	127.0384	109.0643,99.0436,97.0280,81.0331,53.0383
173	379 C49	phenolic acids, MFC00177095	C6 H4 O4	+ 2.48	3.36E+06	141.0182	141.0175	123.0071,113.0228,97.0280,95.0173,81.0321,85.0280,55.0176
174	385 C50	phenolic acids, 4-Oxo-4H-pyran-2-carbaldehyde	C6 H4 O3	+ 2.62	3.7E+06	125.0233	125.0227	97.0279,83.0124,69.0332,53.0310
175	391 C51	phenolic acids, Furo[3,2-b]furan-2,5-dione	C6 H2 O4	+ 2.10	9.28E+05	139.0026	139.0019	111.071,95.0123,68.9968,55.0176
176	443 C52	phenolic acids, Antioxidant CA	C37 H52 O3	+ 19.91	1.17E+08	545.3999	545.3999	55.0539
177	456 C53	phenolic acids, 3-Hydroxy-5-oxo-5-(tetradecyloxy)-3-itetradecol	C34 H64 O7	+ 19.60	1.26E+07	585.4725	585.4733	97.1007,87.0437,85.1008,83.0852,73.0645,71.0852,69.0696,57.0696
178	558 C54	phenolic acids, 5-(2S,3S)-6-Hydroxy-2-(4-hydroxyhexenyl)-4-ite	C28 H52 O8	+ 18.57	1.19E+07	455.4498	455.447	199.0744,138.0883,133.0728,123.1425,107.0487,95.0487
179	583 C55	phenolic acids, C1267	C26 H54 O8	+ 16.44	9.32E+07	496.3991	496.3987	221.1374,177.1114,133.0854,89.0593,71.0852,57.0696
180	617 C56	phenolic acids, C1266	C24 H50 O7	+ 16.44	8.14E+07	451.3629	451.3614	195.1219,177.1114,133.0853,89.0593,71.0852,57.0696
181	619 C57	phenolic acids, 2106657	C24 H42	+ 13.65	3.29E+07	331.3359	331.3380	135.1161,121.1006,97.1006,93.0695,85.1008,79.0538,57.0696
182	631 C58	phenolic acids, MFC00206373	C24 H38 O4	+ 20.52	3.15E+08	391.2843	391.2827	179.0695,167.0331,153.0539,137.0590,71.0852,57.0696
183	657 C59	phenolic acids, 2-Arachidonyl glycerol	C23 H38 O4	+ 13.83	2.42E+06	379.2843	379.2827	133.1006,121.1006,109.1007,107.0850,95.0851,87.0437
184	661 C60	phenolic acids, 5-(8R)-8-Hexadecen-1-yl-1,3-benzenediol	C23 H38 O2	+ 22.28	1.16E+07	347.2945	347.2929	235.1684,179.1058,165.0098,163.0746,161.0596,151.0747,123.0436,83.0852
185	680 C61	phenolic acids, 4-(5,5-dimethyl-1,3-dioxan-2-yl)-4'-heptylbutyr	C23 H38 O3	+ 19.59	2.38E+07	361.2737	361.2720	175.1108,161.0953,159.0795,129.0693,91.0538,69.0696,57.0696
186	718 C62	phenolic acids, C1267	C22 H38 O2	+ 18.44	1.74E+08	333.2748	333.2744	125.0520,89.0593,71.0852,57.0696
187	727 C63	phenolic acids, MFC00038340	C22 H38 O2	+ 18.44	1.74E+08	333.2748	333.2744	151.0746,125.0591,109.0643,107.0486,83.0851,69.0695,55.0540
188	740 C64	phenolic acids, Docosapentaenoic acid	C22 H34 O2	+ 13.11	1.01E+07	331.2632	331.2617	147.1162,133.1006,121.1006,107.0851,95.0851,83.0895,67.0539,55.0540
189	786 C65	phenolic acids, 1-Linolol alcohol	C21 H38 O4	+ 18.08	1.82E+07	355.2843	355.2826	175.1474,147.1162,135.1163,123.1163,109.1007,95.0851,81.0695,67.0539
190	812 C66	phenolic acids, 5-(2-Phenyl-8-ethylbenzene-1,3-diol	C21 H24 O2	+ 8.5	1.35E+06	281.1213	281.1207	179.059,165.0902,151.0747,137.0591,123.0435,69.0695,55.0540
191	825 C67	phenolic acids, 5-(8Z-11Z)-penta-deca-8,11-dien-1-yl-benzene-	C21 H32 O2	+ 16.54	1.22E+07	317.2475	317.2460	177.0902,163.0746,149.0590,137.0591,123.0435,83.0852
192	889 C68	phenolic acids, Ethyl oleate	C20 H38 O2	+ 11.61	1.15E+06	311.2945	311.2929	149.0954,137.0955,125.0955,107.0850,95.0851,81.0695,67.0539,55.0540
193	911 C69	phenolic acids, Ethyl linoleate	C20 H36 O2	+ 20.50	4.42E+06	309.2788	309.2774	161.1318,147.1162,133.1006,109.1007,95.0851,81.0695,69.0696
194	946 C70	phenolic acids, 8Z,12Z-1,4-Eicosatrienoic acid	C20 H34 O2	+ 14.16	5.21E+06	307.2616	307.2616	109.0643,95.0488,69.0695,55.0540
195	964 C71	phenolic acids, 2KCD01887	C20 H32 O2	+ 15.66	1.35E+06	303.2463	303.2463	95.0851,83.0852,69.0696,67.0539,55.0540
196	1072 C72	phenolic acids, PROPYLENEGLYCOLDIOCTANOATE	C19 H36 O4	+ 15.98	7.83E+06	329.2686	329.2673	117.0541,85.0281,61.0281,57.0332
197	1078 C73	phenolic acids, 6132055	C19 H36 O3	+ 19.31	4.59E+07	313.2737	313.2732	125.1319,111.1163,97.1007,85.1008,71.0852,57.0696
198	1181 C74	phenolic acids, (+)-[2(13)-DIHOME	C18 H34 O4	+ 19.38	1.09E+07	315.2530	315.2514	111.0799,109.1007,101.0593,97.0644,95.0851,83.0852,57.0696
199	1189 C75	phenolic acids, 1,2-Di(2-hydroxybutyl)benzoyl-beta-D-glucop	C18 H32 O2	+ 19.38	1.09E+07	293.2126	293.2126	165.1627,155.1424,141.1268,111.1164,97.1008,71.0852,57.0696
200	1250 C76	phenolic acids, Kogonol H	C18 H20 O	+ 20.20	9.63E+06	265.2526	265.2513	153.1267,139.1111,125.0955,111.0799,97.0643,71.0852,57.0696
201	1265 C77	phenolic acids, NP-001445	C18 H30 O5	+ 14.62	4.40E+07	327.2166	327.2151	169.0851,155.0695,127.0384,109.1007,95.0851,69.0696
202	1279 C78	phenolic acids, 9-Oxo-10E,12E)-octadecadienoic acid	C18 H30 O3	+ 10.94	8.20E+07	295.2250	295.2250	179.1421,151.1110,111.0799,99.0800,71.0852,57.0696
203	1286 C79	phenolic acids, Phindelic acid	C18 H30 O2	+ 12.76	2.60E+07	279.2319	279.2305	137.1320,111.1163,97.1008,57.0696
204	1324 C80	phenolic acids, 3,4-Dihydro-8-octyl-(12H)-naphthalene	C18 H28 O2	+ 19.47	2.74E+06	299.2091	299.2086	189.1628,147.0797,133.1006,119.0850,109.1006,91.0538
205	1342 C81	phenolic acids, 4,4'-Disopropylbiphenyl	C18 H22	+ 10.56	1.33E+06	239.1794	239.1787	197.1315,119.0850,105.0694,77.0381
206	1381 C82	phenolic acids, Ethyl 2,5-dimethoxy-1H-oxobenzeneheptanoate	C17 H24 O5	+ 11.72	5.59E+06	309.16605	309.16827	179.1422,165.0539,155.1059,139.1111,137.0591,107.0487
207	1403 C83	phenolic acids, Palmitic acid	C16 H32 O2	+ 16.41	8.25E+06	287.2475	287.2463	61.0281
208	1438 C84	phenolic acids, 2-(2-hydroxyethyl)-2-oxo-3-oxopentanoate	C16 H28 O5	+ 13.30	3.48E+07	293.2126	293.2126	159.1110,137.1318,111.0799,97.1007,69.0695
209	1460 C85	phenolic acids, Benzo-18-crown-6	C16 H24 O6	+ 9.58	9.48E+05	313.1646	313.1631	163.0745,137.0591,119.0486,115.0747,71.0488,59.0489
210	1466 C86	phenolic acids, NP-004038	C16 H24 O3	+ 8.40	1.73E+06	265.1798	265.1786	191.1058,175.1472,153.0903,151.0746
211	1467 C87	phenolic acids, 10-Phenyldecane	C16 H24 O2	+ 11.13	6.68E+06	249.1849	249.1838	133.1420,175.1473,147.1161,133.1005,139.1111,97.0643
212	1508 C88	phenolic acids, 1,2-Di(2-hydroxybutyl)benzoyl-beta-D-glucop	C16 H24 O2	+ 11.13	6.68E+06	249.1849	249.1838	219.0642,209.0435,197.0437,177.0539,133.0728,111.0498,55.0540
213	1607 C89	phenolic acids, 19-NONANEDIOL DIACRYLATE	C15 H24 O4	+ 10.47	5.19E+06	269.1747	269.1734	195.1370,167.1058,155.1059,141.0902,123.1162,83.0852,69.0696
214	1694 C90	phenolic acids, Gemfibrozil	C15 H22 O3	+ 9.78	8.61E+06	251.1642	251.1631	205.1577,149.0954,123.0799,105.0694,87.0437,69.0332
215	1705 C91	phenolic acids, 3,5-di-tert-butyl-4-hydroxybenzaldehyde	C15 H22 O2	+ 9.57	2.74E+07	235.1693	235.1681	207.1736,179.1058,161.0954,151.1110,57.0697
216	1708 C92	phenolic acids, 4-Octylbenzaldehyde	C15 H22 O2	+ 8.73	3.76E+07	219.1743	219.1733	191.1786,121.0643,107.0487,91.0538,57.0696
217	1709 C93	phenolic acids, 1,8-Cyclopentadecadiene	C15 H26 O	+ 8.83	8.61E+06	217.1589	217.1579	175.1109,161.0955,153.1006,125.0956,119.0851,91.0539,83.0489,55.0540
218	1745 C94	phenolic acids, Turmerone	C15 H20 O	+ 8.83	8.61E+06	217.1589	217.1579	145.1094,131.0849,123.1162,111.0799,105.0694,97.1006,91.0538,71.0852,57.0696
219	1748 C95	phenolic acids, (1E,3D)-1,3-Nonadien-1-ylbenzene	C15 H18 O	+ 8.72	2.08E+07	201.16377	201.16309	163.0746,137.0591,119.0486,105.0694,91.0538,83.0852,67.0539
220	1773 C96	phenolic acids, Losoxifenol	C15 H18 O3	+ 8.63	4.75E+07	247.13287	247.13197	191.1786,121.0643,107.0487,91.0538,57.0696
221	1781 C97	phenolic acids, 4-methoxy-6-(2-(4-methoxyphenyl)ethyl)-20H-	C15 H16 O4	+ 8.83	8.61E+06	217.1589	217.1579	175.1109,161.0955,153.1006,125.0956,119.0851,91.0539,83.0489,55.0540
222	1783 C98	phenolic acids, bisphenol A	C15 H16 O2	+ 8.65	1.99E+07	229.1223	229.12143	211.1116,135.0799
223	1874 C99	phenolic acids, MFC00014547	C14 H22 O3	+ 9.51	7.17E+06	239.16417	239.16319	193.1579,141.0903,127.0384,85.0281,71.0853
224	1884 C100	phenolic acids, NP-002040	C14 H20 O3	+ 9.25	2.50E+07	237.1485	237.1475	181.0850,177.1265,163.0746,95.0851
225	1905 C101	phenolic acids, 4,4'-Bis(hydroxy)-4'-oxobutanoic acid	C14 H20 O2	+ 8.59	2.78E+07	233.1485	233.1478	205.1213,165.0903,97.0643,95.0847,59.0489
226	1909 C102	phenolic acids, 2-Pentyl-1-midanone	C14 H18 O	+ 10.09	1.47E+07	203.1430	203.1420	153.1006,105.0694,91.0538
227	1916 C103	phenolic acids, (2S,4R,5S,6S,7R)-5,6,12,14-tetrahydroxy-4-hydrox	C14 H16 O9	+ 4.56	5.24E+08	329.0867	329.0855	207.0642,197.0435,139.0384,85.0280,69.0332
228	1941 C104	phenolic acids, 1,1,8,8-tetrahydroxy-3,6-dimethyl-2-naphthylethan	C14 H14 O3	+ 10.45	3.43E+06	231.1016	231.1006	187.0746
229	1989 C105	phenolic acids, 4-Oxotetradecanoic acid	C14 H26 O2	+ 8.39	1.41E+07	211.1683	211.1668	193.1578,133.1006,111.0493,109.1007,95.0851,67.0539
230	2014 C106	phenolic acids, NP-007909	C13 H20 O3	+ 6.70	2.38E+07	225.1485	225.1476	207.1370,125.0591,123.1163,109.1007,95.0851,83.0852,69.0696
231	2044 C107	phenolic acids, Heptylbenzene	C13 H26 O	+ 9.26	2.67E+06	177.1638	177.1629	135.1162,121.1006,93.0694,79.0538,97.1006
232	2052 C108	phenolic acids, 1-(3-ethyl-2,4-dihydroxy-6-methoxyphenyl)buta	C13 H18 O4	+ 8.78	9.92E+06	239.1278	239.1268	153.0799,111.0436,105.0694,83.0488,55.0540
233	2063 C109	phenolic acids, Hexyloxybenzoic acid	C13 H18 O3	+ 6.68	2.07E+07	223.1329	223.1320	205.1213,165.0903,97.0643,95.0847,59.0489
234	2068 C110	phenolic acids, Hexapentenoic acid	C13 H18 O1	+ 9.09	3.97E+07	235.1430	235.1421	133.1006,105.0694,91.0538
235	2091 C111	phenolic acids, 1-(4-hydroxy-3-(3-methylbut-2-en-1-yl)phenyl)	C13 H16 O2	+ 6.66	9.29E+06	205.1223	205.1216	163.1109,145.1005,135.1162,121.0642,107.0850,105.0694,91.0538
236	2097 C112	phenolic acids, Cyclohexyl phenyl ketone	C13 H16 O	+ 6.69	3.46E+07	189.1274	189.1264	159.0797,143.0848,131.0849,117.0693,91.0538
237	2103 C113	phenolic acids, 4-Pentylphenylacetylene	C13 H16	+ 10.88	8.52E+06	173.1325	173.1316	143.0849,117.0693,95.0338,67.0539
238	2117 C114	phenolic acids, (2S)-5-Methoxy-2-methyl-2,3,8,9-tetrahydro-4H-	C13 H16 O4	+ 8.65	1.00E+07	225.0685	225	

MS	Site	Compound category	Name	Formula	Ion mode	RT	Response	theoretical val	Measured value	MS/MS	
1	4	phenylpropanoid	3,5,7-Trihydroxy-4H-chromen-4-one	C18H05O5	+	2.69	2,48E+07	95.0288	195.0279	177.0173,149.0226,135.0434,123.0435,109.0279	
2	2	8	phenylpropanoid	Umbelliferone	C9H6O3	+	4.42	8,69E+06	163.0390	163.0382	145.0277,123.0434,109.0279,93.0330,55.0176
3	15	phenylpropanoid	Coumarin	C9H6O2	+	5.21	1,20E+06	147.0441	147.0433	119.0485,107.0486,103.0537,77.0382	
4	376	phenylpropanoid	Actigargin-1	C21H24O6	+	7.94	2,57E+06	373.1646	373.1626	373.1626	
5	610	phenylpropanoid	4-(3R,4S)-4-(2E)-3-(3,4-dihydroxyphenyl)propan-2-one	C14H14O4	+	9.38	1,02E+04	255.1024	255.1027	183.0486,163.0392,135.0434,85.0280	
6	827	phenylpropanoid	Diethyl benzalacetate	C14H16O4	+	9.49	1,20E+07	249.1121	249.1110	203.0694,189.0901,175.0538,161.0590,147.0434,91.0538	
7	925	phenylpropanoid	CHEMRRD-BA 6367113	C13H14O3	+	9.72	1,25E+07	219.1016	219.1006	201.0902,191.1057,123.0435,107.0487	
8	1012	phenylpropanoid	7-Hydroxy-4-propylcoumarin	C12H12O3	+	12.91	1,77E+07	205.0859	205.0852	177.0903,163.0745,109.0279	
9	1014	phenylpropanoid	6,7-Dihydroxy-4-methyl-2-oxo-2H-chromen-3-ylidene	C12H10O6	+	4.62	1,44E+08	251.0550	251.0542	191.0329,177.0537,135.0433,71.0121	
10	1102	phenylpropanoid	7-Dihydroxy-4-methyl-2-oxo-2H-chromen-3-ylidene	C12H10O6	+	4.62	1,44E+08	251.0550	251.0542	191.0329,177.0537,135.0433,71.0121	
11	1108	phenylpropanoid	6-Methoxy-4-oxo-4H-chromene-2-carboxylic acid	C11H8O5	+	4.60	8,20E+06	221.0444	221.0436	193.0466,177.0538,175.0383,149.0649,123.0434,107.0486	
12	1080	phenylpropanoid	Scopalone	C11H10O4	+	4.42	1,07E+07	207.0652	207.0646	179.0693,175.0383,165.0538	
13	1085	phenylpropanoid	4,6-Dihydroxy-3-oxo-1,3-dihydro-2-benzofuran-1-one	C10H8O6	+	4.60	7,82E+06	225.0394	225.0385	207.0279,181.0488,179.0330,165.0173,137.0225,109.0279	
14	1087	phenylpropanoid	Fraxetin	C10H8O5	+	4.62	8,27E+07	209.0444	209.0437	191.0329,181.0485,177.0173,165.0538	
15	1095	phenylpropanoid	Scopuletone	C10H8O4	+	4.42	1,07E+07	207.0652	207.0646	179.0693,175.0383,165.0538	
16	1099	phenylpropanoid	hymecromone	C10H8O3	+	4.55	2,56E+06	177.0546	177.0537	149.0589,109.0279,93.0331	
17	1104	phenylpropanoid	2-oxo-2H-chromene-3-carboxylic acid	C10H6O4	+	4.60	1,47E+07	191.0339	191.0329	163.0381,147.0435,145.0277,105.0330	
18	1176	phenylpropanoid	(E)-2-Methoxycinnamaldehyde	C10H10O2	+	4.53	2,37E+06	163.0754	163.0747	131.0485,121.1006,107.0486,91.0538,77.0382,55.0176	
19	31	phenylpropanoid	2-Phenyl-1-propanol	C9H12O	+	8.04	7,94E+06	137.0961	137.0954	119.0849,107.0486,105.0694,91.0538,77.0383,55.0176	
20	43	phenylpropanoid	4-Hydroxy-3-methoxybenzoic acid	C9H8O4	+	4.42	1,07E+07	183.0746	183.0738	123.0798,105.0694,91.0538,77.0383,55.0176	
111	21	1011	phenylpropanoid	3-(2-Methoxyphenyl)-5-oxotetrahydro-3-furancarbaldehyde	C12H12O5	+	6.34	1,75E+06	237.0758	237.0748	163.0746,137.0591,121.0949,106.0643,85.0280
21	210	terpene	Oleonic acid benzoate	C37H52O4	+	16.47	2,13E+08	561.3938	561.3947	561.3947	
22	233	terpene	Ursolic acid	C30H48O3	+	10.19	1,99E+06	457.3676	457.3668	181.1215,163.1477,95.0850,55.0539	
23	241	terpene	18,5,8,5,10S,13S,17S,20R,10D-10-hydroxy-4,5,9,9-tetrahydronaphthalene-1,2-diol	C30H46O3	+	10.98	2,0E+07	455.5520	455.5500	301.2158,193.1216,179.0137,171.3818,95.0851,55.0540	
24	651	terpene	1,2-Dihydroxy-4-methyl-2-oxo-2H-chromen-3-ylidene	NP-0049	+	4.62	1,44E+08	251.0550	251.0542	191.0329,177.0537,135.0433,71.0121	
25	5	281	terpene	1,4-dihydroxy-1,4-dimethyl-7-(propan-2-ylidene)-2,5-dimethyl-2,5-dihydro-3H-pyran-3-one	C15H24O4	+	7.35	1,91E+06	253.1796	253.1786	199.1472,169.1267,171.265,175.1472,125.0954,111.0799,81.0695,67.0539
26	6	661	terpene	(c)-Caryophyllene oxide	C15H24O	+	9.30	2,40E+06	221.1900	221.1892	193.1584,177.1628,163.1474,116.1213,112.1162,106.090
27	7	720	terpene	(8aR,8iR,8aR,8iR)-8-Hydroxy-8a-methyl-3,5-bis(methyl-4-hydroxy-4-methylphenyl)cyclohex-3-ene-1,4-diol	C18H22O2	+	8.17	1,04E+07	211.1693	211.1685	175.1472,151.1474,109.1008,83.0689,69.0695,55.0540
28	8	863	terpene	2-(1E)-1-Buten-3-yn-1-yl-1,3,3-trimethylcyclohex-1-ene-1,2-diol	C18H22O2	+	8.17	1,04E+07	211.1693	211.1685	175.1472,151.1474,109.1008,83.0689,69.0695,55.0540
30	10	902	terpene	2-((1E)-1-Buten-3-yn-1-yl)-1,3,3-trimethylcyclohex-1-ene-1,2-diol	C18H22O2	+	8.16	2,08E+06	175.1481	175.1472	147.1160,133.1055,110.0949,105.0693,91.0538,83.0689,69.0695
31	11	141	terpene	NP-019547	C17H26O5	+	16.23	8,15E+05	309.1707	309.1708	101.0228,90.0129
32	12	838	terpene	3F48	C13H24O3	+	12.33	1,18E+06	229.1789	229.1789	155.1423,99.0436,95.0851,71.0852,57.0696
323	13	1125	steroid	Pulsagon	C20H32O6	+	8.16	1,53E+04	153.1274	153.1266	125.0954,97.0643,91.0538,77.0383,55.0176
32	1	59	quinone	2-Ethynyl-1,4-benzoquinone	C8H4O2	+	4.40	1,65E+06	133.0284	133.0278	101.0340,105.0695,85.0546,71.0487,59.0487,57.0332
2	539	quinone	Embelin	C17H26O4	+	11.79	2,17E+06	295.1904	295.1990	125.0225,101.0228,85.0546,71.0380,71.0852,57.0332	
35	3	101	quinone	2,5,8-Tetrahydroxy-1,4-naphthoquinone	C10H6O6	+	4.60	1,91E+06	223.0237	223.0229	179.0332,167.0694,153.0718,15.0282,15.0227
36	4	106	quinone	6-AVACIN	C10H6O5	+	4.60	2,07E+06	207.0746	207.0738	179.0330,163.0392,151.0384,133.0683,109.0279,93.0331
38	1	1106	quinone	Lawson	C10H6O3	+	6.83	1,26E+06	175.0390	175.0381	131.0484,119.0486,105.0328,103.0537,77.0383
39	1	379	flavonoid	Astibin	C21H22O11	+	5.66	9,91E+05	451.1235	451.1214	451.1214
39	2	380	flavonoid	Myricitrin	C21H22O12	+	7.27	5,11E+06	465.1028	465.1005	465.1005
40	3	617	flavonoid	NP-000924	C16H14O5	+	10.78	6,45E+05	287.0914	287.0900	167.0332,139.0384,121.0717,109.0487,93.0330
41	4	745	flavonoid	1-Fustin	C15H12O5	+	6.69	1,6E+07	289.0710	289.0702	177.0330,153.0539,149.0227,137.0228,127.0384,109.0279,93.0330
42	5	756	flavonoid	Quercetin	C15H10O7	+	9.08	2,70E+07	303.0499	303.0485	165.0174,153.0174,137.0226,125.0223,13.0435,109.0280
43	6	758	flavonoid	Kaempferol	C15H10O6	+	9.78	3,09E+06	287.0550	287.0546	167.0330,151.0384,139.0383,123.0434,121.0277,111.0435,103.0539
44	7	761	flavonoid	Apigenin	C15H10O5	+	5.68	1,06E+07	271.0601	271.0588	153.0176,125.0277,109.0486,109.0279,93.0339
45	1	17	phenolic acids, carb	1H-Isobutene-1,3,4-trione	C9H4O4	+	3.69	7,78E+06	177.01823	177.0174	149.0226,133.0718,121.0279,93.0331,55.0228
46	2	35	phenolic acids, carb	7-ethyl salicylate	C10H10O3	+	4.42	1,07E+07	183.0746	183.0738	123.0798,105.0694,91.0538,77.0383,55.0176
47	3	38	phenolic acids, carb	3,4-Dimethoxybenzoic acid	C9H10O4	+	8.65	4,14E+06	183.0618	183.0643	155.0695,137.0590,123.0434,93.0329,77.0382
48	4	47	phenolic acids, carb	2145	C8H8O2	+	9.63	3,11E+06	137.0597	137.0599	109.0642,91.0538,77.0383,51.0227
49	5	52	phenolic acids, carb	Phenylglyoxylic acid	C8H6O3	+	10.7	3,11E+06	151.0387	151.0382	135.0434,105.0329,91.0538,77.0383,51.0226
50	6	54	phenolic acids, carb	2145	C8H8O2	+	9.63	3,11E+06	137.0597	137.0599	109.0642,91.0538,77.0383,51.0227
51	7	57	phenolic acids, carb	Coumarandione	C8H4O3	+	12.91	4,39E+07	149.0232	149.0226	121.0278,93.0330
52	8	67	phenolic acids, carb	2347	C8H14O2	+	6.68	7,81E+06	143.1065	143.1057	125.0956,97.0077,84.0368,83.0689,69.0695,55.0540
53	9	73	phenolic acids, carb	NP-019360	C8H12O4	+	11.18	1,01E+07	173.08083	173.0801	113.0591,89.0229,81.0695,71.0124,67.0537,66.0696
54	10	76	phenolic acids, carb	Tetrahydro-2-furfuryl acrylate	C12H12O3	+	11.18	1,01E+07	173.08083	173.0801	113.0591,89.0229,81.0695,71.0124,67.0537,66.0696
55	11	78	phenolic acids, carb	Dimesone	C8H12O2	+	9.52	8,22E+05	141.0911	141.0905	141.0902,95.0851,81.0331,53.0383
56	12	79	phenolic acids, carb	ox-dihomoacetic acid	C8H10O6	+	9.07	1,10E+06	203.0501	203.0542	139.0019,129.0504,101.0228,83.0324,67.0589,55.0540
57	13	85	phenolic acids, carb	Tyrosol	C8H10O2	+	3.83	2,71E+06	139.07535	139.0747	121.0277,111.0435,93.0331,77.0382,51.0227
58	14	88	phenolic acids, carb	20330	C7H6O4	+	10.89	2,17E+06	157.04953	157.0486	113.0228,97.0133,93.0386,67.0101
59	15	88	phenolic acids, carb	Gallic acid	C7H6O5	+	8.83	2,19E+06	171.02879	171.027	153.0175,125.0273,125.0273,93.0331,55.0227
60	16	95	phenolic acids, carb	Salicylic acid	C7H6O3	+	3.78	3,42E+06	139.03879	139.0384	121.078,109.0278,93.0331,77.0382,51.0227
61	17	100	phenolic acids, carb	D-pinitol	C7H14O4	+	1.55	9,66E+06	159.08631	159.08551	141.0540,85.0281,71.0489,57.0333
62	18	101	phenolic acids, carb	Butyl salicylate	C11H14O3	+	8.89	2,45E+06	181.10157	181.10094	115.0383,93.0386,73.0383,55.0176
63	19	108	phenolic acids, carb	Ethyl octanoate	C11H20O2	+	1.16	5,48E+06	159.05618	159.05618	141.0539,127.0383,113.0591,89.0286,85.0280,71.0488
64	20	119	phenolic acids, carb	5-hydroxy-4-methoxy-5,6-dihydro-2H-pyran-2-one	C8H8O4	+	6.21	3,67E+07	145.0493	145.0499	127.0384,99.0436,97.0280,85.0369,63.0332,55.0176
65	21	130	phenolic acids, carb	Koic acid	C6H6O4	+	4.34	8,16E+06	140.03388	143.0332	125.0227,115.0385,85.0644,69.0332,55.0020
66	22	134	phenolic acids, carb	Phloroglucinol	C6H4O3	+	9.53	6,67E+07	127.03383	129.0278	109.0278
67	23	135	phenolic acids, carb	Adipic acid	C6H10O4	+	12.37	4,74E+06	147.05818	147.056	129.0540,111.0435,101.0592,83.0538
68	24	182	phenolic acids, carb	Monomethyl succinate	C5H8O4	+	4.9	5,28E+06	133.04953	133.0449	115.0384,101.0287,94.036,73.0281,57.0332
69	25	196	phenolic acids, carb	pentane-1,2,3,4,5-pentol	C5H12O5	+	1.54	1,31E+06	153.0755	153.0575	135.0646,117.0541,99.0436,69.0332,55.0176
70	26	275	phenolic acids, carb	C12E7	C6H5H4O8	+	16.45	6,62E+07	495.38914	495.38277	177.1133,0853,83.0593,85.1008
71	27	276	phenolic acids, carb	NP-014456	C6H5H4O8	+	16.45	6,62E+07	495.38914	495.38277	177.1133,0853,83.0593,85.1008
72	28	326	phenolic acids, carb	BUTYL OLEATE	C22H42O2	+	21.3	9,25E+05	339.32575	339.3241	153.1266,139.1110,125.0954,115.0748,85.1007,71.0851,69.0695
73	29	328	phenolic acids, carb	MFC00003840	C22H36O4	+	18.44	6,40E+06	333.2788	333.2774	111.1663,97.1007,101.0592,71.0852,67.0539,57.0696
74	30	339	phenolic acids, carb	CM2100000	C14H40O2	+	17.56	9,93E+06	357.29993	357.2994	115.0748,101.0748,83.0851,61.0281,57.0332
75	31	343	phenolic acids, carb	1,3-BIS(2-METHOXY-5-HYDROXY-2-FURYL)-1,3-OLEATE	C24H32O10	+	14.8	8,43E+05	441.3337	441.3337	141.167,99.0436,97.0280,85.0369,63.0332,55.0176
76	32	354	phenolic acids, carb	1-Linoleoyl glycerol	C18H38O2	+	15.84	1,06E+07	355.28428	355.28317	179.1785,165.1630,107.007,57.0696
77	33	363	phenolic acids, carb	glycidyl ether	C12H18O3	+	17.56	7,71E+06	339.28937	339.2	

WS site			Compound category	Name	formular	Ion mode	RT	Response	theoretical value	Measured value	MS/MS
1	1	5	phenylpropanoid	3,5,7-Trihydroxy-4H-chromen-4-one	C9 H6 O5	+	3.66	3.11E+06	195.0288	195.0281	167.0334,109.0280
2	2	6	phenylpropanoid	Umbelliferone	C9 H6 O3	+	12.89	1.57E+06	163.0390	163.0383	135.0434,119.0486
3	3	476	phenylpropanoid	6- <i>t</i> -Butyl-4-methylcoumarin	C14 H16 O2	+	11.09	9.98E+04	217.1223	217.1214	57.0696
4	4	512	phenylpropanoid	Nordihelol	C12 H8 O5	+	4.60	4.50E+06	233.0444	233.0435	215.0332,191.0332,135.0435,99.0071,57.0333
5	5	533	phenylpropanoid	NP-020400	C12 H18 O5	+	6.51	1.97E+06	243.1227	243.1216	169.0851,151.0746,137.0591,57.0332
6	6	547	phenylpropanoid	(5,7-Dihydroxy-4-methyl-2-oxo-2H-chromen-3-yl)acetic acid	C12 H10 O6	+	4.59	3.46E+07	251.0550	251.0539	191.0329,179.0333,162.0305,135.0433,71.0124
7	7	550	phenylpropanoid	6-Methoxy-4-oxo-4H-chromene-2-carboxylic acid	C11 H8 O5	+	4.32	2.53E+06	221.0444	221.0437	193.0486,177.0537,175.0381,161.0588
8	575		phenylpropanoid	Scoparone	C11 H10 O4	+	7.32	1.33E+06	207.0652	207.0644	175.0381,165.0539
9	9	577	phenylpropanoid	2,4-Dihydroxy-6-pyruvoylbenzoic acid	C10 H8 O6	+	4.58	1.89E+06	225.0394	225.0385	197.0435,179.0330,163.0382,55.0176
10	10	578	phenylpropanoid	Fraxetin	C10 H8 O5	+	4.60	1.99E+07	209.0444	209.0438	194.0201,181.0486,177.0174,165.0538
11	11	605	phenylpropanoid	(E)-2-Methoxycinnamaldehyde	C10 H10 O2	+	8.42	3.39E+05	163.0754	163.0746	135.0797,131.0485,121.0642,107.0486,91.0538,77.0383,55.0176
12	1	62	steroid	Trenbolone Acetate	C20 H24 O3	-	18.26	6.28E+06	311.1653	311.1652	311.1652
13	2	259	steroid	Methandrol	C20 H32 O2	+	15.62	3.94E+05	305.2475	305.2462	121.1005,107.0850,95.0850,93.0694,57.0332,55.0540
14	1	77	terpene	NP-019547	C17 H26 O5	+	17.80	3.51E+05	309.1707	309.1704	309.1704
15	2	149	terpene	Lup-20(29)-ene-3,28-diol (2E,2'E)bis(3-phenylacrylate)	C48 H62 O4	+	18.55	1.86E+07	703.4721	703.4717	121.1006,91.0538,69.0696,55.0539
16	3	503	terpene		C13 H18 O	+	8.05	3.19E+05	191.1430	191.1412	135.0799,133.1007,109.0643,69.0332,67.0539
17	1	170	flavonoid	5,7-Dihydroxy-2-(4-(4-hydroxyphenyl)-4-oxo-4H-chromen-2-ylidene)-2,3-dihydro-4H-pyran-4-one	C25 H26 O11	+	13.69	6.62E+05	503.1548	503.1550	133.0852,111.0799,107.0487,101.0592,97.0644,57.0696
18	2	441	flavonoid	Taxifolin	C15 H12 O7	+	7.14	5.23E+05	305.0656	305.0642	153.0175,151.0382,149.0225,139.0383,135.0435,127.0383,109.0278
19	3	443	flavonoid	Ouerceitin	C15 H10 O7	+	8.04	1.01E+07	303.0499	303.0485	165.0173,153.0175,123.0434,109.0278
20	1	469	quinone	DK3970000	C14 H20 O2	+	8.57	1.74E+05	221.1536	221.1528	83.0851,57.0696
21	1	13	phenolic acids	(E)-3-cyclohexylacrylic acid	C9 H14 O2	+	5.15	5.23E+05	155.1067	155.1060	137.0954,127.0748,109.1007,83.0852
22	2	20	phenolic acids	D-diacyltartaric anhydride	C8 H8 O7	+	13.87	3.64E+05	217.0343	217.0335	129.0540,97.0278,85.0280
23	3	21	phenolic acids	isovanillic acid	C8 H8 O4	+	1.52	2.08E+06	169.0495	169.0487	151.0383,141.0539,137.0226,123.0434
24	4	26	phenolic acids	Coumarandione	C8 H4 O3	+	12.89	1.23E+07	149.0233	149.0228	121.028
25	5	29	phenolic acids	Ethyl acetosuccinate	C9 H10 O5	+	16.35	1.85E+07	195.0652	195.0646	89.0593,87.0437,75.0438,57.0333
26	6	35	phenolic acids	(2Z)-2-(1,4-Dioxan-2-yl)-2-butenedioic acid	C8 H10 O6	+	1.52	4.10E+05	189.0758	203.0542	129.0539,115.0384,87.0436,71.0487,57.0333
27	7	36	phenolic acids	5-Ethoxy-2-furoic acid	C7 H8 O4	+	4.49	3.24E+06	157.0495	157.0488	139.0384,129.0177,111.0436,97.0644,83.0123
28	8	39	phenolic acids	2-Methoxyresorcinol	C7 H8 O3	+	1.52	1.72E+07	141.0546	141.0540	123.0435,109.0279
29	9	44	phenolic acids	D-pinitol	C7 H14 O6	+	1.52	2.72E+07	195.0863	195.0859	177.0752,159.0646,145.0490,141.0541,127.0385,85.0281,53.0384
30	10	49	phenolic acids	Monomethyl adipate	C7 H12 O4	+	13.71	1.89E+06	161.0808	161.0801	143.0696,129.0540,115.0749,111.0436,101.0593,83.0488
31	11	57	phenolic acids	Ethyl acetosuccinate	C7 H10 O5	+	16.35	1.85E+07	195.0652	195.0646	115.0384,115.0278,87.0437,85.0280,57.0333
32	12	71	phenolic acids	5-Hydroxy-4-methoxy-5,6-dihydro-2H-pyran-2-one	C6 H8 O4	+	3.10	7.28E+07	145.0495	145.0489	127.0384,83.0125,55.0176
33	13	86	phenolic acids	Koic acid	C6 H6 O4	+	4.33	1.87E+06	143.0339	143.0332	125.0227,115.0384,101.0228,85.0280,57.0332
34	14	87	phenolic acids	5-Hydroxymethyl-2-furaldehyde	C6 H6 O3	+	1.52	3.42E+07	127.0390	127.0384	109.0179,99.0436,97.0280,81.0332,69.0332,55.0176
35	15	126	phenolic acids	2,2-Bis(hydroxymethyl)propionic acid	C5 H10 O4	+	1.51	2.69E+06	135.0652	135.0645	117.0541,75.0437,57.0332
36	16	174	phenolic acids	C1216	C24 H50 O7	+	16.38	6.25E+07	451.3629	451.3610	177.1113,133.0854,89.0593,85.1008
37	17	196	phenolic acids	Laureth-5	C22 H46 O6	+	16.38	6.17E+07	407.3367	407.3350	133.0853,89.0593,85.1008
38	18	198	phenolic acids	undecathylene glycol	C22 H46 O12	+	6.52	3.81E+07	503.3062	503.3047	177.1113,133.0853,89.0593
39	19	212	phenolic acids	Methyl 15-phenylpentadecanoate	C22 H36 O2	+	18.34	8.61E+05	333.2788	333.2773	93.0694,79.0538,75.0436,57.0332
40	20	218	phenolic acids	Ethyl 11-oxo-9-phenanthrenehexanoate	C22 H22 O3	+	18.63	2.46E+05	335.1642	335.1653	89.0593
41	21	231	phenolic acids	5-(1'-Pentadec-8-enyl)benzene-1,3-diol	C21 H34 O2	+	18.77	6.48E+05	319.2632	319.2618	235.1684,179.1058,165.0904,137.0591,123.0435,111.1163,71.0852
42	22	241	phenolic acids	3,6,9,12,15,18-Hexaoxahexacosan-1-ol	C20 H42 O7	+	22.33	2.63E+07	395.3003	395.3009	71.0851,57.0696
43	23	243	phenolic acids	C12164	C20 H42 O5	+	16.32	6.47E+07	363.3105	363.3188	195.1218,177.1114,133.0854,89.0593,85.1008
44	24	275	phenolic acids	6132055	C18 H34 O3	+	19.22	1.03E+07	313.2737	313.2723	97.1008,81.0695,71.0852,57.0696
45	25	297	phenolic acids	Nonaethylene Glycol	C18 H38 O10	+	5.90	4.86E+07	415.2538	415.2522	177.1113,133.0854,89.0593,87.0437
46	26	300	phenolic acids	(5R)-5-(1-Hydroxytridecyl)-alpha-D-xylopyranose	C18 H36 O6	+	17.23	7.21E+06	349.2585	349.2563	181.0703,179.0547,75.0438
47	27	302	phenolic acids	(12Z)-9,10,11-trihydroxyoctadec-12-enoic acid	C18 H34 O5	+	17.25	6.10E+07	331.2479	331.2463	185.1164,101.0592,75.0427,71.0852,57.0696
48	28	341	phenolic acids	13(S)-HOTfE	C18 H30 O3	+	13.60	1.35E+06	295.2268	295.2255	179.1421,161.1317,135.1162,121.1006,107.0850,81.0695,71.0850
49	29	342	phenolic acids	1913256	C18 H30 O	+	14.41	1.35E+06	263.2369	263.2357	57.0697
50	30	348	phenolic acids	Methyl (2S,3R,4S)-2-(beta-D-glucopyranosyloxy)-4-(2-hydroxy-1-methyl-1H-imidazol-5-yl)-3-methylpentanoate	C18 H26 O11	+	6.52	7.55E+06	419.1548	419.1533	131.0333,113.0228,97.0280,85.0281,73.0281,71.0124,57.0333
51	31	365	phenolic acids	PEG n8	C16 H34 O9	+	5.58	9.62E+07	371.2276	371.2258	177.1113,133.0853,101.0593,89.0593
52	32	371	phenolic acids	Gemcabene	C16 H30 O5	+	12.21	3.36E+06	303.2166	303.2153	101.0593,97.1008,87.0436,83.0487,55.0540
53	33	407	phenolic acids	6-(7-methyloctyl)-1H-3H-4H-6H-furo[3,4-c]furan-1-ol	C15 H24 O3	+	11.54	9.36E+04	253.1798	253.1788	127.0384,99.0436,87.0280,85.1007,71.0852,57.0696
54	34	422	phenolic acids	3,5-di-tert-Butyl-4-hydroxybenzaldehyde	C15 H22 O2	+	12.39	2.97E+06	235.1693	235.1683	179.1058,161.0952,57.0696
55	35	431	phenolic acids	Atracylon	C15 H20 O	+	12.63	1.52E+05	217.1587	217.1579	135.0798,109.1007,93.0695,95.0487,81.0696,55.0540
56	36	451	phenolic acids	MFC00054545	C14 H26 O5	+	10.75	2.58E+06	275.1853	275.1841	97.0644,89.0593,81.0695,71.0488,59.0488,55.0540
57	37	470	phenolic acids	(2S,4R,5S,6S,7R)-5,6,12,14-tetrahydroxy-4-(hydroxymethyl)-2-methylpentanoic acid	C14 H16 O9	+	4.59	1.43E+08	329.0867	329.0852	211.0228,209.0435,195.0280,103.0386,85.0281,69.0332
58	38	478	phenolic acids	4-Methylbenzophenone	C14 H12 O	+	11.64	2.06E+07	197.0961	197.0952	19.0486,105.0330,91.0538,77.0382
59	39	484	phenolic acids	1,4-Dioxacyclotetradecan-5-one	C13 H24 O3	+	12.34	1.58E+06	229.1798	229.1789	155.1423,99.0436,71.0852,57.0696
60	40	506	phenolic acids	ionene	C13 H18	+	10.76	3.35E+05	175.1481	175.1475	133.1007,119.0850,105.0694,91.0538,83.0851
61	41	509	phenolic acids	3a,8b-Dihydroxy-2-(hydroxymethyl)-4-oxo-4,8b-dihydro-2H-pyran-4-one	C13 H10 O7	+	3.66	5.71E+06	279.0499	279.0486	139.0384,121.0278,119.0485,107.0486,95.0487,85.0281
62	42	511	phenolic acids	Benzophenone	C13 H10 O	+	10.86	1.13E+06	183.0804	183.0798	105.0330,77.0381
63	43	536	phenolic acids	NP-021018	C12 H18 O4	+	15.25	1.06E+06	227.1278	227.1269	1167.0696,139.0747,121.1006,95.0487,83.0851,69.0696
64	44	556	phenolic acids	Methyl 10-oxodecanoate	C11 H20 O3	+	10.82	1.95E+06	201.1485	201.1476	159.1371,141.1265,127.1111,125.0952,101.0592
65	45	560	phenolic acids	3,3-Dimethyl-1,5-dioxaspiro[5.5]undecan-9-one	C11 H18 O3	+	13.56	1.45E+05	199.1329	199.1321	125.0591,111.0797,95.0487,85.0643,57.0332
66	46	568	phenolic acids	4-Ethoxy ethylbenzoate	C11 H14 O3	+	11.47	1.18E+06	195.1016	195.1008	167.0695,149.0591,121.0279,113.0592
67	47	570	phenolic acids	4-Isobutylbenzoic acid	C11 H14 O2	+	10.57	3.13E+05	179.1067	179.1058	133.1004,95.0487
68	48	585	phenolic acids	PEG n5	C10 H22 O6	+	4.29	6.03E+06	239.1489	239.1489	221.1385,177.1113,151.0599,133.0853,89.0593
69	49	589	phenolic acids	NP-019374	C10 H18 O4	+	16.67	6.24E+06	203.1278	203.1272	185.1163,157.1216,125.0954,111.0799,101.0593,83.0488