T3_POS

Library Hit	Area	Height	Adduct / Charge
(6aR, 11aR) 3-Hydroxy-9,10-Dimethoxypterocarpan	1.66E+05	4.49E+04	[M+CH3OH+H]+
1,2-Dichloroethane	2.14E+04	3.44E+03	[M+H]+
15-Hydroxyculmorone	8.23E+03	2.02E+03	[M+H]+
2-PROPENOATE	9.43E+04	1.30E+04	[M+H]+
2-UNDECANONE	4.50E+03	6.49E+02	[M+CH3OH+H]+
3'-Aenylic Acid	2.92E+04	2.66E+03	[M+H]+
4-COUMARATE	5.75E+04	5.62E+03	[M+H]+
5-HYDROXYLYSINE	1.04E+05	5.36E+03	[M+H]+
5-Oxo-2-tetrahydrofurancarboxylic acid	2.82E+04	3.13E+03	[M+H]+
6-PHOSPHOGLUCONATE	1.22E+05	3.17E+04	[M+CH3OH+H]+
7:3 FTB (7:3 fluorotelomer betaine) (pos)	4.87E+04	5.69E+03	[M+H]+
7-Ketocholesterol	1.04E+05	2.11E+04	[M+H]+
Acecarbromal	7.49E+04	2.25E+04	[M+H]+
Acteoside	2.85E+04	7.84E+03	[M+H]+
Adenosine monophosphate	1.85E+04	2.81E+03	[M+H]+
Alpha-Linolenic acid	4.58E+05	1.14E+05	[M+H]+
AMINOISOBUTANOATE	9.93E+04	3.08E+04	[M+CH3OH+H]+
Amphetamine	1.01E+05	6.69E+03	[M+H]+
Androsterone	2.19E+05	6.57E+04	[M+H]+
a-Nortestosteron	4.93E+04	8.90E+03	[M+H]+
ARGININE	3.35E+05	1.32E+05	[M+NH4]+
BENZOATE	1.58E+05	2.68E+04	[M+H]+
BETAINE	1.08E+05	3.21E+04	[M+H]+
Beta-sitosterol	9.13E+05	2.28E+05	[M+H]+
BILIVERDIN	1.46E+05	2.03E+04	[M+H]+
Biperiden	7.10E+04	1.32E+04	[M+H]+
Bisoprolol	1.14E+05	2.32E+04	[M+H]+
Bromacil	2.27E+04	6.19E+03	[M+H]+
Buspirone	2.90E+03	6.72E+02	[M+H]+
Canavanine	2.31E+05	7.53E+04	[M+H]+
Caprolactone	3.98E+04	6.11E+03	[M+H]+
Chelidonic acid	2.20E+04	3.94E+03	[M+H]+
Chlorogenic Acid	3.99E+05	1.01E+05	[M+H]+
CITRAMALATE	1.87E+04	1.40E+03	[M+H]+
CMAmB-FO (carboxymethyldimethylammoniobutyl-p	5.21E+03	7.20E+02	[M+NH4]+
CORTISOL 21-ACETATE	1.95E+05	5.65E+04	[M+H]+
Curcumin	3.52E+06	8.31E+05	[M+H]+
Cyclovalone	9.90E+04	2.75E+04	[M+H]+
CYTIDINE DIPHOSPHATE	5.42E+04	1.42E+04	[M+NH4]+
Danazol	7.35E+05	1.61E+05	[2M+H]+
DECANOATE	9.27E+04	2.72E+04	[M+H]+
DET	3.00E+04	9.18E+03	[M+H]+
Dihydroergocristine	1.08E+05	2.12E+04	[M+H]+
D-Pantothenic Acid Hemicalcium Salt	2.18E+04	5.17E+03	[M+H]+
Epioxandrolone	6.97E+04	1.90E+04	[M+H]+
Eremofortin B	2.55E+04	7.70E+03	[M+H]+
ERUCATE	1.72E+06	3.24E+05	[M+H]+
Fluanisone	3.87E+05	8.45E+04	[M]+
Formononetin	4.01E+05	1.18E+05	[M+H]+
GALACTARATE	4.92E+04	4.14E+03	[M+H]+
GAMMA-LINOLENATE	6.89E+04	3.03E+03	[M+NH4]+
Glycerophosphocholine	1.14E+05	3.23E+04	[M]+
Glycyrrhetinic acid	2.06E+06	3.87E+05	[M+H]+
GUANINE	3.09E+04	3.12E+03	[M+H]+
Homogentisic acid	2.71E+03	4.70E+02	[M+H]+
HYPOXANTHINE	3.33E+04	3.47E+03	[M+H]+

Indoleacrylic acid	1.02E+05	2.88E+04	[M+H]+
INOSINE	6.25E+02	2.83E+02	[M+H]+
Isonicotinamide	5.58E+03	8.29E+02	[M+H]+
ISOPHORONE	1.85E+04	1.81E+03	[M+H]+
Ketotifen	4.85E+03	9.86E+02	[M+H]+
Lasalocid A	1.31E+05	2.00E+04	[M+H]+
LEUCINE	1.92E+05	2.61E+04	[M+H]+
Maltotriose	6.27E+04	1.63E+04	[M+H]+
MESITYL OXIDE	3.86E+03	4.05E+02	[M+H]+
Methyl dihydrojasmonate	1.23E+04	3.96E+03	[M+NH4]+
METHYL GALACTOSIDE	5.70E+04	1.02E+04	[M+H]+
Methyllinoleate	5.75E+05	1.03E+05	[M+H]+
Mexiletine	1.59E+04	1.23E+03	[M+H]+
N-ACETYLGLUTAMATE	1.82E+05	1.45E+04	[M+H]+
N-Acetyl-L-proline	1.10E+05	1.25E+04	[M+H]+
Neomycin	1.24E+04	2.11E+03	[M+H]+
N-HOEAmP-FPrSAPS (pos)	6.46E+04	1.27E+04	[M+H]+
NORADRENALINE	9.82E+03	2.58E+03	[M+H]+
NORLEUCINE	3.64E+03	1.07E+03	[M+H]+
Octadecanamide	3.52E+05	8.45E+04	[M+H]+
Octanal_	2.22E+04	3.07E+03	[M+H]+
OXOPROLINE	3.54E+05	3.80E+04	[M+H]+
PETROSELINATE	7.60E+04	2.12E+04	[M+H]+
PHENYLALANINE	3.20E+05	7.26E+04	[M+NH4]+
PHOSPHORIBOSYL PYROPHOSPHATE	3.53E+05	8.04E+04	[M]+
PHYLLOQUINONE	1.91E+05	3.93E+04	[M+H]+
PYROGLUTAMATE	6.85E+04	7.49E+03	[2M+H]+
Quercetin	3.30E+04	9.86E+03	[M+H]+
Raffinose	1.40E+05	4.44E+04	[M+NH4]+
RIBOSE 1,5-BISPHOSPHATE	1.32E+05	1.50E+04	[M+H]+
S-(Methyl)Glutathione	3.06E+04	3.67E+03	[M+K]+
STEARATE	9.04E+03	1.94E+03	[M+H]+
Tiglic acid	1.11E+04	1.35E+03	[M+CH3OH+H]+
Trichodermin	1.56E+05	1.95E+04	[M+H]+
TRIMETHYLAMINE	4.75E+04	3.91E+03	[M+H]+
TYROSINE	1.69E+05	1.65E+04	[M+NH4]+
URACIL	7.30E+04	5.96E+03	[M+H]+
URIDINE	6.74E+04	6.76E+03	[M+H]+
URIDINE TRIPHOSPHATE	3.41E+05	9.00E+04	[M+H]+
URSODEOXYCHOLATE	1.16E+06	3.02E+05	[M+NH4]+
Uvaol	1.71E+05	4.26E+04	[M+H]+
XANTHINE	3.91E+04	4.13E+03	[M+H]+
Ziprasidone	7.59E+04	1.73E+04	[M+H]+
Betulin	2.08E+04	5.52E+03	[M+H]+
Dictamnine	8.78E+04	2.68E+04	[M+H]+
Patchouli alcohol (loss H20)	2.01E+04	3.29E+03	[M+H]+
Cytidine	1.83E+04	1.93E+03	[M+H]+
Baohuoside I	8.48E+06	2.09E+06	[M+H]+
Epimedin B	7.30E+06	2.07E+06	[M+H]+
Epimedin A	1.89E+06	4.86E+05	[M+H]+
Epimedin C	1.21E+07	3.03E+06	[M]+
Nobiletin	3.09E+04	8.32E+03	[M+H]+
Dihydrotanshinone I	5.02E+04	1.32E+04	[M+H]+
Liquiritin	4.70E+05	7.99E+04	[M+H]+
Glycyrrhizic acid ammonium salt	8.66E+06	1.54E+06	[M+H]+
Pratensein-7-O-glucoside	5.54E+03	8.41E+02	[M+H]+
Trigonelline	1.15E+05	3.55E+04	[M+Na]+
quercetin-3'-O-glucoside	1.02E+05	1.23E+04	[M+H]+

Phellodendrine	1.70E+07	4.10E+06	[M+NH4]+
Obacunone	1.68E+06	4.75E+05	[M+H]+
Tigogenin	5.85E+05	1.02E+05	[M+H]+
Hyperin	1.88E+05	3.74E+04	[M+H]+
Rutin	2.93E+05	8.57E+04	[M+H]+
Ruscogenin	3.16E+04	6.34E+03	[M+H]+
Betulonicacid	1.22E+05	1.69E+04	[M+H]+
Ononin	1.48E+06	4.16E+05	[M+H]+
mangiferin	1.80E+06	4.60E+05	[M+K]+
Acteoside +NH3	2.74E+04	7.29E+03	[M+NH4]+
Calycosin	4.94E+05	1.40E+05	[M+H]+
calycosin-7-o-glucoside	3.18E+06	9.70E+05	[M+H]+
linarin	5.94E+05	1.77E+05	[M]+
Luteolin-7-O-β-D-glucuronide	1.32E+05	3.73E+04	[M+H]+
Pseuoginsenoside F11	1.18E+06	3.32E+05	[M+NH4]+
guanosine	1.40E+05	4.32E+04	[M+H]+
Limonin	5.09E+06	1.41E+06	[M+H]+
Arctigenin	3.60E+03	7.54E+02	[M]+
Proline	4.14E+05	1.30E+05	[M+H]+
Hydroxygenkwanin	4.98E+02	1.45E+02	[M+H]+
Apigenin 7-O-beta-D-glucuronide	1.29E+04	3.31E+03	[M]+
Deacetyl asperulosidic acid methyl ester +NH3	1.25E+05	2.36E+04	[M+H]+
10-Deacetylasperulosidic acid +NH3	2.81E+05	2.33E+04	[M]+
Cistanoside D +NH4	7.44E+03	2.37E+03	[M+H]+
Aempferol-3-O-rutinoside	3.31E+04	9.49E+03	[M+H]+
Diosgenin	2.46E+05	6.04E+04	[M+H]+
Echinacoside +NH3	1.50E+04	4.91E+03	[M+H]+
Dehydrocorydaline	1.15E+05	3.17E+04	[M+H]+
Vitamin B2	5.33E+04	1.49E+04	[M+H]+
Vitamin D2	2.16E+04	4.44E+03	[M+H]+
Schaftoside	9.57E+05	2.14E+05	[M]+
Adenosine	7.62E+03	2.76E+03	[M]+
Adenine	9.38E+04	2.82E+04	[M+H]+
Berberrubine	7.03E+05	2.27E+05	[M+H]+
Methyl linoleate	4.15E+05	7.73E+04	[M+H]+
Palmatine chloride	5.23E+06	1.44E+06	[M+H]+
Stachydrine hydrochloride	1.56E+05	2.77E+04	[M+H]+
Berberine hydrochloride	6.44E+07	1.23E+07	[M]+
3-N-butyl-4,5-dihydrophthalide	3.66E+04	3.06E+03	[M+H]+
Jatrorrhizine	4.55E+06	1.08E+06	[M+H]+
Rhoifolin	8.00E+04	1.94E+04	[M+H]+
Isoliquiritin	1.35E+06	4.62E+05	[M+H]+
Isoliquiritigenin	4.40E+05	1.08E+05	[M+H]+
Isoliensinine	2.09E+05	5.93E+04	[M]+
Isoalantolactone	6.89E+03	2.30E+03	[M+H]+
Leonurine	1.66E+04	3.54E+03	[M+H]+
Icarrin	3.13E+07	8.04E+06	[M+H]+
Cryptotanshinone	8.08E+04	2.07E+04	[M+H]+
Polygalaxanthone VI +Na	6.93E+05	2.03E+05	[M+H]+
Sarsasapogenin	1.07E+06	2.14E+05	[M+H]+
SHIONONE	1.41E+04	2.81E+03	[M+H]+
Astragalin	5.77E+04	1.51E+04	[M+H]+

Precursor Mass	Component Name	Found At Mass
301.108	301.1075 / 10.24 [M+CH3OH+H]+	301.1078
100.075	100.0752 / 18.60	100.0755
253.18	253.1800 / 10.87	253.1802
72.936	72.9362 / 19.69	72.937
171.029	171.0289 / 4.10 [M+CH3OH+H]+	171.029
348.071	348.0707 / 3.57	348.0706
165.054	165.0545 / 3.18 [M+H]+	165.0546
163.133	163.1331 / 1.48 [M+H]+	163.133
131.052	131.0524 / 2.31	131.0525
309.207	309.2065 / 10.49 [M+CH3OH+H]+	309.2065
514.225	514.2248 / 5.02	514.2251
401.341	401.3413 / 17.92	401.3416
279.232	279.2325 / 11.87	279.2327
625.212	625.2117 / 7.33 [M+H]+	625.2123
348.071	348.0706 / 2.17	348.0704
279.233	279.2327 / 13.07	279.2328
104.106	104.1065 / 0.96 [M+CH3OH+H]+	104.1066
136.075	136.0751 / 1.93	136.0753
291.196	291.1960 / 10.49	291.1958
275.201	275.2009 / 11.18	275.2008
175.119	175.1192 / 0.93 [M+NH4]+	175.1193
122.964	122.9639 / 19.64	122.9638
118.086	118.0858 / 1.01	118.0857
415.211	415.2114 / 11.73 [M+H]+	415.2115
583.294	583.2943 / 1.37	583.2941
312.326	312.3264 / 18.46	312.3265
326.379	326.3792 / 12.60	326.3795
261.112	261.1124 / 10.84	261.1121
386.342	386.3417 / 17.28	386.3413
177.087	177.0869 / 1.12 [M+H]+	177.0869
114.988	114.9876 / 0.72	114.9876
185.115	185.1148 / 17.52	185.1148
355.103	355.1030 / 6.25	355.1028
149.023	149.0233 / 1.48	149.0233
578.282	578.2818 / 6.73 [M+NH4]+	578.2915
405.351	405.3508 / 7.97	405.3511
369.118	369.1182 / 6.88	369.1183
367.118	367.1179 / 11.91	367.1179
404.207	404.2066 / 10.90 [M+NH4]+	404.2065
675.677	675.6761 / 18.17 [2M+H]+	675.6767
173.117	173.1171 / 9.60	173.1172
217.097	217.0971 / 6.30	217.0974
612.328	612.3276 / 5.21 [M+H]+	612.3267
220.118	220.1181 / 5.32 [M+H]+	220.118
307.19	307.1897 / 11.02	307.1899
249.148	249.1483 / 11.33	249.1482
339.347	339.3472 / 18.11	339.3463
357.169	357.1694 / 11.06 [M]+	357.1694
269.081	269.0810 / 10.06 [M+H]+	269.0809
211.06	211.0600 / 4.74	211.0602
279.159	279.1593 / 1.48 [M+NH4]+	279.1592
258.11	258.1100 / 0.96 [M]+	258.1102
471.347	471.3468 / 9.98 [M+H]+	471.3469
152.056	152.0564 / 1.81	152.0564
169.014	169.0135 / 3.17	169.0136
137.045	137.0450 / 2.46	137.0454

188.07	188.0704 / 5.73 [M+H]+	188.0705
269.107	269.1073 / 2.60 [M+H]+	269.1072
123.055	123.0551 / 2.16	123.0546
139.002	139.0023 / 3.50	139.0024
310.311	310.3114 / 17.58	310.3113
613.482	613.4824 / 17.66	613.4825
132.102	132.1018 / 3.02	132.1019
505.195	505.1950 / 4.99 [M+H]+	505.1948
99.044	99.0439 / 5.00 [M+H]+	99.0438
244.191	244.1907 / 9.53 [M+NH4]+	244.1906
195.138	195.1379 / 9.58	195.138
295.226	295.2264 / 9.59	295.2269
180.102	180.1020 / 3.29	180.1016
190.071	190.0712 / 1.72	190.0711
158.093	158.0925 / 2.65	158.0924
615.497	615.4974 / 18.61	615.4962
501.321	501.3211 / 10.25	501.3208
170.081	170.0812 / 5.58	170.0813
132.102	132.1019 / 2.40	132.1017
284.295	284.2951 / 16.94	284.2953
129.018	129.0180 / 2.13	129.018
130.05	130.0499 / 2.41 [M+H]+	130.0499
282.278	282.2781 / 15.66	282.2793
166.086	166.0864 / 5.06 [M+NH4]+	166.0863
391.284	391.2842 / 17.57 [M]+	391.2844
451.32	451.3197 / 9.62	451.3206
259.094	259.0931 / 2.40 [2M+H]+	259.093
303.051	303.0505 / 6.68	303.0506
522.202	522.2025 / 1.03 [M+NH4]+	522.2032
311.222	311.2217 / 11.17	311.2215
322.077	322.0771 / 2.18 [M+K]+	322.0772
285.298	285.2980 / 16.66	285.2986
101.022	101.0224 / 2.06 [M+CH3OH+H]+	101.0224
293.211	293.2106 / 9.24	293.2106
60.044	60.0440 / 17.84	60.0441
182.081	182.0813 / 3.17 [M+NH4]+	182.0814
113.034	113.0340 / 1.67	113.034
245.077	245.0770 / 3.45	245.0772
485.326	485.3260 / 11.34	485.3261
393.285	393.2854 / 11.51 [M+NH4]+	393.2857
443.388	443.3878 / 9.13	443.3876
153.04	153.0402 / 1.43	153.0401
413.266	413.2664 / 17.56	413.2665
443.388	443.3879 / 12.74	443.3878
200.07	200.0700 / 10.26	200.0701
205.086	205.0858 / 18.43	205.0862
244.093	244.0927 / 1.78	244.0927
515.191	515.1909 / 10.82	515.1912
809.287	809.2868 / 8.37	809.2868
839.296	839.2964 / 8.28 [M+H]+	839.2966
823.302	823.3018 / 8.44 [M]+	823.3011
403.139	403.1390 / 10.93	403.139
279.102	279.1024 / 12.24	279.1025
419.134	419.1337 / 7.14 [M+H]+	419.134
823.412	823.4116 / 9.97	823.4122
463.255	463.2549 / 6.76	463.2511
138.054	138.0541 / 1.11 [M+Na]+	138.0547
465.208	465.2079 / 2.85	465.2077

342.17	342.1704 / 6.35 [M+NH4]+	342.1705
455.206	455.2060 / 11.45 [M+H]+	455.2063
417.336	417.3361 / 8.96	417.3364
465.103	465.1026 / 7.19	465.1028
611.161	611.1612 / 7.04	611.1607
431.179	431.1791 / 18.41	431.1791
455.351	455.3514 / 8.99	455.3518
431.133	431.1328 / 8.14 [M+H]+	431.1326
423.092	423.0923 / 6.46 [M+K]+	423.0924
642.239	642.2386 / 7.34 [M+NH4]+	642.2406
285.076	285.0758 / 8.77	285.0758
447.128	447.1282 / 7.15 [M+H]+	447.1283
593.187	593.1871 / 8.34 [M]+	593.1862
463.087	463.0868 / 7.30	463.087
801.499	801.4993 / 9.09 [M+NH4]+	801.4995
284.1	284.0998 / 4.85 [M+H]+	284.0993
471.202	471.2016 / 10.45	471.2014
373.128	373.1277 / 9.93 [M]+	373.1321
116.07	116.0702 / 1.08 [M+H]+	116.0703
301.216	301.2164 / 8.69	301.2134
447.092	447.0915 / 8.10 [M]+	447.0917
422.166	422.1656 / 5.53	422.1661
408.15	408.1505 / 4.73 [M]+	408.1507
670.271	670.2709 / 8.09	670.2701
595.166	595.1657 / 7.35	595.1652
415.321	415.3205 / 10.77	415.3206
804.293	804.2929 / 6.44	804.2931
366.171	366.1706 / 8.46	366.1704
377.147	377.1466 / 6.51	377.1458
397.381	397.3814 / 19.51	397.3831
565.156	565.1556 / 6.67 [M]+	565.1559
268.105	268.1046 / 2.61 [M]+	268.1043
136.062	136.0615 / 1.32	136.0614
322.107	322.1072 / 7.96	322.1074
295.227	295.2266 / 13.42	295.2275
352.118	352.1185 / 7.44	352.1184
144.102	144.1018 / 1.23 [M+H]+	144.1017
336.122	336.1224 / 8.14 [M]+	336.1223
193.049	193.0493 / 4.71 [M+H]+	193.0493
338.139	338.1392 / 7.79 [M+H]+	338.1393
579.17	579.1698 / 7.49	579.1703
419.133	419.1332 / 8.07 [M+H]+	419.1332
257.081	257.0808 / 7.17	257.0807
611.325	611.3253 / 5.20 [M]+	611.3253
233.154	233.1544 / 12.34	233.1539
312.326	312.3260 / 17.94	312.3261
677.244	677.2438 / 8.59	677.2435
297.148	297.1483 / 13.28	297.1489
517.17	517.1703 / 8.91	517.1706
417.336	417.3363 / 11.84	417.3362
427.356	427.3561 / 18.07	427.3569
449.108	449.1076 / 7.26	449.1075

T3_NEG

Library Hit	Area	Height
(-)-Syringaresnol-4-O-β-D-apiofuranosyl-(1→2)-β-D-glucopyran	8.40E+04	2.34E+04
(S)-(-)-2-Hydroxyisocaproic Acid	5.65E+04	1.11E+04
1,11-Undecanedicarboxylic acid	7.07E+05	1.89E+05
1,4-Dicaffeoylquinic Acid (Cynarin)	1.33E+05	2.10E+04
10-hydroxydec-2-enoic acid	1.43E+05	4.38E+04
11a-Hydroxyprogesterone	1.50E+06	4.14E+05
Acetyl-11-keto-β-boswellic acid	3.99E+04	9.99E+03
17a-Ethynylestradiol	7.49E+04	7.29E+03
1-AMINOCYCLOPROPANECARBOXYLATE	1.24E+04	2.26E+03
2',4'-DIHYDROXYACETOPHENONE	4.99E+04	1.48E+04
2,4-Di-tert-butylphenol	2.80E+04	7.34E+03
20(R)-Ginsenoside Rh1 +HCOOH	2.06E+05	6.51E+04
20(S)Ginsenoside Rg3 +HCOOH	1.15E+06	3.18E+05
2-Hydroxy-2-methylbutyric acid	2.32E+04	6.59E+03
2-Hydroxyoctanoic acid	2.06E+05	6.77E+04
2-Isopropylmalic acid	6.69E+05	1.53E+05
2-Pyrocatechuic acid	1.24E+05	2.76E+04
3-(4-Hydroxyphenyl)-Propionic Acid	3.74E+06	8.35E+05
3,4 DIHYDROXYMANDELATE	4.81E+05	1.52E+05
3-DEHYDROSHIKIMATE	3.19E+04	9.31E+03
3-HYDROXYMETHYLGLUTARATE	2.91E+05	2.03E+04
3-Methylthiophene	4.18E+04	5.37E+03
4-Bromophenylalanine	2.34E+05	7.31E+04
4-COUMARATE	2.07E+06	6.13E+05
4-HYDROXYBENZALDEHYDE	2.50E+05	7.56E+04
4-HYDROXYBENZOATE	3.52E+05	8.86E+04
4-Hydroxycoumarin	3.78E+04	1.08E+04
5-Oxo-2-tetrahydrofurancarboxylic acid	1.48E+04	1.75E+03
4'-O-β-Glucopyranosyl-5-O-methylvisamminol +HCOOH	6.01E+05	1.56E+05
6-CARBOXYHEXANOATE	4.36E+04	1.33E+04
Acteoside	8.96E+05	2.71E+05
ADENOSINE 2',3'-CYCLIC PHOSPHATE	1.24E+05	9.39E+03
ADIPATE	3.34E+04	7.80E+03
Aflatoxin P1	1.03E+04	3.00E+03
ARACHIDATE	3.91E+04	3.41E+03
Arachidonic acid	5.06E+04	1.49E+04
ASPARAGINE	2.26E+05	8.65E+04
AZELATE	3.43E+06	1.01E+06
BETA-GLYCEROPHOSPHATE	1.04E+05	2.50E+04
Biopterin	2.53E+04	6.17E+03
Caffeic acid	4.68E+05	1.47E+05
Chlorogenic Acid	7.27E+05	1.89E+05
Chrysophanol	9.53E+04	2.65E+04
cis-Aconitic acid	2.14E+05	5.19E+04
CP 47,497 C8-homolog Negative Mode	1.92E+05	5.56E+04
Dodecanedioic acid	1.33E+05	4.51E+04
D-Pantothenic Acid Hemicalcium Salt	1.31E+05	3.83E+04
D-Tagatose	1.01E+06	1.51E+05
D-Xylonic Acid Lithium Salt	1.03E+06	1.91E+05
Estriol	6.12E+05	1.51E+05
Estrone	2.74E+04	6.72E+03
Ethyl dodecanoate	3.31E+04	8.89E+03
Ethyl hexadecanoate1	1.10E+06	2.27E+05
Fatty acid C20:4	7.57E+05	2.20E+05
Formononetin	2.87E+05	8.43E+04
FURFURYL ALCOHOL	4.88E+06	3.42E+05

Genistein	1.25E+05	2.58E+04
GERANYL-PP	1.97E+05	3.06E+04
GLYCERALDEHYDE 3-PHOSPHATE	5.79E+04	1.71E+04
Glycyrrhetinic acid	1.20E+05	3.12E+04
GUANOSINE MONOPHOSPHATE	5.98E+04	3.93E+03
Hexadecanedioic acid	1.94E+05	5.47E+04
HEXADECANOL	1.84E+05	6.54E+04
HISTIDINE	5.18E+04	2.05E+04
Indoleacrylic acid	8.94E+04	1.05E+04
Inosine	3.16E+04	9.54E+03
Isomaltose	2.83E+06	6.02E+05
ITACONATE	3.96E+04	4.98E+03
Kaempferol	1.10E+05	2.62E+04
KYNURENATE	1.04E+04	1.10E+03
L-3-Phenyllactic acid	1.20E+05	3.63E+04
L-Dihydroorotic acid	1.70E+06	4.60E+05
L-Theanine	1.58E+05	5.05E+04
L-TRYPTOPHANAMIDE	2.78E+04	1.94E+03
MALATE	1.44E+06	4.31E+05
MALONATE	9.19E+04	2.04E+04
Maltotriose	2.35E+05	7.27E+04
MESOXALATE	4.55E+04	5.40E+03
Methotrexate	1.24E+05	3.24E+04
Methyllinoleate	5.80E+04	8.16E+03
METHYLMALONATE	3.06E+05	2.24E+04
N,N-DIMETHYL-1,4-PHENYLENEDIAMINE	6.17E+04	1.04E+04
N,N-DIMETHYLARGININE	2.53E+05	1.82E+04
N-ACETYLALANINE	2.22E+04	3.27E+03
N-ACETYLGLUCOSAMINE	1.08E+04	1.92E+03
N-ACETYLGLUTAMATE	4.21E+05	4.05E+04
N-Acetyl-L-tryptophan	1.80E+05	4.81E+04
Nonadecanoic acid	1.73E+05	4.42E+04
Oligomycin B	1.58E+06	1.89E+05
Oxoadipic Acid	2.32E+05	7.44E+04
OXOPROLINE	1.01E+06	1.03E+05
PALMITATE	1.54E+06	3.91E+05
PFBA (perfluoro-n-butanoic acid) (neg)	1.19E+05	3.48E+04
PFHxS (perfluorohexane sulfonate) (neg)	1.00E+06	2.22E+05
PFOS (perfluorooctane sulfonate) (neg)	3.79E+04	3.86E+03
PHENYL ACETATE	8.13E+04	2.16E+04
Phthalic acid	4.17E+05	8.68E+04
Protocatechuic acid	5.40E+04	1.41E+04
Protocatechuic Aldehyde	7.79E+04	2.33E+04
PYRIMIDINE	1.75E+05	2.18E+04
Quinic acid	4.39E+06	1.33E+06
RAFFINOSE	7.76E+04	1.49E+04
SACCHARATE	4.14E+05	8.05E+04
Sambucinol	9.37E+04	1.03E+04
SEBACATE	3.67E+04	8.01E+03
Shikimate 3-phosphate	1.25E+05	3.02E+04
STACHYOSE	1.77E+06	3.62E+05
SUBERATE	6.24E+05	1.98E+05
Sulfadoxine	1.26E+05	2.88E+04
Sulfamethazine	6.47E+05	1.85E+05
Syringic Acid	4.12E+04	1.26E+04
THYMIDINE-MONOPHOSPHATE	1.01E+05	3.16E+04
trans-Ferulic acid	6.10E+05	1.68E+05
Traumatic acid	1.91E+05	5.24E+04

TREHALOSE	2.33E+06	3.32E+05
Turanose	3.48E+04	2.99E+03
TYROSINE	1.73E+05	1.65E+04
Undecanal	2.86E+04	8.09E+03
Undecanedioic acid	4.45E+05	1.28E+05
URATE	7.01E+04	9.90E+03
Uridine	1.91E+05	1.70E+04
Vaccenic acid	1.19E+06	2.75E+05
VALINE	6.58E+04	8.11E+03
XANTHINE	8.68E+04	8.94E+03
Atractylenolide III	1.94E+04	5.14E+03
Baohuoside I	4.11E+06	1.12E+06
Baohuoside I	1.11E+07	2.85E+06
Epibrassinolide +HCOOH	2.77E+05	7.85E+04
Epimedin A +HCOOH	1.36E+06	3.62E+05
Epimedin C	8.11E+05	1.38E+05
Aurantio-Obtusin	2.74E+05	7.38E+04
Daidzin +HCOOH	1.12E+05	3.17E+04
Rehmannioside D +HCOOH	5.94E+05	1.96E+05
Scopoletin	9.26E+04	2.28E+04
Pachymic acid	6.57E+05	1.83E+05
Liquiritin	4.17E+06	1.03E+06
Glycyrrhizic acid ammonium salt	3.20E+07	4.58E+06
Glabridin	1.52E+05	3.94E+04
Quercitrin	3.52E+05	7.74E+04
Quercetin	1.94E+05	4.67E+04
quercetin-3'-O-glucoside	2.49E+04	6.12E+03
Phellodendrine	2.85E+05	7.99E+04
Isomucronulatol-7-O-glucoside	3.26E+05	9.45E+04
Astragaloside I +HCOOH	1.29E+06	3.51E+05
Astragaloside II +HCOOH	1.60E+06	4.94E+05
Asiatic acid	3.05E+04	7.30E+03
Curcumin	4.45E+05	1.30E+05
Gingerglycolipid B +HCOOH	9.03E+04	2.50E+04
Geniposidic acid	2.43E+05	6.48E+04
L(+)-Arginine	2.40E+05	8.40E+04
Corosolic acid	2.29E+05	6.42E+04
PhillyrinForsythin +HCOOH	5.89E+04	1.44E+04
Forsythoside A	4.04E+04	7.12E+03
Forsythoside B	4.52E+05	1.17E+05
Rutin	6.33E+05	1.69E+05
Ononin +HCOOH	2.50E+06	7.05E+05
mangiferin	6.87E+06	1.58E+06
Calycosin	2.19E+06	6.32E+05
Calycosin-7-o-glucoside +HCOOH	9.38E+05	2.72E+05
Gallic acid	4.78E+05	3.59E+04
Calceorioside B	2.20E+05	2.60E+04
Luteolin-7-O-β-D-glucuronide	1.48E+05	3.49E+04
Fungitetraose	1.55E+06	1.82E+05
Pseuoginsenoside F11	6.77E+04	1.59E+04
guanosine	5.63E+05	2.51E+04
Limonin	8.15E+05	1.96E+05
Citric acid	5.98E+06	1.36E+06
arctiin +HCOOH	4.84E+04	4.07E+03
Gypenoside XVII	2.26E+05	6.27E+04
Oleanolic acid	7.39E+04	1.35E+04
Esculetin	1.53E+05	4.95E+04
10-deacetylasperulosidic acid	1.15E+06	7.69E+04

10-deacetylasperulosidic acid	5.07E+04	6.87E+03
Ginsenoside Rb1 +HCOOH	1.65E+06	4.17E+05
Ginsenoside Rb2	1.71E+05	4.99E+04
Ginsenoside Re +HCOOH	1.49E+06	4.30E+05
Ginsenoside Rg1 +HCOOH	2.40E+05	6.20E+04
Ginsenoside Rg2 +HCOOH	8.80E+05	2.80E+05
Ginsenoside-Ro	6.22E+05	1.80E+05
DCistanoside D	1.41E+05	4.37E+04
Ft1 Notoginsenoside Ft1 +HCOOH	1.98E+05	6.09E+04
Phytolaccagenin	6.90E+05	1.29E+05
Monotropein	1.43E+03	4.63E+02
Echinacoside	1.66E+05	4.32E+04
pinoresinol-glucoside	1.57E+05	3.99E+04
Aspartic acid	1.66E+05	5.99E+04
Luteolin	1.64E+05	4.43E+04
Neochlorogenic acid	4.00E+04	9.28E+03
Neo-mangiferin	5.81E+06	1.57E+06
Linoleic acid	8.87E+05	2.35E+05
Isoliquiritin	8.51E+05	2.93E+05
Isoliquiritigenin	1.72E+06	4.98E+05
Isoquercitrin	5.82E+05	1.12E+05
Ciso-Cistanoside C	9.54E+04	2.91E+04
Isorhamnetin	2.54E+05	7.72E+04
Cryptochlorogenic acid	3.40E+06	8.52E+05
Naringenin	1.56E+05	4.07E+04
Tenuifoliside A	1.59E+05	4.85E+04
Vinorelbine	5.90E+05	1.58E+05
Timosaponin BII +HCOOH	2.36E+03	5.51E+02
Gardenoside	1.57E+05	3.06E+04
Raddeanin A	1.68E+05	4.49E+04
Catalpol	5.35E+05	5.97E+04

Adduct / Charge	Precursor Mass	Component Name	Found At Mass
[M-H]-	711.302	711.3008 / 7.34	711.3022
[M-H]-	131.072	131.0713 / 6.97	131.0718
[M-H]-	243.162	243.1606 / 10.54	243.16
[M-H]-	515.142	515.1412 / 5.69	515.1423
[M-H]-	185.119	185.1184 / 8.88	185.1181
[2M-H]-	659.476	659.4742 / 9.60 [2M-H]-	659.4751
[M-H]-	511.344	511.3427 / 14.68	511.3436
[M-H]-	295.229	295.2281 / 14.02	295.2287
[M-H]-	99.926	99.9251 / 16.05	99.9253
[M-H]-	151.041	151.0397 / 8.14	151.0399
[M-H]-	205.161	205.1596 / 13.89	205.1602
[M-H]-	683.438	683.4372 / 9.55	683.4381
[M+FA-H]-	829.497	829.4963 / 11.49 [M+FA-H]-	829.498
[M-H]-	117.056	117.0552 / 5.67	117.0561
[M-H]-	159.104	159.1027 / 7.36 [M-H]-	159.1029
[M-H]-	175.063	175.0616 / 6.21 [M-H]-	175.0616
[M-H]-	153.021	153.0196 / 5.60	153.0193
[M-H]-	165.057	165.0561 / 6.18 [M-H]-	165.0562
[M-H]-	183.104	183.1030 / 7.30	183.1032
[M-H]-	171.104	171.1033 / 8.08 [M-H]-	171.1028
[M-H]-	161.047	161.0456 / 3.83 [M-H]-	161.046
[M-H]-	96.961	96.9598 / 5.01	96.96
[M-H]-	242.177	242.1760 / 9.54	242.1761
[M-H]-	163.042	163.0405 / 7.29	163.0405
[M-H]-	121.03	121.0292 / 6.96 [M-H]-	121.0295
[M-H]-	137.025	137.0244 / 8.28	137.0243
[M-H]-	161.062	161.0607 / 8.14	161.0609
[M-H2O-H]-	129.02	129.0193 / 1.99 [M-H2O-H]-	129.0197
[M-H]-	497.328	497.3267 / 11.68	497.3276
[M+FA-H]-	159.067	159.0664 / 6.95 [M+FA-H]-	159.0666
[M-H]-	623.2	623.1993 / 7.36	623.1997
[M-H]-	328.047	328.0457 / 4.19	328.0462
[M-H]-	145.051	145.0500 / 5.77 [M-H]-	145.0513
[M-H]-	297.244	297.2431 / 14.51	297.2437
[M-H]-	311.17	311.1689 / 16.49	311.1701
[M-H]-	303.234	303.2328 / 15.50 [M-H]-	303.2337
[M-H]-	131.048	131.0465 / 0.90	131.0466
[M-H]-	187.099	187.0981 / 7.94	187.0982
[M-H]-	171.068	171.0666 / 7.50	171.067
[M-H]-	236.058	236.0570 / 6.04	236.0578
[M+Na-2H]-	179.036	179.0353 / 6.61 [M+Na-2H]-	179.0353
[M]-	354.092	354.0911 / 6.28 [M]-	354.0918
[M-H]-	253.052	253.0505 / 12.00	253.051
[M+Na-2H]-	173.01	173.0090 / 1.36 [M+Na-2H]-	173.0097
[M-H]-	331.25	331.2484 / 9.51 [M-H]-	331.2488
[M+AcO-H]-	229.146	229.1450 / 9.94 [M+AcO-H]-	229.1448
[M-H]-	218.104	218.1031 / 5.49	218.1034
[M-H]-	179.057	179.0563 / 1.03 [M-H]-	179.0563
[M-H]-	165.042	165.0407 / 0.96 [M-H]-	165.0407
[M-H]-	287.224	287.2227 / 9.90	287.223
[M-H]-	269.25	269.2485 / 16.80	269.249
[M-H]-	227.202	227.2013 / 15.16	227.2022
[M-H]-	283.266	283.2652 / 17.43 [M-H]-	283.2654
[M-H]-	303.161	303.1602 / 10.78	303.1605
[M-H]-	267.067	267.0660 / 10.78	267.0664
[M-H]-	96.961	96.9600 / 1.38 [M-H]-	96.9604

[M-H]-	269.214	269.2126 / 12.46			269.2128
[M-H]-	313.24	313.2385 / 11.01	[M-H]-		313.2387
[M-H]-	169.088	169.0871 / 9.89			169.0875
[M-H]-	469.334	469.3328 / 14.03			469.3332
[M-H]-	362.052	362.0506 / 4.23			362.0515
[M-H]-	285.207	285.2060 / 12.35			285.2064
[2M-H]-	483.248	483.2462 / 6.77	[2M-H]-		483.2476
[M-H]-	154.064	154.0624 / 0.89			154.0624
[M-H]-	186.042	186.0411 / 2.41			186.0416
[M-H]-	267.074	267.0733 / 5.15			267.0733
[M+Cl]-	377.086	377.0854 / 1.05	[M+Cl]-		377.0856
[M-H2O-H]-	129.02	129.0194 / 2.89	[M-H2O-H]-		129.0198
[M-H]-	285.042	285.0411 / 9.44			285.0405
[M-H]-	188.094	188.0926 / 3.56			188.0932
[M-H]-	165.057	165.0560 / 7.39			165.0559
[M-H]-	157.052	157.0510 / 6.77	[M-H]-		157.0513
[M-H]-	173.12	173.1190 / 8.10			173.1184
[M-H]-	202.11	202.1085 / 4.39			202.1092
[M-H]-	133.016	133.0145 / 1.27	[M-H]-		133.0146
[M-H]-	103.005	103.0035 / 1.34			103.0037
[M-H]-	503.163	503.1621 / 1.05	[M-H]-		503.1614
[M-H]-	116.929	116.9283 / 8.84			116.9284
[M-H]-	453.193	453.1915 / 12.05			453.1926
[M-H]-	293.181	293.1795 / 16.53	[M-H]-		293.1804
[M-H]-	117.02	117.0193 / 2.73			117.0195
[M-H]-	134.895	134.8941 / 18.20			134.8945
[M-H]-	201.061	201.0596 / 3.91			201.0602
[M-H]-	130.088	130.0873 / 2.85			130.0875
[M-H]-	220.148	220.1467 / 14.47			220.1469
[M-H]-	188.058	188.0568 / 2.81			188.0571
[M-H]-	245.095	245.0938 / 7.46	[M-H]-		245.0942
[M-H]-	297.243	297.2418 / 13.44			297.2426
[M-H2O-H]-	805.406	805.4044 / 10.97	[M-H2O-H		805.4051
[M-H]-	159.104	159.1030 / 8.58			159.1027
[M-H]-	128.037	128.0356 / 2.41			128.0358
[M-H]-	255.235	255.2336 / 16.27	[M-H]-		255.2337
[M-H]-	213.114	213.1134 / 10.18			213.1135
[2M-H]-	799.272	799.2701 / 7.50	[2M-H]-		799.2708
[M-H]-	499.169	499.1675 / 3.41			499.1683
[M-H]-	134.895	134.8942 / 16.42			134.8945
[M-H]-	165.021	165.0197 / 6.51			165.0197
[M-H]-	153.02	153.0193 / 6.36			153.0196
[M-H]-	137.025	137.0243 / 6.22	[M-H]-		137.0244
[M-H]-	78.96	78.9589 / 0.94			78.9591
[M-H]-	191.058	191.0567 / 1.09	[M-H]-		191.0567
[M-H]-	503.178	503.1770 / 6.62			503.1783
[M-H]-	209.068	209.0670 / 1.20	[M-H]-		209.0671
[M-H]-	265.15	265.1486 / 15.88			265.1487
[M-H]-	201.079	201.0775 / 6.41			201.0778
[M-H2O-H]-	253.218	253.2173 / 15.38	[M-H2O-H		253.2176
[M-H2O-H]-	665.216	665.2152 / 1.16	[M-H2O-H]-		665.2154
[M+AcO-H]-	173.083	173.0823 / 7.23	[M+AcO-H]-		173.0824
[M-H]-	309.208	309.2070 / 12.52			309.2078
[M-H]-	277.219	277.2179 / 15.02	[M-H]-		277.2183
[M+FA-H]-	197.047	197.0458 / 6.84	[M+FA-H]-		197.0461
[M-H]-	321.114	321.1132 / 11.22			321.1134
[M-H]-	193.052	193.0510 / 7.50	[M-H]-		193.0508
[M-H]-	227.13	227.1289 / 9.58			227.1291

[M-H]-	341.11	341.1093 / 1.19	[M-H]-	341.1092
[M+FA-H]-	387.116	387.1145 / 4.93	[M+FA-H]-	387.1154
[M-H]-	180.068	180.0665 / 3.16		180.0674
[M-H]-	169.125	169.1235 / 10.17	[M-H]-	169.1234
[M-H]-	215.13	215.1293 / 9.29	[M-H]-	215.1292
[M-H]-	167.022	167.0210 / 2.37		167.0217
[M+FA-H]-	289.069	289.0677 / 3.49	[M+FA-H]-	289.0687
[M-H]-	281.25	281.2488 / 16.42		281.2493
[M-H]-	115.921	115.9204 / 10.53	[M-H]-	115.9201
[M-H]-	151.027	151.0261 / 3.07	[M-H]-	151.0268
[M-H]-	247.135	247.1343 / 11.38		247.1347
[M-H]-	513.178	513.1768 / 8.64		513.1771
[M-H]-	513.178	513.1769 / 10.85		513.1772
[M-H]-	525.36	525.3586 / 15.06		525.3596
[M+FA-H]-	883.292	883.2913 / 8.31	[M+FA-H]-	883.2921
[M-H]-	821.291	821.2897 / 8.45		821.2902
[M+AcO-H]-	329.067	329.0664 / 9.48	[M+AcO-H]-	329.0667
[M-H]-	461.168	461.1666 / 6.60		461.1676
[M-H]-	731.228	731.2264 / 5.25		731.2273
[M-H]-	191.037	191.0354 / 7.57	[M-H]-	191.0351
[M-H]-	527.377	527.3756 / 15.28		527.376
[M-H]-	417.121	417.1200 / 7.26	[M-H]-	417.1204
[M-H]-	821.398	821.3966 / 9.97	[M-H]-	821.3975
[M-H]-	323.13	323.1287 / 11.98	[M-H]-	323.1292
[M-H]-	447.094	447.0933 / 7.65		447.0939
[M-H]-	301.036	301.0349 / 8.78		301.0358
[M-H]-	463.219	463.2184 / 7.77	[M-H]-	463.2201
[M+FA-H]-	386.163	386.1616 / 6.59	[M+FA-H]-	386.1618
[M-H]-	463.162	463.1607 / 8.54		463.161
[M+FA-H]-	913.484	913.4827 / 11.57	[M+FA-H]-	913.4829
[M-H]-	871.473	871.4723 / 10.27	[M-H]-	871.4729
[M-H]-	487.344	487.3425 / 11.28	[M-H]-	487.344
[M-H]-	367.105	367.1034 / 7.69	[M-H]-	367.104
[M-H]-	723.383	723.3823 / 12.38		723.3839
[M-H]-	373.116	373.1146 / 5.49		373.1138
[M-H]-	173.106	173.1049 / 0.89	[M-H]-	173.1046
[M-H]-	471.347	471.3462 / 12.91		471.3476
[M+TFA-H]-	579.209	579.2080 / 8.32	[M+TFA-H]-	579.2096
[M-H]-	623.222	623.2206 / 5.43		623.2218
[M-H]-	755.425	755.4241 / 10.78		755.424
[M-H]-	609.148	609.1466 / 7.06		609.1471
[M-H]-	475.126	475.1247 / 8.17		475.1255
[M-H]-	421.08	421.0785 / 6.49	[M-H]-	421.079
[M-H]-	283.062	283.0614 / 8.79		283.0617
[M-H]-	491.122	491.1205 / 7.17		491.1206
[M-H]-	169.016	169.0150 / 4.72	[M-H]-	169.0147
[M-H]-	477.126	477.1247 / 5.47		477.1247
[M+TFA-H]-	461.073	461.0720 / 7.22	[M+TFA-H]-	461.0732
[M+FA-H]-	711.224	711.2228 / 2.88	[M+FA-H]-	711.2231
[M-H]-	799.488	799.4869 / 9.05	[M-H]-	799.4875
[M-H]-	282.086	282.0849 / 4.35		282.0851
[M-H]-	469.186	469.1848 / 10.47	[M-H]-	469.1856
[M-H2O-H]-	191.021	191.0201 / 1.31	[M-H2O-H]-	191.0205
[M-H]-	579.287	579.2861 / 16.46	[M-H]-	579.2871
[M-H]-	945.545	945.5438 / 9.77	[M-H]-	945.5447
[M-H]-	455.355	455.3538 / 15.57		455.3548
[M-H]-	177.02	177.0192 / 6.61		177.0199
[M-H]-	389.11	389.1092 / 3.55	[M-H]-	389.1094

[M-H2O-H]-	389.146	389.1451 / 6.00	[M-H2O-H]-	389.1458
[M-H]-	1153.605	1153.6038 / 9.09	[M-H]-	1153.606
[M-H]-	1077.588	1077.5864 / 9.26	[M-H]-	1077.5884
[M-H]-	991.553	991.5524 / 7.92		991.5525
[M-H]-	845.494	845.4924 / 7.98	[M-H]-	845.4933
[M-H2O-H]-	829.499	829.4982 / 9.41	[M-H2O-H]-	829.4988
[M-2H]2-	955.494	955.4931 / 9.37	[M-2H]2-	955.4948
[M-H]-	651.232	651.2311 / 8.35		651.2317
[3M+K-2H]-	961.544	961.5416 / 10.26	[3M+K-2H]-	961.5415
[4M+2K-3H]-	531.176	531.1730 / 7.00	[4M+2K-3H]-	531.1731
[M-H]-	389.11	389.1088 / 4.24	[M-H]-	389.1089
[M-H]-	785.254	785.2530 / 6.47	[M-H]-	785.2544
[M+FA-H]-	565.193	565.1922 / 7.46	[M+FA-H]-	565.1937
[M-H]-	132.032	132.0304 / 0.90		132.0307
[M-H]-	285.041	285.0403 / 8.73		285.041
[M-H]-	353.146	353.1450 / 6.42		353.1459
[M+Cl]-	583.133	583.1319 / 5.93	[M+Cl]-	583.1323
[M-H]-	279.235	279.2335 / 15.66	[M-H]-	279.2336
[M-H]-	417.12	417.1190 / 8.09		417.1192
[M-H]-	255.067	255.0661 / 9.88	[M-H]-	255.0663
[M-H]-	463.088	463.0870 / 7.26	[M-H]-	463.0887
[M-H]-	637.217	637.2159 / 7.84	[M-H]-	637.2158
[M-H]-	315.255	315.2536 / 12.49		315.2544
[M-H]-	353.089	353.0876 / 6.24	[M-H]-	353.0886
[M-H]-	271.063	271.0614 / 9.31		271.0614
[M-H]-	681.298	681.2966 / 15.57		681.2983
[M-H]-	777.41	777.4086 / 10.60	[M-H]-	777.4087
[M-H]-	965.428	965.4270 / 8.68	[M-H]-	965.4202
[M-H]-	403.126	403.1250 / 5.50		403.1253
[M+Br]-	895.396	895.3952 / 8.77	[M+Br]-	895.3966
[M-H]-	407.121	407.1198 / 2.27		407.1198