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Table. S1. The detail data for 411 phenolic compounds.

No.	Compounds	Formula	Class I	Class II	CAS	Q1 (Da)	Q3 (Da)	Molecular weight (Da)	Ionization model	LF-OMTMS-D-1	LF-OMTMS-D-2	LF-OMTMS-D-3	MF-OMTMS-D-1	MF-OMTMS-D-2	MF-OMTMS-D-3	HF-OMTMS-D-1	HF-OMTMS-D-2	HF-OMTMS-D-3
1	1-O-p-Coumaroylquinic acid	C16H18O8	Phenolic acids	Phenolic acids	-	337.09	163.04	338.1002	[M-H]-	21296398	14902495.2	21428995.6	20670086.7	21733345.8	14248843.9	21202013.4	19982307.5	22732608.9
2	2-Hydroxycinnamic acid*	C9H8O3	Phenolic acids	Phenolic acids	583-17-5	163.04	119.05	164.0473	[M-H]-	11702959.9	10889151.1	10546549	10235525	10080350.3	10128075.3	14582851.4	14189657.7	13865588.7
3	α-Hydroxycinnamic Acid*	C9H8O3	Phenolic acids	Phenolic acids	5801-57-0	163.0401	119.0502	164.0473	[M-H]-	11484080.1	11357105.5	11321427.9	10374426.5	10119731.4	10238949.7	13246908.5	14873876.3	14013284.8
4	3-Hydroxycinnamic Acid*	C9H8O3	Phenolic acids	Phenolic acids	14755-02-3	163.04	119.05	164.0473	[M-H]-	10174947.9	11073831.7	10269587.5	9745958.58	9401503.95	9845393.46	13637118.3	14054314.9	14139235
5	Butyl isobutyl phthalate*	C16H22O4	Phenolic acids	Phenolic acids	17851-53-5	279.16	149.03	278.1518	[M+H]+	11071447.8	10278557.2	12307095.8	8649993.58	10247829	9184439.39	9708835.52	9706888	10783181
6	4-O-Methylgallic Acid	C8H8O5	Phenolic acids	Phenolic acids	4319-02-2	183.03	124.02	184.0372	[M-H]-	1908573.42	2230906.26	2075349.38	5283832.11	4507638.31	5285518.21	9004367.93	9663017.17	11061022.2
7	Methyl gallate	C8H8O5	Phenolic acids	Phenolic acids	99-24-1	183.03	124.02	184.0372	[M-H]-	1639766.93	1845745.97	1861219.3	4596875.12	4004415.44	4460316.52	7442354.24	7909577.23	9224934.07
8	3-O-p-Coumaroylquinic acid	C16H18O8	Phenolic acids	Phenolic acids	87099-71-6	337.09	191.06	338.1002	[M-H]-	6870805.25	7136648.59	7047089.74	7362037.14	6657524.44	7202262.83	7223062.97	7745198.68	7798558.15
9	4-(3,4,5-Trihydroxybenzoxy)benzoic acid	C14H10O7	Phenolic acids	Phenolic acids	-	289.04	137.02	290.0427	[M-H]-	7082310.23	6764209.51	5080971.72	5453492.9	4743469.84	5147226.73	6505821.73	4972151.24	7055673.61
10	Phthalic anhydride	C8H4O3	Phenolic acids	Phenolic acids	85-44-9	149.02	65.04	148.016	[M+H]+	7374407.55	7225989.86	8174042.31	7100987.46	7126100.42	5165476.37	5355508.35	6928134.32	6202811.26
11	Ferulic acid*	C10H10O4	Phenolic acids	Phenolic acids	537-98-4	193.05	134.04	194.0579	[M-H]-	4534444.84	4191517.32	4261634.13	4844286.08	4437516.71	4424536.87	5229883.2	5090616.61	5126196.42
12	3-Galloylquinic acid	C14H16O10	Phenolic acids	Phenolic acids	17365-11-6	343.07	191.06	344.0751	[M-H]-	3498357.24	3378167.91	3169330.56	4135508.8	4016862.62	4218911.06	4045162.17	4330015.55	4308978.89
13	5-O-p-Coumaroylquinic acid	C16H18O8	Phenolic acids	Phenolic acids	1899-30-5	337.09	191.06	338.1002	[M-H]-	2960321.06	3327446.52	3501419.94	3662756.27	3567016.82	3845672.16	3960694.27	4195955.97	4096184.45
14	Dimethyl phthalate	C10H10O4	Phenolic acids	Phenolic acids	131-11-3	195.06	163.04	194.0579	[M+H]+	4971658.9	6031624.99	4717620.12	3110305.29	3963354	4178728.31	4147008.73	3878484.55	4215180.49
15	4-Hydroxybenzoic acid	C7H6O3	Phenolic acids	Phenolic acids	99-96-7	137.02	93.03	138.0317	[M-H]-	3058025.61	3159386.16	2923961.22	3072831.12	3158008.42	3072402.47	3833794.25	3770062.88	3722624.21
16	4-Hydroxybenzaldehyde	C7H6O2	Phenolic acids	Phenolic acids	123-08-0	121.03	92.03	122.0368	[M-H]-	3542189.6	3655526	3445210.69	3160460.73	2835170.56	2656221.14	3195330.63	3048636.5	3106045.13
17	2,5-Dihydroxybenzaldehyde	C7H6O3	Phenolic acids	Phenolic acids	1194-98-5	137.02	93.03	138.0317	[M-H]-	2413115.61	2532170.59	2251703.09	2452020.85	2471300.13	2458317.07	2925034.73	3097795.72	2946586.78
18	Isoferulic Acid*	C10H10O4	Phenolic acids	Phenolic acids	25522-33-2	193.0506	134.0374	194.0579	[M-H]-	2701623.19	2461465.16	2555785.23	2578774.79	2637701.7	2733818.27	3075105.33	3018062.22	2821667.4
19	Caffeic acid	C9H8O4	Phenolic acids	Phenolic acids	331-39-5	179.03	135.05	180.0423	[M-H]-	1779940.56	1783909.98	1565851.87	2979366.16	2990165.95	2935740.88	2821906.27	2552963.37	2510066.49
20	Gallic acid	C7H6O5	Phenolic acids	Phenolic acids	149-91-7	169.01	125.02	170.0215	[M-H]-	1939874.56	1845183.9	1627606.25	2312807.78	2284382.49	2260598.55	2328110.5	2517485.33	2379630.2
21	2-(Formylamino)benzoic acid	C8H7NO3	Phenolic acids	Phenolic acids	3342-77-6	164.04	120.05	165.0426	[M-H]-	1971785.84	1763745.51	1824241.35	1692164.88	1685718.67	1604513.07	2198784.79	2211278.27	2126756.08
22	Vanillin; 4-Hydroxy-3-Methoxybenzaldehyde*	C8H8O3	Phenolic acids	Phenolic acids	121-33-5	151.04	136.02	152.0473	[M-H]-	2254368.65	1930479	2126812.62	1939643.9	2082162.29	2031453.36	2019461.67	2372500.53	2075203
23	2,5-Dihydroxybenzoic acid; Gentisic Acid*	C7H6O4	Phenolic acids	Phenolic acids	490-79-9	153.02	109.03	154.0266	[M-H]-	2342169.36	2329211.34	2329523.03	2204344.25	2059050.05	2357386.34	1973992.24	2080327.44	2124394.75
24	2,3-Dihydroxybenzoic Acid*	C7H6O4	Phenolic acids	Phenolic acids	303-38-8	153.02	109.03	154.0266	[M-H]-	2342169.36	2329211.34	2329523.03	2204344.25	2059050.05	2357386.34	1973992.24	2080327.44	2124394.75
25	3,4-Dihydroxybenzoic acid (Protocatechuic acid)*	C7H6O4	Phenolic acids	Phenolic acids	99-50-3	153.02	109.03	154.0266	[M-H]-	2466642.51	2403845.31	2260731.63	2233766.3	2010634.14	2076159.69	1993379.29	1997891.62	2181255.23
26	3-O-Methylgallic acid	C8H8O5	Phenolic acids	Phenolic acids	3934-84-7	183.03	124.02	184.0372	[M-H]-	1405659.69	1370557.79	1546313.29	1420482.54	1462529.15	1469950.3	1500293.88	1454404.23	1563933.04
27	Coniferin	C16H22O8	Phenolic acids	Phenolic acids	531-29-3	341.12	179.07	342.1315	[M-H]-	1135655.5	966010.304	1109370.62	1392240.57	1330933.05	1488469.33	1266152	1458409.03	1492672.92
28	Nordihydrocapsiate	C17H26O4	Phenolic acids	Phenolic acids	220012-53-3	293.18	221.16	294.1831	[M-H]-	1373675.77	1674848.33	1446870.01	1009801.81	1232574.26	1600082.14	1274003.68	1336727.8	1191364.74
29	Methyl cumalate*	C7H6O4	Phenolic acids	Phenolic acids	6018-41-3	153.02	109.03	154.0266	[M-H]-	1445859.24	1231188.11	1251315.11	1250822.75	1216791.51	1318675.72	1096351.34	1144797.72	1103544.47
30	4-MethoxycinnaMaldehyde	C10H10O2	Phenolic acids	Phenolic acids	1963-36-6	163.08	91.05	162.0681	[M+H]+	1243590.38	1387805.82	1485428.86	1158803.82	1214953.02	1286335.58	1121625.63	1073411.17	1043180.69
31	Protocatechuic acid 1-O-(Glucosylvanilloyl)*	C21H22O12	Phenolic acids	Phenolic acids	-	465.1	303.05	466.1111	[M-H]-	511603.74	482634.43	443232.007	739135.838	652690.659	625912.341	867805.378	887829.337	955663.305
32	1-O-Salicyloyl-β-D-glucose*	C13H16O8	Phenolic acids	Phenolic acids	60517-74-0	299.08	137.02	300.0845	[M-H]-	632258.831	569863.945	582547	1001252.82	1098266.5	1153194.71	845789.207	862957.039	913109.615
33	Glucosyloxybenzoic acid*	C13H16O8	Phenolic acids	Phenolic acids	-	299.08	137.02	300.0845	[M-H]-	632258.831	569863.945	582547	1001252.82	1098266.5	1153194.71	845789.207	862957.039	913109.615
34	Glucosyringic acid	C15H20O10	Phenolic acids	Phenolic acids	33228-65-8	359.1	197.05	361.1129	[M-H]-	381272.481	400952.663	418414.809	541639.534	641514.247	581905.868	871079.112	879989.923	842525.061
35	Salidroside	C14H20O7	Phenolic acids	Phenolic acids	10338-51-9	299.11	137.02	300.1209	[M-H]-	508882.839	572592.748	538798.078	1012072.03	932553.426	887629.365	870551.543	844649.839	838650.881
36	4-Nitrophenol	C6H5NO3	Phenolic acids	Phenolic acids	100-02-7	140.03	98.96	139.0269	[M+H]+	13075656.9	12180580	12042611.1	1373444.53	1607729.14	1652747.62	739515.902	697427.545	1039870.08
37	Benzamide	C7H7NO	Phenolic acids	Phenolic acids	55-21-0	122.06	105.03	121.0528	[M+H]+	1012020.78	943822.597	1003477.17	909934.302	802345.65	879871.594	702852.815	812880.411	759953.857
38	2-O-Galloyl-D-glucose*	C13H16O10	Phenolic acids	Phenolic acids	-	331.07	169.01	332.0743	[M-H]-	813166.149	824879.908	593137.883	67384.0007	694096.907	539178.301	899573.003	99801.5007	1147701.17
39	Phloroglucinol; 1,3,5-Benzenetriol	C6H6O3	Phenolic acids	Phenolic acids	108-73-6	127.04	81.03	126.0317	[M+H]+	714628.637	627568.598	787268.967	594816.02	433908.206	609273.353	604966.631	642249.354	888436.512
40	Dunalianoside A*	C21H22O10	Phenolic acids	Phenolic acids	-	433.11	271.06	434.1213	[M-H]-	588759.706	532545.225	512086.933	658345.108	649776.945	657321.077	666652.911	708015.939	749820.819

41	Isovanillin	C8H8O3	Phenolic acids	Phenolic acids	621-59-0	153.05	65.04	152.0473	[M+H]+	878706.424	546059.105	780874.689	671992.127	710702.094	715966.104	660641.854	732529.26	670926.615
42	3-O-caffeoylshikimic acid*	C16H16O8	Phenolic acids	Phenolic acids	-	335.08	179.03	336.084518	[M-H]-	734506.915	654661.519	643056.232	729031.839	655087.996	769771.319	643725.077	609511.464	764317.217
43	4-caffeoylshikimic acid*	C16H16O8	Phenolic acids	Phenolic acids	-	335.08	179.03	336.0845	[M-H]-	734506.915	654661.519	643056.232	729031.839	655087.996	769771.319	643725.077	609511.464	764317.217
44	5-O-Caffeoylshikimic acid	C16H16O8	Phenolic acids	Phenolic acids	73263-62-4	335.08	135.05	336.0845	[M-H]-	667748.306	591361.995	586490.57	600922.746	627108.661	676127.595	636566.02	616599.976	673927.841
45	4-O-p-Coumaroylquinic acid	C16H18O8	Phenolic acids	Phenolic acids	32451-86-8	337.09	163.04	338.1002	[M-H]-	594097.945	595002.857	529494.069	568103.96	549829.136	563676.052	641283.814	616842.485	640149.225
46	2,4-Di-Tert-Butylphenol*	C14H22O	Phenolic acids	Phenolic acids	96-76-4	205.1598	189.1267	206.1671	[M-H]-	553984.891	750167.022	739801.771	711499.92	682784.191	665814.18	674379.363	674473.305	537110.624
47	Eugenol	C10H12O2	Phenolic acids	Phenolic acids	97-53-0	165.09	91.05	164.0837	[M+H]+	702101.047	555971.137	881084.612	492526.11	385616.479	519423.307	581867.102	706318.571	586444.511
48	4-Hydroxyacetophenone	C8H8O2	Phenolic acids	Phenolic acids	99-93-4	135.05	92.03	136.0524	[M-H]-	717663.02	558622.981	698741.845	657997.991	588899.976	565758.214	649941.702	613657.967	609550.625
49	Phenyl acetate	C8H8O2	Phenolic acids	Phenolic acids	122-79-2	135.05	92.03	136.0524	[M-H]-	731175.481	705949.871	694122.63	699536.306	694564.67	598263.915	606767.337	616729.86	639185.849
50	2,6-Di-tert-butylphenol*	C14H22O	Phenolic acids	Phenolic acids	128-39-2	205.16	189.13	206.1671	[M-H]-	589965.389	724764.194	799790.502	726001.277	740009.989	793488.446	639362.13	681931.139	519784.418
51	Sinapic acid	C11H12O5	Phenolic acids	Phenolic acids	530-59-6	223.06	193.02	224.0685	[M-H]-	67682.4881	51625.1426	70575.7545	847206.383	822014.463	775020.98	601498.424	571260.099	582672.942
52	6-O-Caffeoyl-D-glucose*	C15H18O9	Phenolic acids	Phenolic acids	-	341.09	179.03	342.0951	[M-H]-	426442.323	483655.185	468934.794	530510.672	496104.37	470269.325	581614.96	550035.345	607033.544
53	1-O-Caffeoyl-β-D-glucose*	C15H18O9	Phenolic acids	Phenolic acids	14364-08-0	341.09	179.04	342.0951	[M-H]-	509530.417	454094.82	438177.612	520798.706	565359.858	563778.965	595428.085	597623.099	530222.364
54	Neochlorogenic acid (5-O-Caffeoylquinic acid)*	C16H18O9	Phenolic acids	Phenolic acids	906-33-2	353.09	191.06	354.0951	[M-H]-	487989.753	520193.216	504333.15	482315.919	537326.25	580285.528	599666.449	567363.215	545652.258
55	1-O-Sinapoyl-β-D-glucose	C17H22O10	Phenolic acids	Phenolic acids	-	385.11	223.06	386.1213	[M-H]-	212109.388	199120.152	167958.93	441696.215	403300.411	361277.348	531168.15	568670.925	598515.126
56	Syringic acid	C9H10O5	Phenolic acids	Phenolic acids	530-57-4	197.05	123.01	198.0528	[M-H]-	409717.774	414310.705	372650.617	407886.454	423712.715	433542.506	571926.813	584438.389	509473.445
57	4-O-Glucosyl-sinapate	C17H22O10	Phenolic acids	Phenolic acids	-	385.11	223.06	386.1213	[M-H]-	233971.392	217114.868	158441.556	392183.177	411381.042	365319.001	553757.678	530453.506	530171.073
58	Chlorogenic acid (3-O-Caffeoylquinic acid)*	C16H18O9	Phenolic acids	Phenolic acids	327-97-9	353.09	191.06	354.0951	[M-H]-	425723.484	428685.7	397611.491	435013.42	454706.575	472680.784	524869.9	529585.91	485296.996
59	Grevilloside F	C15H18O9	Phenolic acids	Phenolic acids	1094004-50-8	341.09	135.04	342.0951	[M-H]-	342952.673	367819.683	396250.374	486353.097	501052.501	500650.32	526055.039	473815.696	523596.195
60	Dunalianoside C*	C21H22O11	Phenolic acids	Phenolic acids	-	449.11	287.06	450.1162	[M-H]-	518667.895	522915.672	507535.248	521707.073	501809.643	502861.665	515201.212	483988.607	495701.843
61	1-O-Vanilloyl-D-Glucose	C14H18O9	Phenolic acids	Phenolic acids	-	329.11	167.03	330.0951	[M-H]-	378063.466	525558.827	515748.276	466098.608	406110.64	408986.162	496986.136	509645.139	455365.597
62	davidioside C*	C15H16O9	Phenolic acids	Phenolic acids	-	339.07	177.02	340.0794	[M-H]-	639721.675	574549.934	609063.852	538795.541	477102.881	554598.819	513742.107	441476.817	499223.796
63	5-Glucosyloxy-2-Hydroxybenzoic acid methyl ester	C14H18O9	Phenolic acids	Phenolic acids	-	329.09	167.04	330.0951	[M-H]-	399557.957	509168.987	530107.065	450931.707	380126.016	413365.081	470831.702	490936.868	474591.382
64	Caffeic aldehyde	C9H8O3	Phenolic acids	Phenolic acids	141632-15-7	165.05	91.05	164.0473	[M+H]+	582348.648	682501.958	887953.761	654124.17	354051.134	534017.857	455892.883	495924.882	467250.41
65	Trihydroxycinnamoylquinic acid	C16H20O10	Phenolic acids	Phenolic acids	-	371.1	249.06	372.1056	[M-H]-	786962.529	734650.924	796333.812	453501.895	418413.342	404032.77	469295.665	416175.959	499740.162
66	Methyl 4-hydroxybenzoate*	C8H8O3	Phenolic acids	Phenolic acids	99-76-3	151.04	136.02	152.0473	[M-H]-	435647.573	427823.414	448080.712	407686.826	437846.544	406886.352	427137.753	476159.318	424049.118
67	2,4-Dinitrophenol	C6H4N2O5	Phenolic acids	Phenolic acids	51-28-5	183	109.02	184.012	[M-H]-	439376.116	508445.488	511463.745	399147.855	394972.709	393018.824	406909.368	409169.032	417552.728
68	p-Coumaric acid	C9H8O3	Phenolic acids	Phenolic acids	501-98-4	165.05	119.05	164.0473	[M+H]+	567508.557	545021.781	570883.814	439163.151	378960.357	367438.247	416390.739	379983.585	414860.555
69	3,4-Dihydroxybenzeneacetic acid*	C8H8O4	Phenolic acids	Phenolic acids	102-32-9	167.03	123.05	168.0423	[M-H]-	248875.5	251541.925	254251.949	327330.221	355517.917	356430.288	392318.465	413750.684	379294.687
70	5-O-Galloyl-D-hamamelose*	C13H16O10	Phenolic acids	Phenolic acids	-	331.07	169.02	332.0743	[M-H]-	342493.727	324260.753	317027.437	362328.969	331714.946	342211.388	354761.707	374990.155	397033.897
71	1-O-Galloyl-β-D-glucose*	C13H16O10	Phenolic acids	Phenolic acids	58511-73-2	331.07	169.01	332.0743	[M-H]-	326466.636	336864.77	340358.355	332982.867	314006.17	332823.157	347066.618	386063.2	375642.488
72	6-O-Galloyl-β-D-glucose*	C13H16O10	Phenolic acids	Phenolic acids	13186-19-1	331.07	169.01	332.0743	[M-H]-	326466.636	336864.77	340358.355	332982.867	314006.17	332823.157	347066.618	386063.2	375642.488
73	Digalloylglucose*	C20H20O14	Phenolic acids	Phenolic acids	-	483.08	169.05	484.0853	[M-H]-	317600.488	233573.625	252005.446	218704.181	216840.689	221537.945	345324.202	374360.009	357197.223
74	Isochlorogenic acid B*	C25H24O12	Phenolic acids	Phenolic acids	14534-61-3	515.12	353.09	516.1268	[M-H]-	124007.044	134100.565	56395.9674	192667.045	206357.307	161357.101	357945.013	307172.002	408684.191
75	Gallic Acid Ethyl Ester; Ethyl gallate	C9H10O5	Phenolic acids	Phenolic acids	831-61-8	197.05	124.02	198.0528	[M-H]-	296431.153	272613.638	248213.888	295796.229	293622.854	292308.525	347889.455	345646.182	379644.345
76	3-O-Galloyl-D-glucose*	C13H16O10	Phenolic acids	Phenolic acids	-	331.07	169.01	332.0743	[M-H]-	355913.065	332707.465	324660.989	360855.901	315014.782	343134.955	311871.912	388335.114	353718.01
77	Diisobutyl phthalate*	C16H22O4	Phenolic acids	Phenolic acids	84-69-5	279.1591	149.0233	278.1518	[M+H]+	564387.718	375798.198	464588.938	401763.108	435552.929	48953.1758	270698.959	419107.855	353194.706
78	4-Hydroxyphenylacetic acid*	C8H8O3	Phenolic acids	Phenolic acids	156-38-7	151.04	107.05	152.0473	[M-H]-	296546.039	287452.427	271771.969	239057.116	300712.939	289455.069	270789.166	392226.915	376726.934
79	Anthranilic Acid	C7H7NO2	Phenolic acids	Phenolic acids	118-92-3	138.06	92.05	137.0477	[M+H]+	446324.721	445458.289	424822.753	302091.305	373967.16	368393.632	321906.074	329903.314	364490.036
80	Propyl 4-hydroxybenzoate	C10H12O3	Phenolic acids	Phenolic acids	94-13-3	179.07	92.03	180.0786	[M-H]-	128036.021	191142.762	182271.853	175293.768	142987.459	166710.154	322799.987	303607.167	332747.7
81	Phthalic acid	C8H6O4	Phenolic acids	Phenolic acids	88-99-3	165.02	77.04	166.0266	[M-H]-	3513766.02	551707.251	496446.621	504460.479	1402577.15	1339783.39	399007.304	256740.868	300455.978
82	Isochlorogenic acid C*	C25H24O12	Phenolic acids	Phenolic acids	57378-72-0	515.12	353.09	516.1268	[M-H]-	174059.354	123743.667	52852.2884	169494.902	201174.38	171724.407	361707.093	203432.574	381541.603

83	Isochlorogenic acid A*	C25H24O12	Phenolic acids	Phenolic acids	2450-53-5	515.12	353.09	516.1268	[M-H]-	174059.354	123743.667	52852.2884	169494.902	201174.38	171724.407	361707.093	203432.574	381541.603
84	Vanillin acetate	C10H10O4	Phenolic acids	Phenolic acids	881-68-5	195.06	93.03	194.0579	[M+H]+	414192.878	374190.626	367965.706	348951.783	425854.829	392873.281	322035.13	300259.382	301584.017
85	Gallic acid-4-O-glucoside	C13H16O10	Phenolic acids	Phenolic acids	84274-52-2	331.07	313.06	332.0743	[M-H]-	271137.477	289950.592	302790.234	296521.924	299419.961	308885.082	290608.328	322648.674	290052.666
86	5,7-Dihydroxy-1(3H)-isobenzofuranone	C8H6O4	Phenolic acids	Phenolic acids	27979-58-4	165.02	121.03	166.0266	[M-H]-	1437920.02	380428.216	384602.316	363325.056	718302.788	680936.66	308320.422	326658.737	266560.365
87	Anthranilate-1-O-Sophoroside	C19H27NO12	Phenolic acids	Phenolic acids	-	460.15	117.9	461.1533	[M-H]-	124537.013	105402.523	100106.265	157796.936	96979.7062	89077.3583	211831.465	396056.033	286404.02
88	Homogentisic acid*	C8H8O4	Phenolic acids	Phenolic acids	451-13-8	167.03	123.05	168.0423	[M-H]-	209542.723	217688.017	207527.069	247662.018	281619.769	283172.911	290791.107	293040.779	284031.984
89	Cryptochlorogenic acid (4-O-Caffeoylquinic acid)*	C16H18O9	Phenolic acids	Phenolic acids	905-99-7	353.09	191.06	354.0951	[M-H]-	257889.048	251447.223	251490.32	272168.383	268924.214	292295.043	306902.593	256017.978	293213.384
90	1,4-Di-O-Galloyl-D-glucose	C20H20O14	Phenolic acids	Phenolic acids	-	483.08	169.01	484.0853	[M-H]-	292582.122	118251.653	103792.377	271386.315	29100.241	125217.515	452075.296	179199.134	189935.066
91	p-Coumaric acid methyl ester	C10H10O3	Phenolic acids	Phenolic acids	19367-38-5	177.06	145.03	178.063	[M-H]-	82370.7343	91256.3521	68274.9224	154604.628	137868.464	162926.426	243090.921	269990.583	287048.618
92	1-O-Galloyl-6-O-p-Coumaroyl-β-D-glucose	C22H22O12	Phenolic acids	Phenolic acids	-	477.1	169.01	478.1111	[M-H]-	198633.905	221204.062	153837.747	189196.14	160824.254	185355.869	225691.19	260547.049	307428.556
93	6-O-Caffeoylarbutin	C21H22O10	Phenolic acids	Phenolic acids	136172-60-6	433.11	271.06	434.1213	[M-H]-	226674.874	246172.858	241978.332	224728.869	224892.614	267585.832	223635.706	292024.03	277669.563
94	2,6-dimethoxy-hydroquinone-4-O-β-D-glucopyranoside	C14H20O9	Phenolic acids	Phenolic acids	-	331.1	169.01	332.1107	[M-H]-	223545.885	241042.19	219062.273	214669.564	225094.176	233459.63	264850.75	259350.167	257990.232
95	4,6-(S)-Hexahydroxydiphenoyl-β-D-glucose	C20H18O14	Phenolic acids	Phenolic acids	36378-48-0	481.06	301	482.0697	[M-H]-	293089.186	239349.291	245331.899	228786.863	233872.562	204473.978	269837.708	250902.116	237347.809
96	2-Hydroxybenzaldehyde (Salicylaldehyde)	C7H6O2	Phenolic acids	Phenolic acids	90-02-8	121.03	77.04	122.0368	[M-H]-	2764194.21	436514.427	439629.685	345807.165	1071184.92	1123139.58	299817.561	218150.919	224687.642
97	Brevifolin carboxylic acid	C13H8O8	Phenolic acids	Phenolic acids	18490-95-4	291.01	247.02	292.0219	[M-H]-	256936.963	243751.952	271571.768	203855.541	236154.055	206609.075	246284.326	224261.516	268190.227
98	1,6-Di-O-galloyl-β-D-glucose	C20H20O14	Phenolic acids	Phenolic acids	-	483.08	169.01	484.0853	[M-H]-	109686.464	116668.776	118412.874	119600.214	118909.685	28966.3651	218814.764	215353.273	249063.101
99	3-Aminosalicylic acid	C7H7NO3	Phenolic acids	Phenolic acids	570-23-0	152.04	108.05	153.0426	[M-H]-	200063.965	201924.586	192330.223	204845.352	209217.069	213041.04	227517.903	215555.455	235440.458
100	3-(4-Hydroxyphenyl)-propionic acid*	C9H10O3	Phenolic acids	Phenolic acids	501-97-3	165.06	119.05	166.063	[M-H]-	205750.122	191151.987	208831.022	186963.565	196047.534	202911.313	221865.19	233090.571	212983.711
101	Cinnamic acid	C9H8O2	Phenolic acids	Phenolic acids	140-10-3	149.06	103.06	148.0524	[M+H]+	228087.39	151321.419	247400.01	288660.113	181448.439	222104.051	216725.793	206750.273	214358.831
102	Vanillic acid	C8H8O4	Phenolic acids	Phenolic acids	121-34-6	167.03	108.02	168.0423	[M-H]-	188089.974	180719.859	190538.568	122400.862	145836.403	127783.585	195607.128	218961.691	220248.67
103	Ferulic acid-4-O-glucoside	C16H20O9	Phenolic acids	Phenolic acids	117405-51-3	355.1	193.05	356.1107	[M-H]-	120312.397	113618.044	138113.453	135244.991	192765.237	149403.037	201850.204	199817.667	212091.986
104	Protocatechualdehyde	C7H6O3	Phenolic acids	Phenolic acids	139-85-5	139.04	65.04	138.0317	[M+H]+	200642.856	211684.755	169493.193	212249.136	191191.714	209884.923	155305.56	200143.782	182849.465
105	Methyl-3-(3-hydroxyphenyl)Propionate	C10H12O3	Phenolic acids	Phenolic acids	61389-68-2	181.09	121.06	180.0786	[M+H]+	252726.435	188618.976	251663.477	228240.235	257738.963	263260.079	195366.38	153803.692	187914.033
106	5'-Glucosyloxyjasmanic acid	C18H28O9	Phenolic acids	Phenolic acids	-	387.17	207.1	388.1733	[M-H]-	134897.153	120234.049	133607.332	153207.186	137881.93	152748.311	152803.539	206954.512	165792.425
107	2,6-Dimethoxybenzaldehyde*	C9H10O3	Phenolic acids	Phenolic acids	3392-97-0	165.06	119.05	166.063	[M-H]-	146685.723	151785.439	152634.287	136907.446	171535.031	140465.689	161593.27	165485.768	197264.455
108	Benzoic acid	C7H6O2	Phenolic acids	Phenolic acids	65-85-0	123.04	79.05	122.0368	[M+H]+	195894.104	131735.316	224623.567	132155.179	228366.963	205961.649	189597.663	169121.926	162030.013
109	2,3-Di-O-Galloyl-β-D-Glucose*	C20H20O14	Phenolic acids	Phenolic acids	-	483.08	169.01	484.0853	[M-H]-	149092.476	113137.201	112015.845	109134.541	108509.543	95634.5915	191148.526	158249.392	156771.234
110	1-O-Gentisoyl-β-D-glucoside*	C13H16O9	Phenolic acids	Phenolic acids	23445-11-6	315.07	153.02	316.0794	[M-H]-	133290.94	127851.165	59225.4511	149651.799	177479.637	250164.419	190188.277	176328.378	135313.474
111	Protocatechuic acid-4-O-glucoside*	C13H16O9	Phenolic acids	Phenolic acids	-	315.07	153.02	316.0794	[M-H]-	133290.94	127851.165	59225.4511	149651.799	177479.637	250164.419	190188.277	176328.378	135313.474
112	Salicylic acid	C7H6O3	Phenolic acids	Phenolic acids	69-72-7	137.03	108.02	138.0317	[M-H]-	123418.533	147573.118	150087.117	142132.544	137124.833	142480.432	156885.849	145888.056	190007.671
113	β-Hydroxy-(3,4-dihydroxyphenylethanolyl)-glucoside	C14H20O9	Phenolic acids	Phenolic acids	-	331.1	151.04	332.111	[M-H]-	134299.584	147654.422	143817.882	148102.906	151709.723	148645.572	159458.608	158840.604	172518.045
114	Syringin	C17H24O9	Phenolic acids	Phenolic acids	118-34-3	371.13	209.08	372.142	[M-H]-	26181.1108	39617.5073	34101.9887	44592.319	46416.4177	48345.9109	146821.55	159697.241	164291.079
115	Ethyl phenylacetate	C10H12O2	Phenolic acids	Phenolic acids	101-97-3	165.09	91.05	164.0837	[M+H]+	102001.416	141400.537	92317.0289	74464.0648	85407.2648	122546.077	145673.857	109817.524	202893.712
116	3,5-Digalloylshikimic acid	C23H26O11	Phenolic acids	Phenolic acids	95753-52-9	477.14	169	478.1475	[M-H]-	114132.143	150119.672	75138.0023	126777.11	124720.011	120540.97	150470.924	118328.406	162196.928
117	Chlorogenic acid methyl ester	C17H20O9	Phenolic acids	Phenolic acids	29708-87-0	367.1	190.9	368.1107	[M-H]-	229528.454	199893.996	218023.87	156205.415	162977.919	152535.002	119609.429	146040.372	160698.503
118	3-[(1-Carboxyvinyl)oxy]benzoic acid	C10H8O5	Phenolic acids	Phenolic acids	16929-37-6	207.03	119.05	208.0372	[M-H]-	93685.1496	82857.4583	84188.681	122456.033	115596.713	137598.326	133016.111	117706.975	136398.501
119	Dicaffeoylshikimic acid	C25H22O11	Phenolic acids	Phenolic acids	-	499.13	163.04	498.1162	[M+H]+	71277.4249	66283.2612	63204.8429	69115.9706	85694.7832	99952.3533	111580.308	115122.529	145803.876
120	Syringaldehyde; 4-Hydroxy-3,5-Dimethoxybenzaldehyde	C9H10O4	Phenolic acids	Phenolic acids	134-96-3	181.05	151	182.0579	[M-H]-	402237.873	414834.822	426257.518	149769.625	129218.273	131697.483	129340.974	126155.323	116874.211
121	Salicylic acid-2-O-glucoside	C13H16O8	Phenolic acids	Phenolic acids	10366-91-3	299.08	137.02	300.0845	[M-H]-	87054.0576	88848.9528	83854.7895	102326.754	132139.352	123633.271	174989.262	188112.96	7207.49914
122	4-Hydroxyphenyllactic Acid*	C9H10O4	Phenolic acids	Phenolic acids	306-23-0	181.05	135.04	182.0579	[M-H]-	79294.5225	77103.6179	80490.5112	67591.7237	86282.3499	88390.1643	113052.009	120304.576	123481.156
123	3-hydroxyphenylacetic acid*	C8H8O3	Phenolic acids	Phenolic acids	621-37-4	151.04	107.05	152.0473	[M-H]-	85988.932	96179.1872	83606.0734	91559.7798	93239.2323	77221.0625	101953.428	110374.961	128263.981
124	Methyl 2,4-dihydroxyphenylacetate*	C9H10O4	Phenolic acids	Phenolic acids	67828-42-6	181.05	135.04	182.0579	[M-H]-	71700.1836	69461.34	72721.5692	68251.6428	68696.7994	69002.802	106171.108	102100.276	123815.807

125	1-O-(3,4-Dihydroxy-5-methoxy-benzoyl)-glucoside	C14H18O10	Phenolic acids	Phenolic acids	-	345.08	139.04	346.09	[M-H]-	96337.9683	96513.0182	90055.0799	113402.954	114584.509	121217.111	105261.904	110579.64	107163.727
126	4-hydroxy-3-methoxyphenyl 1-O-β-D-(6'-O-galloyol)-glucopyranoside	C20H22O12	Phenolic acids	Phenolic acids	-	453.1	313.05	454.1111	[M-H]-	109039.825	78852.0554	85218.8625	113661.05	88060.8669	100701.079	103338.969	102118.392	116034.008
127	Dihydroferulic acid glucoside	C16H22O9	Phenolic acids	Phenolic acids	-	357.12	195.07	358.1264	[M-H]-	63783.8001	68345.5457	31835.3275	112334.945	46871.8188	59995.3163	105500.675	71390.8059	132595.041
128	Hydroxyferulic acid glucoside	C16H20O10	Phenolic acids	Phenolic acids	-	371.1	209.05	372.1056	[M-H]-	21622.5733	17285.5489	24205.4392	31185.886	35143.3854	28442.724	78494.2591	101771.556	105003.788
129	Protocatechuic Acid Methyl Ester	C8H8O4	Phenolic acids	Phenolic acids	2150-43-8	167.04	108.02	168.0423	[M-H]-	36598.6763	40338.0378	38246.9661	55487.9739	52184.5367	60647.3002	91005.4091	97446.9494	91950.5657
130	2-(3,4-dihydroxyphenyl)ethanediol 1-O-β-D-glucopyranoside*	C14H20O9	Phenolic acids	Phenolic acids	-	331.1	153.02	332.1107	[M-H]-	64701.7832	56496.476	67708.8004	63067.3107	56462.8977	69003.1084	90902.8892	92039.2547	84880.5011
131	Tachioside*	C13H18O8	Phenolic acids	Phenolic acids	109194-60-7	301.09	123.01	302.1002	[M-H]-	100533.55	104298.47	97381.2817	87164.9032	102806.278	103616.107	89239.6001	89207.7571	85928.5422
132	1-O-p-Coumaroyl-β-D-glucose*	C15H18O8	Phenolic acids	Phenolic acids	7139-64-2	325.09	163.04	326.1002	[M-H]-	171136.58	187270.546	185622.841	63895.7604	162287.218	220614.135	95816.9825	75298.0298	83094.5878
133	p-Coumaric acid-4-O-glucoside*	C15H18O8	Phenolic acids	Phenolic acids	117405-48-8	325.09	163.04	326.1002	[M-H]-	171136.58	187270.546	185622.841	63895.7604	162287.218	220614.135	95816.9825	75298.0298	83094.5878
134	5-Acetylsalicylic acid	C9H8O4	Phenolic acids	Phenolic acids	13110-96-8	181.05	107.05	180.0423	[M+H]+	122128.203	119247.773	84585.5918	85255.0204	88784.7172	79424.7645	81547.4396	103868.164	63072.7066
135	2-Hydroxy-3-phenylpropanoic acid	C9H10O3	Phenolic acids	Phenolic acids	7326-19-4	165.06	103.06	166.063	[M-H]-	76311.4646	88706.0059	86660.1093	93993.528	75573.044	85654.8196	70726.1825	93152.5671	81476.9906
136	3-Galloyl-6-O-Benzoyl Glucose*	C20H20O11	Phenolic acids	Phenolic acids	-	435.09	169.02	436.1006	[M-H]-	106021.546	73712.8553	54834.2064	62291.0017	67102.5104	53228.8074	59223.4142	62208.6432	123509.164
137	4-O-Galloylquinic Acid	C14H16O10	Phenolic acids	Phenolic acids	110170-37-1	343.07	191.06	344.0743	[M-H]-	73499.8142	74205.6115	75629.5175	77951.9165	75581.8189	78767.7047	84487.6087	78864.006	79127.9141
138	Koaburaside*	C14H20O9	Phenolic acids	Phenolic acids	41653-73-0	331.1	153.02	332.1107	[M-H]-	62603.956	79701.7455	46309.4485	68817.1753	65377.7534	78131.464	77633.5848	81724.4581	78954.1031
139	Furanofructosyl-α-D-(6-mustard acyl)glucoside*	C23H32O15	Phenolic acids	Phenolic acids	-	547.17	223.1	548.1741	[M-H]-	19805.8132	25638.9081	26627.4012	60548.6177	59312.2023	62004.2692	65787.2513	60338.0982	95464.1831
140	Antiarol; 3,4,5-Trimethoxyphenol	C9H12O4	Phenolic acids	Phenolic acids	642-71-7	185.08	125.06	184.0736	[M+H]+	67005.2634	61370.9616	69113.4452	71085.3692	81588.9744	40841.6248	74437.3456	62957.739	83685.6583
141	Homovanilloylquinic acid	C16H20O9	Phenolic acids	Phenolic acids	-	355.1	121.03	356.1107	[M-H]-	81097.9654	75015.9472	76700.013	82707.7844	77907.414	87779.0231	72693.8072	74642.1214	73535.7831
142	(S)-2-Hydroxy-3-(4-Hydroxyphenyl)Propanoic Acid	C9H10O4	Phenolic acids	Phenolic acids	23508-35-2	181.05	135.04	182.0579	[M-H]-	48417.6638	50927.5481	38499.159	45126.6067	47274.7303	43434.721	73035.336	67432.7322	77030.5652
143	Rosmarinic acid-3'-O-glucoside	C24H26O13	Phenolic acids	Phenolic acids	910028-78-3	521.13	359.08	522.1373	[M-H]-	72424.3837	79847.049	70337.9237	58507.1099	85852.2621	86179.417	70559.173	70298.5714	75174.5817
144	2-Galloyl-6-O-Benzoyl Glucose*	C20H20O11	Phenolic acids	Phenolic acids	-	435.09	169.01	436.1006	[M-H]-	80510.6493	40058.0705	39817.5775	54822.463	44079.6156	54931.8354	61206.0242	65625.2315	85004.3699
145	6'-O-Sinapoylsucrose*	C23H32O15	Phenolic acids	Phenolic acids	-	547.17	223.06	548.1741	[M-H]-	32635.528	26572.0367	33755.8683	68595.2131	71042.921	67245.7393	58601.8377	76037.2278	76128.5774
146	2-β-D-Glucopyranosyloxy-5-hydroxyphenylacetic acidmethylester	C15H20O9	Phenolic acids	Phenolic acids	-	343.1	181.05	344.1107	[M-H]-	61263.9682	71441.661	57977.7141	75765.7789	64305.8765	65665.5312	68868.7991	61662.6617	79220.5325
147	3-Hydroxy-4-isopropylbenzylalcohol-3-O-glucoside	C16H24O7	Phenolic acids	Phenolic acids	-	327.14	165.09	328.1522	[M-H]-	75422.2311	74008.8934	36217.1337	56701.0272	56092.5807	55702.8184	63723.4854	73415.0664	59464.8581
148	Isotachioside*	C13H18O8	Phenolic acids	Phenolic acids	31427-08-4	301.09	123.01	302.1002	[M-H]-	39656.7763	47774.1843	38265.5852	51910.8974	40693.5773	43755.9739	40250.9662	80383.0309	58054.7328
149	Phenylpropionic acid-O-β-D-glucopyranoside	C15H18O8	Phenolic acids	Phenolic acids	-	325.09	119.05	326.1002	[M-H]-	85413.8313	85792.3897	77704.1048	80352.6664	76886.2875	74262.7137	67833.7657	46189.6814	62057.5086
150	Tyrosol; 4-Hydroxyphenylethanol	C8H10O2	Phenolic acids	Phenolic acids	501-94-0	139.08	55.02	138.0681	[M+H]+	40712.9451	36194.5192	48488.2588	35184.1701	21606.3609	38887.6622	50912.6011	47870.2866	75926.2803
151	2-hydroxymethyl benzoic acid	C8H8O3	Phenolic acids	Phenolic acids	612-20-4	151.04	77.04	152.0473	[M-H]-	38733.0634	37685.3384	39137.56	41770.2945	42301.826	42839.8752	68827.0882	52479.948	52598.242
152	6'-O-Feruloyl-D-sucrose	C22H30O14	Phenolic acids	Phenolic acids	118230-77-6	517.16	175.04	518.1636	[M-H]-	130516.908	101534.547	111348.013	76860.274	67249.3685	75092.9769	54266.135	58504.079	54435.8059
153	Hydroxytyrosol	C8H10O3	Phenolic acids	Phenolic acids	10597-60-1	153.06	123.05	154.063	[M-H]-	32896.4931	27563.4999	35414.6281	31756.647	33560.6508	56404.8925	53532.2413	57392.5915	55356.467
154	Syringaldehyde-4-O-glucoside	C15H20O9	Phenolic acids	Phenolic acids	-	343.11	181.05	344.1107	[M-H]-	43873.8288	52559.8965	39251.0307	41925.4665	40954.0309	57755.8512	56498.7375	40098.4109	56233.3277
155	2-Amino-3-methoxybenzoic acid	C8H9NO3	Phenolic acids	Phenolic acids	3177-80-8	168.06	94.06	167.0582	[M+H]+	41358.8688	46777.5217	48698.7564	41157.1503	46092.1639	43873.8667	51270.9869	48079.1544	52764.8101
156	3-Hydroxy-4-methoxybenzoic acid; Isovanillic Acid	C8H8O4	Phenolic acids	Phenolic acids	645-08-9	169.05	65.04	168.0423	[M+H]+	26302.9742	33552.923	45903.2896	14973.4057	30487.9704	41552.5637	43973.2735	55330.6995	46629.4538
157	1-O-Feruloyl-β-D-glucose	C16H20O9	Phenolic acids	Phenolic acids	7196-71-6	355.1	193.05	356.1107	[M-H]-	40505.9646	66378.5797	39041.4719	49031.5885	40533.0083	44616.4828	42205.0964	47459.8685	45341.3163
158	6-O-Feruloyl-β-D-glucose	C16H20O9	Phenolic acids	Phenolic acids	137887-25-3	355.1	193.05	356.1107	[M-H]-	18818.7429	39220.3408	21902.3326	27702.0722	23451.5989	43772.6049	46805.045	42665.2023	36698.6188
159	Trans-5-O-(p-Coumaroyl)shikimate	C16H16O7	Phenolic acids	Phenolic acids	-	321.1	147.04	320.0896	[M+H]+	53421.4157	43850.7208	64821.444	96675.3213	100383.236	65157.6769	41871.0093	30124.0956	50451.0122
160	Benzyl-(2"-O-xylosyl)glucoside	C18H26O10	Phenolic acids	Phenolic acids	-	401.14	269.1	402.1526	[M-H]-	37228.7833	37044.613	29357.7272	30805.0998	32803.4803	23077.1663	36542.6691	33253.3557	44544.6455
161	4-O-Galloylarbutin	C19H20O11	Phenolic acids	Phenolic acids	-	423.09	169.01	424.1008	[M-H]-	71658.8096	15452.2732	83189.8094	20700.2637	71310.3249	53789.8478	25091.0898	19160.2784	69165.3804
162	3,4-Digalloylshikimic acid	C21H18O13	Phenolic acids	Phenolic acids	-	477.06	169.01	478.0747	[M-H]-	43542.9396	29308.8404	18180.8009	66464.6814	49753.405	68634.9905	44064.8648	36431.2674	31244.184
163	Benzyl β-primeveroside	C18H26O10	Phenolic acids	Phenolic acids	130622-31-0	401.15	269.11	402.1526	[M-H]-	37304.7333	35562.6874	47157.8633	38729.8338	35280.0416	34519.1257	39562.4948	38109.2837	33635.1058
164	4-O-Glucosyl-3,4-dihydroxybenzyl alcohol	C13H18O8	Phenolic acids	Phenolic acids	-	301.09	139.05	302.1002	[M-H]-	43057.758	47138.9832	42176.612	14206.1104	36492.9254	34923.8595	37311.9384	41228.0035	32390.2264
165	4'-Hydroxypropiophenone	C9H10O2	Phenolic acids	Phenolic acids	70-70-2	149.07	92.03	150.0681	[M-H]-	41930.6609	37876.2663	39133.2729	36896.5518	41325.4621	41872.5098	37354.5858	35673.6151	36859.6552
166	4,7,9,9'-Tetrahydroxy-3,3'-dimethoxy-8-O-4'-neolignan*	C20H26O7	Phenolic acids	Phenolic acids	-	377.16	329.14	378.1679	[M-H]-	35568.5104	34830.5422	34013.2075	30592.3454	30005.4166	37049.3411	29814.1128	48821.3952	30308.1895

167	Monogalloyl-diglucose	C19H26O15	Phenolic acids	Phenolic acids	-	493.12	169.01	494.1272	[M-H]-	25327.764	29262.1693	22847.5877	27752.1499	32129.1234	33531.0659	33817.065	33581.0402	34511.8483
168	1-O-Caffeoyl-4-O-galloyl-β-D-glucose	C22H22O13	Phenolic acids	Phenolic acids	-	493.1	169.01	494.106	[M-H]-	35351.6863	29847.5114	28848.8067	21547.4348	27954.1798	19443.2316	31058.8473	23064.3854	43606.7867
169	Vanillic acid-4-O-glucoside	C14H18O9	Phenolic acids	Phenolic acids	32142-31-7	329.09	209.04	330.0951	[M-H]-	44292.9454	37178.1915	36337.3726	24645.1513	42700.4029	40731.655	33659.706	28462.4751	35287.8342
170	Demethyl coniferin	C15H20O8	Phenolic acids	Phenolic acids	-	327.11	165.05	328.1158	[M-H]-	33870.3407	30419.0579	39900.5689	28851.1283	25780.4808	25048.3647	34001.6562	23078.2019	35329.5226
171	p-Hydroxypheny-β-D-allopyranoside*	C12H16O7	Phenolic acids	Phenolic acids	-	271.08	108.02	272.0896	[M-H]-	25611.3018	26103.1247	26433.0364	23189.1619	24962.4472	23287.5357	32027.7899	28590.3067	30556.7011
172	Phenylmethyl β-L-glucopyranoside	C13H18O6	Phenolic acids	Phenolic acids	176018-22-7	269.1	59.02	270.1103	[M-H]-	35629.2509	43523.776	26526.4706	34162.1006	37680.0416	29291.7481	26514.4465	28141.5143	33654.0149
173	Pyrocatechol	C6H6O2	Phenolic acids	Phenolic acids	120-80-9	109.03	81.03	110.0368	[M-H]-	30915.4335	24909.5732	18608.3065	24204.3551	38772.722	24523.9163	30550.8423	18757.9247	37569.0742
174	3-Galloylshikimic acid	C14H14O9	Phenolic acids	Phenolic acids	110082-91-2	325.06	93.03	326.0638	[M-H]-	13634.4992	18047.964	12519.9093	18061.6049	18430.0777	19379.5088	26322.2701	31095.7231	26108.6696
175	Arbutin*	C12H16O7	Phenolic acids	Phenolic acids	497-76-7	271.08	108.02	272.0896	[M-H]-	25312.1681	18803.6653	24410.5886	23433.7059	19183.551	23261.6887	25108.7965	30088.0347	27247.4661
176	4-O-β-D-glucopyranosylferulic acid	C16H20O9	Phenolic acids	Phenolic acids	-	355.1039	175.04	356.1107	[M-H]-	38402.3938	47367.4348	31885.244	33841.3323	29588.9242	28133.3056	23942.1788	27235.0297	28717.1451
177	3-O-p-Coumaroylshikimic acid	C16H16O7	Phenolic acids	Phenolic acids	-	319.08	145.03	320.0896	[M-H]-	170082.597	154794.44	177883.278	87644.4679	95962.3411	58961.5481	35573.319	22103.8375	20459.1898
178	1-(4-Methoxyphenyl)-1-propanol	C10H14O2	Phenolic acids	Phenolic acids	5349-60-0	165.09	149.06	166.0994	[M-H]-	23677.1595	26696.4105	26027.6379	21826.5413	23775.2497	28621.2502	30516.6505	28090.4347	19156.3641
179	Caffeoyl(p-Hydroxybenzoyl)tartaric acid	C20H16O11	Phenolic acids	Phenolic acids	-	431.06	137.03	432.0693	[M-H]-	24136.3301	17791.3975	21905.7887	31430.3535	33196.2316	30116.6813	22762.1586	20089.0927	34301.065
180	3,5-Dihydroxyacetophenone	C8H8O3	Phenolic acids	Phenolic acids	51863-60-6	151.04	65.04	152.0473	[M-H]-	24988.0444	22796.3467	24555.3986	24499.6627	8682.2747	17726.6644	17799.3173	28068.4197	28842.8022
181	Salicin	C13H18O7	Phenolic acids	Phenolic acids	138-52-3	285.1	123.05	286.1053	[M-H]-	17156.4753	22179.3738	19357.3044	16042.5795	19115.0829	22290.1024	16590.5987	14638.0127	41567.6771
182	5-O-Galloylshikimic acid	C14H14O9	Phenolic acids	Phenolic acids	-	325.06	169.02	326.0638	[M-H]-	32074.1499	33963.8659	38902.6298	41603.1599	35156.9098	40393.7878	42514.4177	7199.84116	14315.1996
183	(2E)-3-[4-(β-D-glucopyranoside)-phenylacrylic]-acid	C15H18O8	Phenolic acids	Phenolic acids	-	325.09	119.05	326.1002	[M-H]-	16046.8799	14805.9957	22942.1818	29274.1487	18153.3805	18874.2581	23674.8784	21060.5304	18647.5609
184	Hydroquinone	C6H6O2	Phenolic acids	Phenolic acids	123-31-9	109.03	81.03	110.0368	[M-H]-	23456.4108	23928.4706	26462.8213	25810.5106	19125.111	16873.6214	14209.7185	26740.938	18616.8972
185	Benzyl glucoside	C13H18O6	Phenolic acids	Phenolic acids	4304-12-5	269.1	101.02	270.1103	[M-H]-	30390.5815	20715.9454	16700.0419	14183.0256	21692.6306	12289.9159	12931.7639	24758.1147	16900.1787
186	3,4,5-Trimethoxycinnamic acid	C12H14O5	Phenolic acids	Phenolic acids	90-50-6	237.08	103.02	238.0841	[M-H]-	9881.283	9036.32121	10019.9959	16666.3532	17038.4308	16575.5804	18818.5605	18046.7679	17614.4418
187	Syringoyl-D-Glucose	C15H20O10	Phenolic acids	Phenolic acids	-	359.1	239.06	360.1056	[M-H]-	15818.286	21315.6371	9937.89381	15159.7467	12275.6394	12598.027	20527.8088	9218.72636	20454.8778
188	1-O-p-Cumaroylglycerol	C12H14O5	Phenolic acids	Phenolic acids	106055-11-2	237.08	163.04	238.0841	[M-H]-	8891.55885	9941.6436	5830.98664	8259.15299	15497.2531	8438.88999	14721.719	17562.6505	16799.8852
189	2-Naphthol*	C10H8O	Phenolic acids	Phenolic acids	135-19-3	143.05	115.05	144.0575	[M-H]-	14285.7863	12955.04	17856.4894	13068.471	15206.9387	13758.2945	14016.6575	14596.5811	12200.5977
190	1-Naphthol*	C10H8O	Phenolic acids	Phenolic acids	90-15-3	143.05	115.06	144.0575	[M-H]-	17273.6788	12098.9792	10995.3345	8904.12352	10125.0734	13496.2797	11733.0252	15721.6292	12272.1884
191	3-(3-Hydroxyphenyl)-3-hydroxypropanoic acid	C9H10O4	Phenolic acids	Phenolic acids	3247-75-4	181.05	121.03	182.0579	[M-H]-	28301.6598	30866.0182	36936.8576	17946.5169	13417.7803	15960.0078	16562.4768	9053.81698	11896.1351
192	Gallacetophenone	C8H8O4	Phenolic acids	Phenolic acids	528-21-2	169.05	65.03	168.0423	[M+H]+	9341.41236	5125.72107	13767.2202	9	9	9	8447.29501	6859.86122	10110.0637
193	Phenethyl caffeate	C17H16O4	Phenolic acids	Phenolic acids	104594-70-9	283.1	135.04	284.1049	[M-H]-	10402.5147	10123.1402	11298.5735	8067.88032	8571.06107	7802.19458	6191.75717	8272.36413	6300.39923
194	Leonuriside A	C14H20O9	Phenolic acids	Phenolic acids	121748-12-7	331.1	108.02	332.1107	[M-H]-	4088.68573	4807.08808	3929.98908	3593.34564	4186.77407	4397.67368	5706.53577	6142.8583	4825.7476
195	1-O-Galloyl-2-O-Cinnamoyl-β-D-glucose	C22H22O11	Phenolic acids	Phenolic acids	56994-83-3	461.11	169.01	462.1162	[M-H]-	4310.65203	2766.71468	4364.26436	9	9	9	4681.53625	5491.30164	2562.07945
196	Malonyl Tachioside	C16H20O11	Phenolic acids	Phenolic acids	-	387.09	139.04	388.1006	[M-H]-	6872.26003	14005.0833	8063.74126	12474.8571	3972.76234	9	5855.65672	2844.36218	9
197	4-Ethylbenzoic acid*	C9H10O2	Phenolic acids	Phenolic acids	619-64-7	149.06	105.07	150.0681	[M-H]-	3883.29298	2809.8484	4003.77929	2186.35837	2464.80973	3330.54573	1684.09673	2090.98242	2743.12633
198	3,4-Dimethylbenzoic acid*	C9H10O2	Phenolic acids	Phenolic acids	619-04-5	149.06	105.07	150.0681	[M-H]-	3883.29298	2809.8484	4003.77929	2186.35837	2464.80973	3330.54573	1684.09673	2090.98242	2743.12633
199	3-hydroxybenzaldehyde	C7H6O2	Phenolic acids	Phenolic acids	100-83-4	123.04	77.04	122.0368	[M+H]+	74598.9366	87853.8471	170774.783	9	9	9	9	9	9
200	Apigenin-6-C-glucoside (Isovitexin)*	C21H20O10	Flavonoids	Flavones	38953-85-4	431.1	311.05	432.1056	[M-H]-	5836585.11	5792391.39	5209346.87	6884193.76	6177770.95	6488187.08	8853498.12	7226531.14	11557314.4
201	5,7,3',4',5'-Pentahydroxyflavan (Tricetiflavan)	C15H14O6	Flavonoids	Flavanols	-	289.07	151.04	290.079	[M-H]-	9247063.21	9100485.18	7791423.02	7441375.48	6727153.01	7515780.73	8022417.18	6840810.24	9675293.05
202	Vitexin-2''-O-rhamnoside	C27H30O14	Flavonoids	Flavones	64820-99-1	579.17	433.11	578.1636	[M+H]+	6478980.53	6523577.62	6053909.26	5453621.92	5644332.48	6335858.9	7182740.92	6940084.9	7422218.68
203	Apigenin-8-C-Glucoside (Vitexin)*	C21H20O10	Flavonoids	Flavones	3681-93-4	433.11	313.07	432.1056	[M+H]+	3794268.41	3481811.68	3517331.35	4316052.21	4284778.89	4492679.19	5491907.58	5786141.9	6810794.54
204	2'-Hydroxy-3,4,5,4',6'-pentamethoxychalcone	C20H22O7	Flavonoids	Chalcones	-	375.14	357.13	374.1366	[M+H]+	5813234.72	5920839.24	5037332.37	5669146.89	5679887.12	5461024.7	5077916.41	5604779.31	5502196.22
205	Quercetin-3-O-glucoside (Isoquercitrin)*	C21H20O12	Flavonoids	Flavonols	482-35-9	463.09	300.03	464.0955	[M-H]-	421057.313	446645.47	263769.876	1212120.92	1032665.45	1402252.61	3713237.53	3512582.88	4708750.8
206	3,5,7,3'4'-Pentamethoxyflavone	C20H20O7	Flavonoids	Flavones	1247-97-8	373.13	343.08	372.1209	[M+H]+	3712089.73	3217023.67	3371860.49	3481562.06	3271371.66	3580872.09	3541029.91	3554488.77	3718483.73
207	Kaempferol-3-O-robinobioside(Biorobin)	C27H30O15	Flavonoids	Flavonols	17297-56-2	593.15	285.04	594.1585	[M-H]-	1860308.54	1763558.85	1254703.28	2294989.15	2186037.01	1879017.57	2982260.31	3097500.8	3858842.35
208	Quercetin-4'-O-glucoside (Spiraeoside)*	C21H20O12	Flavonoids	Flavonols	20229-56-5	463.09	301.04	464.0955	[M-H]-	450519.092	426162.926	320578.55	1018447.34	1006256.02	1102172.2	2888189.87	2889136.48	4055777.68

209	Hesperetin-5-O-glucoside	C22H24O11	Flavonoids	Flavanones	69651-80-5	463.12	301.07	464.1319	[M-H]-	455748.531	529312.347	341796.548	1028142.43	1008044.13	1111913.27	2688568.49	2834596.69	3880119
210	Quercetin-7-O-glucoside*	C21H20O12	Flavonoids	Flavonols	491-50-9	463.09	301.04	464.0955	[M-H]-	452057.822	445017.272	272312.892	892933.843	826908.124	1180745.7	2491273.46	2507147.37	3691012.63
211	Quercetin 3-xylosyl-(1->6)-glucoside	C26H28O16	Flavonoids	Flavones	-	595.14	134.05	596.137735	[M-H]-	1371754.41	1081944.86	1340157.67	1415160.4	1304481.21	1440066.33	2511555.3	2572278.21	2210860.43
212	Gallocatechin 3-O-gallate*	C22H18O11	Flavonoids	Flavanols	5127-64-0	457.08	169.01	458.0849	[M-H]-	1341849.05	803428.136	888131.166	2267294.22	1977962.24	2014408.23	1943235.25	2155624.37	2045512.92
213	4'-O-Glucosylvitexin	C27H30O15	Flavonoids	Flavones	38950-94-6	595.17	433.12	594.1585	[M+H]+	1908101	2035668.27	1914801.15	1897242	1727236.73	1995618.18	1912882.2	1960299.81	2004628.02
214	Kaempferol-7-O-glucoside*	C21H20O11	Flavonoids	Flavonols	16290-07-6	447.09	285.04	448.1006	[M-H]-	303188.176	305734.892	247274.819	698574.801	638674.174	732649.002	1596767.78	1743625.48	2301864.76
215	Kaempferol-3-O-galactoside (Trifolin)*	C21H20O11	Flavonoids	Flavonols	23627-87-4	447.09	285.04	448.1006	[M-H]-	321004.479	305908.575	213722.393	686313.416	615340.738	761976.392	1627863.71	1528297.64	2264533.45
216	Quercetin-3-O-robinobioside	C27H30O16	Flavonoids	Flavonols	52525-35-6	609.15	300.03	610.1534	[M-H]-	678256.876	726892.212	541386.57	840664.061	779403.879	916269.372	1397347.77	1415233.34	1511621.39
217	Luteolin-4'-O-glucoside*	C21H20O11	Flavonoids	Flavones	6920-38-3	449.11	287.05	448.1006	[M+H]+	939965.77	861731.742	600392.947	1222739.83	1127253.31	893579.175	1267243.61	1590345.82	1329505.03
218	Kaempferol-3-O-glucoside (Astragalin)*	C21H20O11	Flavonoids	Flavonols	480-10-4	449.1078	287.0553	448.1006	[M+H]+	927220.27	840695.168	751285.006	840198.244	837901.11	872426.212	633001.838	1456413.66	1918861.67
219	Epicatechin*	C15H14O6	Flavonoids	Flavanols	490-46-0	291.0863	139.0397	290.079	[M+H]+	1506755.68	1381641.25	1289976.52	1070080.88	1058108.46	1123042.14	1200705.73	1107058.49	1337390.45
220	Kaempferol-4'-O-glucoside*	C21H20O11	Flavonoids	Flavonols	-	449.11	287.06	448.1006	[M+H]+	667303.552	827759.447	632765.889	751084.088	639730.857	1064282.28	823546.88	808504.971	1852982.48
221	Quercetin-3-O-rutinoside (Rutin)	C27H30O16	Flavonoids	Flavonols	153-18-4	609.15	301.04	610.1534	[M-H]-	572950.012	490353.212	391357.203	771459.519	645255.724	602315.463	1041467.82	1008284.22	1302361.87
222	Isohemiphloin	C21H22O10	Flavonoids	Flavanones	3682-02-8	433.11	313.07	434.1213	[M-H]-	1076164.53	989065.023	1152685.77	1251644.03	973290.589	1002998.44	1084672.8	1028849.74	1047747.16
223	Taxifolin-3'-O-glucoside*	C21H22O12	Flavonoids	Flavanonols	31106-05-5	465.13	303.05	466.1111	[M-H]-	633476.852	542042.692	537202.355	672062.595	651898.233	760872.729	1017922.16	997527.923	1114865.47
224	1,8-dihydroxy-4,5-dimethoxy-3- [[(2s,3r,4s,5s,6r)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy] xanthen-9-one*	C21H22O12	Flavonoids	Other Flavonoids	-	465.1	303.05	466.1111	[M-H]-	566317.374	593562.085	564520.955	741938.24	660482.932	633920.978	999574.541	807933.597	1154453.7
225	Isovitexin-2"-O-rhamnoside	C27H30O14	Flavonoids	Flavones	-	579.17	313.07	578.1636	[M+H]+	866414.131	898738.222	1010474.56	850749.466	953400.384	884558.049	968164.956	981412.883	961340.845
226	Quercetin-5-O-β-D-glucoside*	C21H20O12	Flavonoids	Flavonols	-	465.1	303.05	464.0955	[M+H]+	45547.113	223357.746	52420.8654	51853.607	261755.79	119535.977	1223228.62	462232.857	1005375.81
227	3,4,2',4',6'-Pentahydroxychalcone	C15H12O6	Flavonoids	Chalcones	73692-51-0	289.07	163.04	288.0634	[M+H]+	1001597.46	873981.243	636644.372	501899.369	555207.997	602992.732	923575.883	829700.252	855243.349
228	Epicatechin glucoside	C21H24O11	Flavonoids	Flavanols	-	451.12	289.07	452.1319	[M-H]-	1484760.19	1255589.71	158429.246	1093178.16	69252.9855	1024562.77	104607.513	1121044.75	1210074.53
229	Isosaponarin(Isovitexin-4'-O-glucoside)	C27H30O15	Flavonoids	Flavones	19416-87-6	595.17	313.07	594.1585	[M+H]+	711597.206	694321.3	738377.34	663937.095	603569.848	723885.365	726034.916	821342.233	768824.303
230	Apigenin-6-C-(2"-glucuronyl)xyloside	C26H26O15	Flavonoids	Flavones	-	579.13	283.06	578.1272	[M+H]+	775172.137	648034.494	754237.46	746799.563	504238.143	657899.383	639707.302	664011.8	851045.576
231	Naringenin-4'-O-glucoside*	C21H22O10	Flavonoids	Flavanones	-	433.12	271.06	434.1213	[M-H]-	520345.862	502233.971	538413.582	641616.596	573160.398	597089.1	634969.712	726860.122	762040.687
232	Quercetin-3-O-galactoside (Hyperin)*	C21H20O12	Flavonoids	Flavonols	482-36-0	465.1	303.06	464.0955	[M+H]+	47752.0677	87093.3459	103810.889	97602.4412	187106.517	341454.76	570531.5	539067.655	993533.223
233	Isohyperoside*	C21H20O12	Flavonoids	Flavonols	35589-21-0	465.1019	303.0613	464.0955	[M+H]+	47752.0677	87093.3459	103810.889	97602.4412	187106.517	341454.76	570531.5	539067.655	993533.223
234	Tricin-7-O-Glucoside*	C23H24O12	Flavonoids	Flavones	32769-01-0	493.13	331.08	492.1268	[M+H]+	372456.865	295201.575	229996.45	356320.833	366148.605	428503.241	606027.932	600641.881	893746.1
235	Butin-7-O-glucoside*	C21H22O10	Flavonoids	Flavanones	-	433.11	271.06	434.1213	[M-H]-	557497.21	531237.545	461234.855	608051.827	571661.816	608179.001	696379.512	669752.543	700753.71
236	Apigenin-6,8-di-C-arabinoside*	C25H26O13	Flavonoids	Flavones	-	535.14	499.12	534.1373	[M+H]+	280789.028	232218.082	237742.066	331725.158	278345.886	366898.877	591020.457	747719.467	706862.414
237	Luteolin-7-O-glucoside (Cynaroside)*	C21H20O11	Flavonoids	Flavones	5373-11-5	449.11	287.07	448.1006	[M+H]+	751454.992	745490.243	673975.821	756535.887	813354.635	889618.969	1123256.69	204029.984	622022.144
238	Apigenin-6-C-arabinoside-8-C-xyloside*	C25H26O13	Flavonoids	Flavones	-	535.14	499.12	534.1373	[M+H]+	233154.294	200923.356	142325.856	318267.061	297703.044	291924.217	558817.046	544011.435	722476.652
239	Jaceosidin-7-O-Glucoside*	C23H24O12	Flavonoids	Flavones	25474-11-7	493.14	331.08	492.1268	[M+H]+	312085.076	291704.138	204325.993	300853.502	343062.752	412460.939	525550.497	458339.847	705757.633
240	Apigenin-6-C-(2"-glucosyl)arabinoside	C26H28O14	Flavonoids	Flavones	-	565.16	427.1	564.1479	[M+H]+	497919.496	432943.242	390366.69	526285.349	577932.497	515247.615	590617.04	559363.254	534182.443
241	Isoschaftoside	C26H28O14	Flavonoids	Flavones	52012-29-0	565.16	409.09	564.1479	[M+H]+	530183.403	465530.138	385933.646	456993.672	464112.649	504119.389	495918.931	530111.726	622044.972
242	6-C-Glucosyl-2-Hydroxynaringenin	C21H22O11	Flavonoids	Flavanones	-	449.11	269.05	450.1162	[M-H]-	622605.705	592203.539	580460.878	509786.007	503945.026	518470.013	532900.638	472169.728	580890.756
243	Dihydrokaempferide	C16H14O6	Flavonoids	Flavanonols	137225-59-3	303.09	229.08	302.079	[M+H]+	117396.499	103089.214	46845.3147	182132.706	204947.162	216551.27	405379.433	479405.108	667434.72
244	Luteolin-3'-O-glucoside*	C21H20O11	Flavonoids	Flavones	-	449.11	287.06	448.1006	[M+H]+	130910.861	207164.836	78585.6587	150759.481	238609.228	383656.371	456053.283	366829.487	713858.377
245	Aromadendrin-7-O-glucoside*	C21H22O11	Flavonoids	Flavanonols	28189-90-4	449.11	287.06	450.1162	[M-H]-	592612.88	554614.122	516828.33	465993.459	464400.414	445071.465	534298.052	547507.708	431856.211
246	1,3,6,7-tetrahydroxy-2-(3,4,5-trihydroxyoxan-2-yl)xanthen-9-one	C18H16O10	Flavonoids	Other Flavonoids	-	391.07	229.05	392.0743	[M-H]-	495270.985	537092.724	458337.69	583264.968	537063.024	582548.694	313809.196	841470	210597.376
247	Chrysoeriol-5-O-glucoside	C22H22O11	Flavonoids	Flavones	-	461.11	299.1	462.1162	[M-H]-	83106.0587	77629.9028	66624.5139	175186.703	142297.016	183497.46	414026.924	412310.032	508464.314
248	Eriodictyol-8-C-glucoside*	C21H22O11	Flavonoids	Flavanones	1023271-51-3	449.11	287.06	450.1162	[M-H]-	491374.041	457508.751	511191.619	405982.912	430345.385	384586.878	481862.318	437316.705	399574.779
249	1,2,3,7,8-pentahydroxy-6-methylanthracene-9,10-dione	C15H10O7	Flavonoids	Other Flavonoids	-	303.05	229.05	302.0427	[M+H]+	99831.9101	85280.9251	51441.5114	133382.123	80641.8851	133614.942	340836.461	355545.155	609335.195
250	1,2,4,5-tetrahydroxy-7-(hydroxymethyl)anthracene-9,10-dione	C15H10O7	Flavonoids	Other Flavonoids	-	303.05	229.05	302.0427	[M+H]+	140537.646	139785.902	118658.31	178106.834	149577.533	192621.764	364150.811	338671.738	540749.444

251	2'-Hydroxy-3,4,5,3',4',6'-hexameth-oxychalcone	C21H24O8	Flavonoids	Chalcones	-	405.15	387.14	404.1471	[M+H]+	461340.971	501929.585	459878.425	399944.705	464528.849	406576.569	403962.77	463542.684	367149.076
252	Apigenin-6-C-(2"-xylosyl)glucoside*	C26H28O14	Flavonoids	Flavones	-	565.16	433.11	564.1479	[M+H]+	333743.418	346698.584	405872.942	381196.348	335812.312	251681.648	310452.964	341231.102	399143.571
253	Mearnsetin	C16H12O8	Flavonoids	Flavones	16805-10-0	333.06	153.02	332.0532	[M+H]+	153152.431	291992.32	226961.178	381291.505	332786.77	323218.559	418438.548	109029.971	504862.359
254	Apigenin-7-O-glucuronide	C21H18O11	Flavonoids	Flavones	29741-09-1	447.09	271.06	446.0849	[M+H]+	518265.124	430714.857	517346.844	286423.858	422921.324	391866.854	340021.946	376875.851	280110.448
255	Luteolin-8-C-glucoside (Orientin)*	C21H20O11	Flavonoids	Flavones	28608-75-5	449.11	299.05	448.1006	[M+H]+	182824.284	231396.652	136379.477	271656.438	262619.889	242788.072	156291.498	381753.157	446422.275
256	Dihydrocharcone-4'-O-glucoside	C21H24O10	Flavonoids	Chalcones	-	435.13	273.08	436.1369	[M-H]-	137271.818	183443.787	160008.404	228598.192	200516.464	187068.002	313584.351	261320.753	390943.699
257	Epiafzelechin	C15H14O5	Flavonoids	Flavanols	24808-04-6	275.09	107.05	274.0841	[M+H]+	393945.359	388790.051	414289.855	285267.712	254858.22	293407.883	298323.343	279155.115	384507.511
258	Apigenin-6-C-xyloside-8-C-arabinoside	C25H26O13	Flavonoids	Flavones	-	535.14	517.13	534.1373	[M+H]+	243352.264	327854.022	161821.33	297092.592	74768.5436	214703.327	274032.53	332926.779	348482.981
259	Myricetin-3-O-β-D-glucoside*	C21H20O13	Flavonoids	Flavonols	19833-12-6	481.1	319.04	480.0904	[M+H]+	45864.2363	20217.0018	36986.9134	48819.5046	61128.6154	121946.415	222404.131	169910.077	555107.598
260	Phloretin-2'-O-glucoside (Phlorizin)	C21H24O10	Flavonoids	Chalcones	60-81-1	435.13	167.04	436.1369	[M-H]-	140831.342	158222.236	136766.89	204430.175	188087.713	204755.088	322098.32	280008.762	328650.6
261	Dihydrokaempferol-7-O-glucoside*	C21H22O11	Flavonoids	Flavanonols	-	449.11	287.06	450.1162	[M-H]-	178359.169	153127.003	274837.171	216656.058	211060.127	391223.755	259445.103	306358.019	339852.767
262	Isovitexin-2"-O-xyloside	C26H28O14	Flavonoids	Flavones	-	565.15	433.11	564.1479	[M+H]+	320092.802	307896.351	316389.038	263515.588	282668.46	320066.567	282180.369	295158.025	322562.985
263	Vitexin-2"-O-xyloside*	C26H28O14	Flavonoids	Flavones	-	565.16	433.11	564.1479	[M+H]+	312324.93	282348.002	339424.693	287345.572	241923.167	263937.956	283958.246	279456.039	296647.454
264	Kaempferol-3-O-rutinoside(Nicotiflorin)*	C27H30O15	Flavonoids	Flavonols	17650-84-9	595.17	287.05	594.1585	[M+H]+	194030.598	233574.715	228124.942	148185.587	513689.669	281698.147	137908.887	189417.606	486766.043
265	Apigenin-5-O-glucoside	C21H20O10	Flavonoids	Flavones	28757-27-9	433.11	271.06	432.1056	[M+H]+	142250.657	205073.595	121645.775	193535.33	187499.301	156103.74	312343.742	244391.249	235727.368
266	Myricetin-3-O-galactoside*	C21H20O13	Flavonoids	Flavonols	15648-86-9	481.1	319.06	480.0904	[M+H]+	56549.4511	83095.0938	59535.1425	101139.214	74857.9555	149763.993	193494.252	219157.717	338783.025
267	Naringenin-7-O-glucoside (Prunin)*	C21H22O10	Flavonoids	Flavanones	529-55-5	433.11	271.07	434.1213	[M-H]-	234261.876	221115.459	236194.716	320062.667	208092.491	215626.661	184461.941	310806.95	251312.874
268	Luteolin-7-O-neohesperidoside (Lonicerin)*	C27H30O15	Flavonoids	Flavones	25694-72-8	595.17	287.06	594.1585	[M+H]+	205449.911	245848.105	74343.9845	167207.372	129873.83	146593.835	122647.121	179136.041	409344.021
269	Luteolin-7-O-rutinoside*	C27H30O15	Flavonoids	Flavones	3563-98-2	595.17	287.06	594.1585	[M+H]+	205449.911	245848.105	74343.9845	167207.372	129873.83	146593.835	122647.121	179136.041	409344.021
270	Kaempferol-3-O-glucorhamnoside*	C27H30O15	Flavonoids	Flavonols	40437-72-7	595.17	287.06	594.1585	[M+H]+	205449.911	245848.105	74343.9845	167207.372	129873.83	146593.835	122647.121	179136.041	409344.021
271	Apigenin-6,8-di-C-glucoside (Vicenin-2)	C27H30O15	Flavonoids	Flavones	23666-13-9	595.17	457.13	594.1585	[M+H]+	207100.221	209770.579	213172.595	177385.092	174279.653	235012.193	223153.974	220554.101	240129.397
272	Quercetin-3-O-glucoside-7-O-rhamnoside*	C27H30O16	Flavonoids	Flavonols	-	611.16	303.05	610.1534	[M+H]+	46238.9091	40814.9306	58613.484	202471.985	130829.77	97312.7206	98857.2499	121877.482	462935.175
273	Quercetin-7-O-rutinoside*	C27H30O16	Flavonoids	Flavonols	147714-62-3	611.1607	303.0499	610.1534	[M+H]+	91716.0438	85653.284	81972.6981	137539.152	91566.7258	128019.286	196899.24	243087.218	213331.446
274	Quercetagetin-7-O-glucoside(Quercetagitrin)*	C21H20O13	Flavonoids	Flavonols	548-75-4	481.1	319.05	480.0904	[M+H]+	131275.1	105591.389	67338.1193	132081.438	156735.326	154318.766	199203.469	202883.456	248545.427
275	4,4'-dihydroxy-2'-methoxychalcone	C16H14O4	Flavonoids	Chalcones	-	271.1	121.03	270.0892	[M+H]+	373165.643	113626.514	304896.584	323391.397	32721.4925	280488.341	225673.632	184978.014	228500.675
276	Apigenin-4'-O-glucoside*	C21H20O10	Flavonoids	Flavones	-	433.11	271.07	432.1056	[M+H]+	151513.213	65636.2796	107375.948	97716.0391	145530.175	183786.789	205160.597	183971.948	246829.243
277	Apigenin-8-C-Arabinoside	C20H18O9	Flavonoids	Flavones	-	403.1	367.08	402.0951	[M+H]+	166592.782	132214.498	85536.6441	157509.263	137931.983	61446.8169	152884.876	278600.49	193832.625
278	Galangin-7-O-glucoside*	C21H20O10	Flavonoids	Flavones	-	433.11	271.06	432.1056	[M+H]+	171821.23	140057.692	110986.612	174601.944	111519.953	180409.42	227286.311	180786.036	211064.593
279	Apigenin-8-C-(2"-glucosyl)arabinoside	C26H28O14	Flavonoids	Flavones	-	565.16	457.11	564.1479	[M+H]+	213559.553	145149.098	143954.609	179008.255	137104.851	141929.544	211773.368	210031.938	162093.227
280	Eriodictyol-3'-O-glucoside*	C21H22O11	Flavonoids	Flavanones	-	449.11	287.06	450.1162	[M-H]-	69223.5614	99956.4194	116992.639	127147.955	104770.605	105182.969	188511.808	176912.536	216914.182
281	3',4',5',5,7-Pentamethoxyflavone*	C20H20O7	Flavonoids	Flavones	53350-26-8	373.13	343.08	372.1209	[M+H]+	119970.617	143959.673	137743.252	187173.776	172325.533	181431.417	195295.553	191651.57	195019.047
282	3',5',5,7-Tetrahydroxy-4'-methoxyflavanone-3'-O-glucoside	C22H24O12	Flavonoids	Flavones	-	481.13	319.05	480.1268	[M+H]+	114247.164	53326.8325	46812.561	134634.88	91223.3085	132293.528	193731.241	159080.079	228011.961
283	Gallocatechin gallate*	C22H18O11	Flavonoids	Flavanols	4233-96-9	459.09	139.04	458.0849	[M+H]+	115079.263	69377.5915	55648.551	103940.497	126203.89	145878.846	119226.36	209919.923	213158.256
284	Naringenin-7-O-Neohesperidoside(Naringin)*	C27H32O14	Flavonoids	Flavanones	10236-47-2	579.17	271.06	580.1792	[M-H]-	183871.467	141474.019	174962.127	164659.39	151180.855	167097.914	163678.845	183609.215	169807.453
285	7-Hydroxyflavanone	C15H12O3	Flavonoids	Flavanones	6515-36-2	239.07	207.04	240.078644	[M-H]-	300403.383	87211.5257	78277.4914	115661.647	78907.1284	88319.38	106834.877	131268.209	273073.026
286	7-Benzyloxy-5-hydroxy-3',4'-methylenedioxyflavonoid	C23H16O6	Flavonoids	Flavones	-	387.16	207.1	388.0947	[M-H]-	97510.3762	126543.989	102294.58	133091.104	165926.919	142022.358	154283.928	169114.981	168923.368
287	Quercetin-3-O-(4"-O-glucosyl)rhamnoside*	C27H30O16	Flavonoids	Flavonols	59262-54-3	611.16	303.05	610.1534	[M+H]+	274511.249	132977.267	40022.4299	117124.239	15301.0333	261303.096	173250.348	203671.382	110811.39
288	Epigallocatechin-3-O-gallate*	C22H18O11	Flavonoids	Flavanols	989-51-5	459.09	139.04	458.0849	[M+H]+	115580.939	52967.4908	40147.324	115489.322	117676.104	83886.4975	127104.577	144187.455	201328.996
289	kaempferol-3-p-coumaroyldiglucoside	C36H36O18	Flavonoids	Flavonols	-	755.19	285.04	756.1902	[M-H]-	117268.522	105668.494	100560.487	138508.322	114224.666	117403.205	148034.43	157017.801	158452.893
290	Quercetin-3-O-arabinoside	C20H18O11	Flavonoids	Flavonols	22255-13-6	433.08	300.03	434.0849	[M-H]-	3838.1627	17635.6479	9095.33105	34482.5626	26288.4918	34445.9846	136090.317	121103.935	198967.017
291	4'-Hydroxy-3,5-dimethoxydihydrochalcone	C17H18O4	Flavonoids	Chalcones	-	287.14	121.03	286.1205	[M+H]+	94078.3358	119871.505	134773.478	153516.792	195221.756	111565.504	150739.285	179181.771	111027.07
292	Rhamnazine-5-O-β-D-glucoside*	C24H26O12	Flavonoids	Flavones	-	507.15	345.1	506.1419	[M+H]+	93033.7153	73633.9876	82807.587	126750.55	114897.427	127643.5	130876.683	118234.773	176017.376

293	Luteolin-6-C-glucoside-7-O-rhamnoside	C27H30O15	Flavonoids	Flavones	-	595.17	449.11	594.1585	[M+H]+	118858.254	121668.979	101996.977	149322.783	126447.192	101613.702	158214.551	110627.576	144162.578
294	Delphinidin-3-O-galactoside	C21H21O12+	Flavonoids	Anthocyanidins	28500-00-7	465.1	303.05	465.1028	[M]+	97899.5241	97108.4852	78717.0358	101695.214	113309.681	107411.862	136035.243	134774.758	140515.839
295	Hispidulin-7-O-glucoside(Homoplantaginin)*	C22H22O11	Flavonoids	Flavones	17680-84-1	463.13	301.09	462.1162	[M+H]+	74284.0295	28251.3965	53761.2333	59559.9335	53436.7424	58319.069	111456.964	122348.595	157087.633
296	3,4,5,3'-tetrahydroxybenzophenone	C13H10O5	Flavonoids	Other Flavonoids	-	247.06	153.02	246.0528	[M+H]+	123950.952	135085.498	149619.428	137421.256	142528.379	122879.803	137059.572	118477.25	125741.885
297	Diosmetin-7-O-glucoside*	C22H22O11	Flavonoids	Flavones	20126-59-4	463.12	301.07	462.1162	[M+H]+	52274.8949	39769.0796	48970.1666	70394.6035	59101.4948	77905.3299	95491.3583	121108.147	162059.019
298	Diosmetin-7-O-galactoside*	C22H22O11	Flavonoids	Flavones	-	463.12	301.07	462.1162	[M+H]+	52274.8949	39769.0796	48970.1666	70394.6035	59101.4948	77905.3299	95491.3583	121108.147	162059.019
299	Luteolin-6-C-glucoside (Isoorientin)*	C21H20O11	Flavonoids	Flavones	4261-42-1	447.09	357.06	448.1006	[M-H]-	69377.4701	65111.5094	49727.0306	88072.9878	70554.7361	88068.6816	112204.053	119074.838	118337.546
300	Eriodictyol-7-O-glucoside*	C21H22O11	Flavonoids	Flavanones	38965-51-4	451.12	289.07	450.1162	[M+H]+	74917.9812	32301.8191	78684.7956	75203.7543	71389.7115	69243.6806	97916.81	75826.9046	122337.84
301	Catechin*	C15H14O6	Flavonoids	Flavanols	154-23-4	291.09	139.04	290.079	[M+H]+	134715.048	110181.163	120004.049	89171.6485	71566.1045	89753.348	93876.467	95924.17	92020.704
302	Isovitexin-8-O-xyloside	C26H28O14	Flavonoids	Flavones	-	565.16	367.1	564.1479	[M+H]+	73595.843	71995.869	67995.2677	62900.8994	64095.4242	82123.5756	81603.1828	92553.8874	98964.8297
303	6-C-MethylKaempferol-3-glucoside*	C22H22O11	Flavonoids	Flavones	-	463.12	301.08	462.1162	[M+H]+	57274.0681	49970.4547	39988.9431	65303.5476	68223.6658	59118.9455	97493.4284	67024.8659	102229.386
304	Catechin gallate*	C22H18O10	Flavonoids	Flavanols	130405-40-2	443.1	139.04	442.09	[M+H]+	30559.198	35595.7972	56399.3813	21572.6801	77363.5532	50919.7879	67238.574	80449.9533	118719.019
305	Apigenin-7-O-rutinoside (Isorhoifolin)*	C27H30O14	Flavonoids	Flavones	552-57-8	579.17	271.04	578.1636	[M+H]+	89566.0018	104186.88	66813.7214	65199.8023	86799.1732	63441.0934	117712.052	65420.3222	76702.2066
306	Kaempferol-3-O-(6"-O-acetyl)glucoside	C23H22O12	Flavonoids	Flavonols	-	489.11	285.04	490.1111	[M-H]-	50196.6508	64710.2501	48558.4423	60651.7585	69240.4941	72248.4054	65389.4748	95090.5272	95387.6855
307	Chrysoeriol-7-O-(6"-acetyl)glucoside	C24H24O12	Flavonoids	Flavones	-	503.12	341.1	504.1268	[M-H]-	168966.426	153913.934	120954.431	102398.761	109280.63	75514.3139	83787.802	82724.499	80535.8994
308	Chrysoeriol-7-O-rutinoside	C28H32O15	Flavonoids	Flavones	-	607.17	299	608.1741	[M-H]-	41223.0104	44567.6314	39992.0865	59658.099	52114.7574	56040.9361	86453.4529	71329.2647	81526.5165
309	Dihydromyricetin (Ampelopsin)	C15H12O8	Flavonoids	Flavanonols	27200-12-0	319.05	301.04	320.0532	[M-H]-	43107.95	35213.6558	55349.8069	61164.5416	63143.2225	68322.9338	81781.2383	77063.7588	69194.6394
310	Dihydrokaempferol-3-O-glucoside*	C21H22O11	Flavonoids	Flavanonols	31049-08-8	451.12	289.08	450.1162	[M+H]+	65723.8744	54675.0966	56859.8784	62591.6985	68038.6401	110416.262	55948.2741	44720.8062	124580.062
311	artemisidin A	C27H30O18	Flavonoids	Flavones	-	643.15	481.1	642.1432	[M+H]+	52767.4093	54467.5738	53299.4166	74664.4195	43647.2465	67022.398	70188.8654	83419.8013	57603.6957
312	3'-O-Methyl-epicatechin	C16H16O6	Flavonoids	Flavanols	76549-34-3	305.1	139.04	304.0947	[M+H]+	47985.7429	51938.0814	49093.5358	49277.8092	38046.3607	38105.728	71690.5957	73930.8451	61142.4155
313	Tangeretin (4',5,6,7,8-Pentamethoxyflavone)*	C20H20O7	Flavonoids	Flavones	481-53-8	373.13	343.09	372.1209	[M+H]+	57571.8427	62834.6383	63727.3309	64967.7315	64116.5773	64855.5106	63353.7977	65493.9684	65944.6512
314	Naringenin-7-O-Rutinoside(Narirutin)*	C27H32O14	Flavonoids	Flavanones	14259-46-2	579.17	271.06	580.1792	[M-H]-	57826.8513	57024.5562	60254.8016	53091.3916	52521.8433	54693.7776	60762.3715	47931.1581	67682.7631
315	3',5,5',7-Tetrahydroxyflavanone-7-O-glucoside*	C21H22O11	Flavonoids	Flavanones	-	451.12	289.07	450.1162	[M+H]+	78069.43	60969.104	75578.9393	99712.7637	60306.0001	78026.5229	47894.4818	52302.0594	74217.1196
316	Nobiletin (5,6,7,8,3',4'-Hexamethoxyflavone)	C21H22O8	Flavonoids	Flavones	478-01-3	403.14	373.1	402.1315	[M+H]+	69056.2354	61222.3504	53705.9941	52163.9743	52188.436	56076.8766	59139.4562	67127.0034	45884.7271
317	Phloretin-4'-O-glucoside (Trilobatin)	C21H24O10	Flavonoids	Chalcones	4192-90-9	435.13	315.09	436.1369	[M-H]-	42139.2155	26037.967	29204.5131	47693.6378	54008.0626	50158.3347	55691.9786	56610.1333	59805.3709
318	Kaempferol-3-O-(6"-malonyl)galactoside*	C24H22O14	Flavonoids	Flavonols	-	535.11	287.05	534.101	[M+H]+	44116.3525	53563.3813	23958.3127	62364.0153	71907.8538	42560.3697	30682.2008	60193.5939	79681.8758
319	Kaempferol-3-O-(6"-malonyl)glucoside*	C24H22O14	Flavonoids	Flavonols	-	535.11	287.05	534.101	[M+H]+	52813.9744	53058.5614	40911.7938	80209.4525	39306.544	49393.0832	46837.9367	46992.7496	76646.9808
320	Mearnsetin-3-O-glucoside	C22H22O13	Flavonoids	Flavones	-	493.1	331.05	494.106	[M-H]-	43819.5506	70378.173	52422.4719	62819.0994	58870.1509	63950.1914	60220.5999	59417.5399	47530.0813
321	7-O-Methylaloesin	C20H24O9	Flavonoids	Other Flavonoids	-	409.15	247.09	408.142	[M+H]+	70653.8655	57409.0471	61642.9678	78664.2274	46785.9471	34375.9376	17797.7475	69459.8246	77496.4592
322	7-Methoxy-3-[1-(3-pyridyl)methylidene]-4-chromanone	C16H13NO3	Flavonoids	Other Flavonoids	-	268.103	136.0607	267.089543	[M+H]+	15637.5391	15567.4503	14743.6227	25728.3686	22253.2267	22519.6441	60399.64	52106.736	49885.0175
323	Kaempferol-7-O-rhamnoside*	C21H20O10	Flavonoids	Flavonols	20196-89-8	431.1	285.04	432.1056	[M-H]-	6200.01583	5497.19546	5191.73057	12616.8573	12188.2078	19606.7336	45087.4413	50242.1265	59120.0665
324	Isorhamnetin-3-O-gallate	C23H16O11	Flavonoids	Flavonols	-	469.12	317.08	468.0693	[M+H]+	55051.558	42742.2741	41459.0829	43368.3115	44754.9672	55145.8486	51209.5935	51676.8572	51427.18
325	Luteolin-7-O-(6"-malonyl)glucoside*	C24H22O14	Flavonoids	Flavones	-	535.11	287.05	534.101	[M+H]+	77686.8273	51427.6806	45550.3073	65196.7252	46041.36	56160.7919	47264.6442	57124.7214	37657.0559
326	Kaempferol-3-O-rhamnoside (Afzelin)(Kaempferin)*	C21H20O10	Flavonoids	Flavonols	482-39-3	431.1	285.04	432.1056	[M-H]-	2064.07716	2037.10358	5377.79918	16352.6692	13742.9433	14468.611	34165.5006	44782.9984	61369.0685
327	Epitheaflavic acid-3-O-Gallate	C28H20O14	Flavonoids	Flavanols	34218-97-8	579.08	289.07	580.0853	[M-H]-	58956.2515	86561.6577	25415.4232	18284.9863	50533.795	16751.267	28897.9763	65394.7847	34886.4427
328	Myricetin-3-(2"-galloyl)rhamnoside	C28H24O16	Flavonoids	Flavonols	-	617.11	471.06	616.106435	[M+H]+	74262.0494	14735.4005	11818.3397	16586.512	24351.1354	16191.3625	50563.4585	37539.1711	37525.0182
329	Apigenin-7-O-(6"-p-Coumaryl)glucoside	C30H26O12	Flavonoids	Flavones	-	579.15	271.06	578.1424	[M+H]+	32069.0113	33456.3918	38987.3449	47313.8694	33534.2607	44897.8755	26101.8675	52080.274	44597.2345
330	Quercetin-3,7-Di-O-glucoside	C27H30O17	Flavonoids	Flavonols	-	627.14	303.05	626.1483	[M+H]+	46718.9111	26073.058	25140.208	39909.0657	35241.0746	45049.852	32215.3516	42862.3812	38040.9937
331	5,6,7,4'-Tetramethoxyflavone	C19H18O6	Flavonoids	Flavones	1168-42-9	343.12	282.09	342.1103	[M+H]+	37934.9839	36822.7904	47959.0356	28220.1048	33862.0662	38746.6429	38953.0043	37501.3694	34022.2974
332	3'-O-Methyltricetin-7-O-(6"-malonyl)glucoside*	C25H24O15	Flavonoids	Flavones	-	565.12	317.07	564.1115	[M+H]+	164016.026	140763.168	239354.557	65283.2	136255.603	87391.9354	14899.3026	47736.4379	43012.3947
333	Tamarixetin-3-O-(6"-malonyl)glucoside*	C25H24O15	Flavonoids	Flavonols	-	565.12	317.07	564.1115	[M+H]+	164016.026	140763.168	239354.557	65283.2	136255.603	87391.9354	14899.3026	47736.4379	43012.3947
334	Hispidulin-8-C-glucoside*	C22H22O11	Flavonoids	Flavones	-	463.13	343.09	462.1162	[M+H]+	24014.9199	18233.5228	28867.3819	34650.5936	23269.2989	19238.1771	39516.6609	23417.5946	42673.8439

335	Chrysoeriol-8-C-glucoside (Scoparin)*	C22H22O11	Flavonoids	Flavones	301-16-6	463.11	343.08	462.1162	[M+H]+	10553.4928	14519.0271	10784.839	52419.0769	25198.7601	20291.3849	24900.7101	50658.3432	25303.21
336	Rhamnazine-4'-O-β-D-glucoside*	C24H26O12	Flavonoids	Flavones	-	507.15	345.1	506.1419	[M+H]+	21565.7692	22842.8181	29386.1404	40488.5714	34906.941	41614.1831	28821.4132	33197.2494	32764.5433
337	Sieboldin	C21H24O11	Flavonoids	Chalcones	18777-73-6	451.12	289.07	452.1319	[M-H]-	23199.7445	12417.5251	8915.89364	29435.6484	17675.1531	25671.9541	34402.352	23617.3162	30083.386
338	Apigenin-7-O-neohesperidoside (Rhoifolin)*	C27H30O14	Flavonoids	Flavones	17306-46-6	579.17	271.06	578.1636	[M+H]+	31089.3852	8592.06649	15180.6318	8467.02693	13992.3509	19611.0495	18641.2267	26386.1989	41519.2995
339	6-Hydroxykaempferol-3,6-O-Diglucoside	C27H30O17	Flavonoids	Flavonols	-	627.16	303.1	626.1483	[M+H]+	9378.24552	19006.0394	10949.4837	23946.1366	21136.9694	20612.5065	38907.6407	9014.95649	33905.9583
340	Epicatechin-4'-O-β-D-glucopyranoside*	C21H24O11	Flavonoids	Flavanols	-	451.13	289.07	452.1319	[M-H]-	36464.7201	37717.9766	30761.739	22224.3165	26117.984	27157.3452	26857.5879	26602.827	25419.6073
341	Tricin-7-O-saccharic acid	C23H22O14	Flavonoids	Flavones	-	521.09	329.2	522.101	[M-H]-	8147.95387	21293.4576	12358.012	14111.0258	19617.6594	16793.4572	11644.2195	37574.8599	29367.339
342	Epicatechin-6-C-β-D-glucopyranoside*	C21H24O11	Flavonoids	Flavanols	-	451.1263	289.0729	452.1319	[M-H]-	21396.4475	18733.1194	19658.5161	18794.9103	21220.397	18616.2351	25366.5401	26001.2564	23635.1516
343	Gallocatechin*	C15H14O7	Flavonoids	Flavanols	970-73-0	307.08	139.04	306.074	[M+H]+	36391.8485	12862.8025	6004.1815	45507.143	36682.376	34801.9405	27168.7485	24403.9005	21254.164
344	3,3',4',5,6,7,8-Heptahydroxyflavan	C15H14O8	Flavonoids	Flavanols	-	323.07	139.04	322.0689	[M+H]+	34220.1034	27759.7684	16752.3801	16801.0535	28411.9656	31358.0913	28977.7489	19948.9315	22860.6842
345	Quercetin	C15H10O7	Flavonoids	Flavonols	117-39-5	303.05	137.02	302.0427	[M+H]+	28697.8374	16963.9398	23908.4459	29396.3357	20734.8896	12080.9084	23506.0789	23841.707	21758.04
346	Afzelechin (3,5,7,4'-Tetrahydroxyflavan)	C15H14O5	Flavonoids	Flavanols	2545-00-8	275.09	139.04	274.0841	[M+H]+	26661.1337	14404.586	18189.1199	26970.21	12079.5251	22670.1973	21361.0565	21822.253	20789.0661
347	Epicatechin-3'-O-β-D-glucopyranoside*	C21H24O11	Flavonoids	Flavanols	-	451.13	289.07	452.1319	[M-H]-	20753.4056	16888.5214	21926.4553	15057.0392	19317.7819	19741.0032	24089.8739	19226.0095	18364.0401
348	catechin-4-β-D-galactopyranoside	C21H24O11	Flavonoids	Flavanols	-	451.12	289.07	452.1319	[M-H]-	18914.9285	21202.7597	23804.6914	13982.5777	15858.673	16207.0099	19690.4358	19307.5917	21878.867
349	1,3,7-trihydroxy-2-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]xanthen-9-one	C19H18O10	Flavonoids	Other Flavonoids	-	405.08	243.03	406.09	[M-H]-	14549.4396	17460.1073	14728.69	17629.508	16191.8938	11363.3609	16871.6647	23972.2582	16700.4743
350	2',4'-Dihydroxy-4-methoxychalcone; (E)-Cardamonin	C16H14O4	Flavonoids	Chalcones	19309-14-9	271.1	167.04	270.0892	[M+H]+	18552.8284	19289.5654	21933.7876	14953.9084	20039.1257	17012.395	14033.3264	16686.5836	20712.8673
351	Cyanidin-3-O-rutinoside (Keracyanin)	C27H31O15+	Flavonoids	Anthocyanidins	28338-59-2	595.17	287.06	595.1657	[M]+	10788.6283	5790.79091	2054.6892	17235.7333	12927.2429	9219.39804	18487.6255	24600.0045	7802.33488
352	Quercetin-3-O-(6''-O-acetyl)galactoside	C23H22O13	Flavonoids	Flavonols	-	505.1	300.03	506.106	[M-H]-	7113.04991	4960.10167	13732.459	10065.1301	13680.5075	13692.5365	15396.9666	16691.6428	12077.7319
353	Catechin-5-O-glucoside	C21H24O11	Flavonoids	Flavanols	-	451.12	289.07	452.1319	[M-H]-	12117.8589	10683.1292	10100.4351	10438.711	11957.5942	14814.9699	11540.4429	14146.9041	13366.7694
354	Quercetin-3-O-sophoroside (Baimaside)	C27H30O17	Flavonoids	Flavonols	18609-17-1	627.16	303.06	626.1483	[M+H]+	22512.9695	5745.74029	12028.7823	7790.40721	24923.9107	30120.7377	23728.433	7882.90511	6811.81848
355	3,5,6,7,8,3',4'-Heptamethoxyflavone	C22H24O9	Flavonoids	Flavonols	1178-24-1	433.15	403.11	432.142	[M+H]+	10310.0666	13746.6141	9751.46268	11481.234	12829.242	9143.32287	12701.7427	9279.68354	12209.5241
356	Pinocembrin-7-O-rutinoside*	C27H32O13	Flavonoids	Flavanones	118985-31-2	563.18	255.07	564.1843	[M-H]-	3989.89369	7376.5526	2672.98104	2688.44937	8551.39609	9120.49679	10951.9105	9391.72411	9062.15973
357	Pinocembrin-7-O-neohesperidoside*	C27H32O13	Flavonoids	Flavanones	13241-31-1	563.18	255.07	564.1843	[M-H]-	8257.81235	8287.34314	8217.74044	1754.76405	6762.2251	7186.62045	8633.99445	8967.36356	11314.5668
358	5,7-Dihydroxy-4-methoxyflavone-3-O-xylose-(1-6)-glucose	C27H30O15	Flavonoids	Flavones	-	595.19	127.04	594.1585	[M+H]+	12131.8783	3784.28485	6819.97481	23219.9196	11642.5354	8218.7912	10423.1015	11522.6032	6271.49984
359	Epigallocatechin*	C15H14O7	Flavonoids	Flavanols	970-74-1	307.08	139.04	306.074	[M+H]+	9708.56763	8893.7715	7334.572	6548.424	10558.8503	7306.1745	9387.1695	6260.21029	5141.46439
360	Kaempferol-3-O-(6''-p-Coumaroyl)glucoside (Tiliroside)*	C30H26O13	Flavonoids	Flavonols	20316-62-5	593.13	285.04	594.1373	[M-H]-	2132.73959	3641.81743	1526.27729	1647.00294	9988.92518	2549.97166	4262.86494	8745.46501	4598.6506
361	Luteolin-7-O-(6''-caffeoyl)rhamnoside*	C30H26O13	Flavonoids	Flavones	-	593.1301	285.0399	594.1373	[M-H]-	2132.73959	3641.81743	1526.27729	1647.00294	9988.92518	2549.97166	4262.86494	8745.46501	4598.6506
362	(3R)-5,7-Dihydroxy-8-methyl-3-(2',4'-dihydroxybenzyl)-chroman-4-one	C17H16O6	Flavonoids	Other Flavonoids	-	315.09	125.02	316.0947	[M-H]-	6560.4605	3473.50436	2551.51416	2140.95715	3077.195	10708.0936	4158.80645	2352.07706	9080.24138
363	Neoeriocitrin	C27H32O15	Flavonoids	Flavones	13241-32-2	595.17	459.11	596.1741	[M-H]-	6909.81013	5380.82892	4023.02945	2163.84015	4983.56359	10773.2762	559.113846	4849.36861	7705.40061
364	Kaempferol-6,8-di-C-glucoside	C27H30O16	Flavonoids	Flavonols	-	611.16	593.15	610.1539	[M+H]+	263774.17	221704.535	99418.1041	412537.065	65935.8079	140895.93	9	9	9
365	1-hydroxy-7-[[(2s,3r,4s,5r,6r)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]xanthen-9-one	C19H18O9	Flavonoids	Other Flavonoids	-	391.1	229.05	390.095082	[M+H]+	100372.139	24482.3355	93096.8073	80652.9541	104218.775	149761.682	9	9	9
366	coumarin	C9H6O2	Lignans and Coumarins	Coumarins	-	147.04	91.05	146.0368	[M+H]+	3299021.01	3227578.22	3215914.64	2479454.91	2527754.56	2480932.72	2375637.71	2311080.01	2233490.02
367	7-Methoxycoumarin	C10H8O3	Lignans and Coumarins	Coumarins	531-59-9	177.05	89.04	176.0473	[M+H]+	2366341.72	2224277.32	2176483.61	2143443.4	2075982.99	2064551.72	2229326.44	2098479.83	2176171.92
368	Esculetin-7-O-glucoside*	C15H16O9	Lignans and Coumarins	Coumarins	-	339.07	177.02	340.0794	[M-H]-	626472.662	613020.395	575785.302	541860.074	485517.638	538474.535	547978.269	514286.403	519191.403
369	Cichoriin*	C15H16O9	Lignans and Coumarins	Coumarins	531-58-8	339.07	177.02	340.0794	[M-H]-	552881.655	640224.249	596573.842	584104.617	507781.275	535864.137	505175.424	499881.676	550131.892
370	Esculin (6,7-Dihydroxycoumarin-6-O-glucoside)*	C15H16O9	Lignans and Coumarins	Coumarins	531-75-9	339.07	177.02	340.0794	[M-H]-	543487.729	576084.655	612589.578	508332.112	501267.662	534521.093	448140.306	469956.067	524677.23
371	Daphnin*	C15H16O9	Lignans and Coumarins	Coumarins	486-55-5	339.07	177.02	340.079432	[M-H]-	543487.729	576084.655	612589.578	508332.112	501267.662	534521.093	448140.306	469956.067	524677.23
372	6-hydroxycoumarin	C9H6O3	Lignans and Coumarins	Coumarins	6093-68-1	163.04	89.04	162.0317	[M+H]+	583112.002	750378.232	497355.917	433732.778	466346.093	433698.039	398893.744	409251.209	376104.991
373	3,4-Methylenedioxy cinnamyl alcohol	C10H10O3	Lignans and Coumarins	Lignans	58095-76-4	177.06	117.04	178.063	[M-H]-	125035.853	126325.899	103579.523	197410.52	174732.587	218860.669	326126.522	357601.976	386924.024
374	Sideretin (5,7,8-Trihydroxy-6-methoxycoumarin)	C10H8O6	Lignans and Coumarins	Coumarins	-	223.03	149.03	224.0321	[M-H]-	34713.2969	21825.7902	39624.1152	371555.797	482337.015	357999.29	263513.889	318065.915	344403.181
375	Esculetin (6,7-Dihydroxycoumarin)	C9H6O4	Lignans and Coumarins	Coumarins	305-01-1	177.02	133.03	178.0266	[M-H]-	210173.208	203718.304	185155.347	274652.095	245331.174	234634.476	236304.15	268217.957	226236.989
376	7-hydroxy-2H-1-benzopyran-2-one	C9H6O3	Lignans and Coumarins	Coumarins	-	163.04	89.04	162.0317	[M+H]+	102267.455	101448.831	106078.974	108197.606	121465.72	139050.223	68434.0143	101206.886	328405.588

377	Fraxetin (7,8-Dihydroxy-6-methoxycoumarin)	C10H8O5	Lignans and Coumarins	Coumarins	574-84-5	209.04	149.02	208.0372	[M+H]+	227281.283	231268.344	207945.379	192538.563	189794.188	157334.311	149839.022	173963.027	160365.725
378	Lariciresinol-4'-O-glucoside	C26H34O11	Lignans and Coumarins	Lignans	143663-00-7	521.2	359.15	522.2101	[M-H]-	103402.656	127528.456	108162.59	113881.544	103636.281	117655.245	122893.698	105223.063	127669.171
379	6-MethylCoumarin	C10H8O2	Lignans and Coumarins	Coumarins	92-48-8	161.06	115.05	160.0524	[M+H]+	81751.0919	91412.895	85433.3306	91779.26	117474.239	97644.0099	99396.3664	95760.4834	107903.448
380	7-Hydroxycoumarin;Umbelliferone	C9H6O3	Lignans and Coumarins	Coumarins	93-35-6	161.02	133.03	162.0317	[M-H]-	74645.1111	88427.0541	71154.9717	107160.143	89495.1211	94972.5267	111409.416	96643.1581	77045.5851
381	Ethyl 3-coumarincarboxylate	C12H10O4	Lignans and Coumarins	Coumarins	1846-76-0	219.06	173.03	218.0579	[M+H]+	77889.4788	74215.1092	108097.709	67304.1042	68677.4982	77631.5666	84514.8266	69819.5172	102133.6
382	Massoniresinol; Vladinol A	C20H24O8	Lignans and Coumarins	Lignans	96087-10-4	391.14	59.01	392.1471	[M-H]-	91635.1375	140956.368	74919.9532	111517.366	91035.3922	87752.6899	97921.889	65534.158	87168.933
383	4-Hydroxycoumarin	C9H6O3	Lignans and Coumarins	Coumarins	1076-38-6	161.02	117.03	162.0317	[M-H]-	59594.6739	52766.474	49260.9932	51125.9417	60487.1076	64637.2961	67608.3063	78079.7052	74298.4726
384	Erythro-Guaiacylglycerol-β-dihydroconiferyl Ether glucoside	C26H36O12	Lignans and Coumarins	Lignans	-	539.21	491.19	540.2207	[M-H]-	85785.5505	87455.5182	71500.9501	50974.9422	84924.9907	66467.28	70069.5202	68602.9907	78856.5545
385	Dihydrodehydrodiconiferyl alcohol-4-O-glucoside*	C26H34O11	Lignans and Coumarins	Lignans	-	521.2	359.15	522.2101	[M-H]-	77407.4538	93142.9406	72829.6244	57867.6501	60022.7057	56349.3853	62987.3579	66336.1499	75838.7627
386	Isolariciresinol-9'-O-glucoside*	C26H34O11	Lignans and Coumarins	Lignans	63358-12-3	521.2	359.15	522.2101	[M-H]-	66742.1135	54634.4018	66657.6603	64453.8357	67918.0413	69004.0608	62295.5204	62155.6774	62001.6495
387	Sesamol	C7H6O3	Lignans and Coumarins	Lignans	533-31-3	139.04	98.98	138.0317	[M+H]+	62649.7625	45473.5437	72369.7826	44492.9144	57268.6556	47924.1594	53354.2354	55084.7843	62513.148
388	3,4-Dihydro-4-(4'-hydroxyphenyl)-5,7-dihydroxycoumarin glucoside*	C21H22O10	Lignans and Coumarins	Coumarins	-	435.13	273.08	434.1208	[M+H]+	58356.5293	60707.8034	82184.7907	137703.701	74944.8678	66869.5152	48984.923	52310.7876	56328.3826
389	Skimmin (7-Hydroxycoumarin-7-O-glucoside)	C15H16O8	Lignans and Coumarins	Coumarins	93-39-0	325.09	163.04	324.0845	[M+H]+	48858.4995	60032.7253	86980.5373	58797.3083	64693.2014	68121.0983	49756.0951	57947.3552	47188.9947
390	Erythro-Guaiacylglycerol-β-dihydroconiferyl Ether*	C20H26O7	Lignans and Coumarins	Lignans	135820-77-8	377.16	329.14	378.1679	[M-H]-	35568.5104	34830.5422	34013.2075	30592.3454	30005.4166	37049.3411	29814.1128	48821.3952	30308.1895
391	Daphnetin	C9H6O4	Lignans and Coumarins	Coumarins	486-35-1	177.02	121.03	178.0266	[M-H]-	43565.7587	33272.1891	26515.1706	29689.7064	37644.8258	29918.0544	32922.544	26982.0089	26935.6639
392	Sesamin	C20H18O6	Lignans and Coumarins	Lignans	607-80-7	355.1	163.04	354.1103	[M+H]+	30225.1097	10788.871	29473.0803	22645.386	34290.0128	33388.8161	42205.6819	17030.6045	25149.379
393	Secoisolariciresinol 4-O-glucoside	C26H36O11	Lignans and Coumarins	Lignans	-	523.22	361.14	524.2258	[M-H]-	22009.7548	30317.3622	28388.7353	27970.2312	31942.3569	23115.0018	36271.0974	24191.1337	22935.596
394	Demethyl-erythro-Guaiacylglycerol β-Sinapyl Ether	C20H24O8	Lignans and Coumarins	Lignans	-	391.14	343.12	392.1471	[M-H]-	30663.7843	19759.9235	20437.5922	21042.5192	34248.8466	23130.4708	23872.8192	29384.7219	18262.0405
395	Epipinoresinol*	C20H22O6	Lignans and Coumarins	Lignans	24404-50-0	357.1344	151.0442	358.1416	[M-H]-	10752.0317	19723.0419	15164.1372	15148.6686	15074.9625	19036.8515	20164.4152	20919.5217	19662.1938
396	Scopoletin-7-O-glucoside (Scopolin)	C16H18O9	Lignans and Coumarins	Coumarins	531-44-2	355.1	193.05	354.0951	[M+H]+	17471.3118	21654.0461	13495.1185	30559.9382	22547.2285	13272.9815	14646.7055	21148.3037	23921.7239
397	1-Hydroxypinoresinol-1-O-Glucoside	C26H32O12	Lignans and Coumarins	Lignans	81495-71-8	535.18	373.13	536.1894	[M-H]-	12693.9279	15181.1415	14686.3068	9950.31484	10028.9393	11729.0385	21161.6468	14872.9586	23426.0647
398	Esculetin-7-O-quinic acid	C16H16O9	Lignans and Coumarins	Coumarins	-	351.07	105.1	352.0794	[M-H]-	19356.4251	20560.1549	23124.5459	13242.8158	17489.6799	17088.0701	16190.8347	21865.5005	17897.3332
399	Matairesinol-4'-O-glucoside (Matairesinoside)	C26H32O11	Lignans and Coumarins	Lignans	23202-85-9	538.23	359.15	520.1945	[M+NH4]+	8785.30555	21711.7421	26006.5309	31372.1591	14414.4886	9783.0458	16503.2086	23446.8867	15945.2282
400	Pinoresinol*	C20H22O6	Lignans and Coumarins	Lignans	487-36-5	357.13	151.04	358.1416	[M-H]-	18077.7977	15863.405	16180.1862	18046.3724	13049.9606	16661.248	17110.9103	18609.0867	16312.0907
401	7R,8S-erythro-3',4,9,9'-tetrahydroxy-3-methoxy-8-O-4'-neolignan-7-O-glucopyr-anoside,	C25H34O12	Lignans and Coumarins	Lignans	-	525.2	179.07	526.205	[M-H]-	8318.10185	13923.6602	21998.0897	19747.9438	5906.80871	8332.35305	18461.6879	20591.4632	10476.6712
402	Secoisolariciresinol-9'-O-glucoside	C26H36O11	Lignans and Coumarins	Lignans	63320-67-2	523.22	475.2	524.2258	[M-H]-	11817.546	9936.83465	10074.2947	15199.4268	11552.6447	11722.8734	10960.2314	11128.6967	4285.4874
403	dihydrodehydrodiconiferyl alcohol-9-O-β-D-glucopyranoside	C26H34O11	Lignans and Coumarins	Lignans	-	521.2	491.19	522.2101	[M-H]-	4954.10082	14146.7918	6752.07499	8827.68773	8929.54933	10234.1273	10858.9051	1759.40207	10193.601
404	Procyanidin B1*	C30H26O12	Tannins	Proanthocyanidins	20315-25-7	577.14	425.09	578.1424	[M-H]-	86689.6959	70753.0391	74523.5745	70469.1228	71321.4145	76719.3374	53583.186	55881.7932	69285.4373
405	Gambiriin A1	C30H28O12	Tannins	Tannin	76250-49-2	581.17	139.04	580.1581	[M+H]+	9	9	9	9	9	9	34956.7798	23536.8073	30023.7983
406	Procyanidin B3*	C30H26O12	Tannins	Proanthocyanidins	23567-23-9	577.14	407.08	578.1424	[M-H]-	24480.2633	26649.7362	16454.0329	24251.4269	27186.7795	26849.2437	24829.6116	18224.4591	39452.9479
407	Procyanidin B2*	C30H26O12	Tannins	Proanthocyanidins	29106-49-8	577.14	407.08	578.1424	[M-H]-	25649.1197	17561.2106	21660.2535	14371.6035	25110.8173	23285.3998	22147.1522	18949.4899	15964.0912
408	Phyllanemblinin B*	C27H22O18	Tannins	Tannin	-	633.07	301	634.0806	[M-H]-	8228.33313	10144.7116	4957.65349	11335.123	9608.50834	20853.7047	17502.7289	12221.9424	27312.6636
409	Theaflagallin	C20H16O9	Tannins	Tannin	102208-15-1	399.07	233.05	400.0794	[M-H]-	10036.9678	16237.7003	7088.75091	20454.4768	10633.7923	15533.7487	12488.2827	18918.9215	16063.1133
410	Isocorilagin*	C27H22O18	Tannins	Tannin	-	633.07	301	634.0806	[M-H]-	4255.37907	3922.46236	3551.18054	9879.03539	14502.6115	8380.65647	11952.7554	14023.8439	17925.1421
411	Sanguiin H4*	C27H22O18	Tannins	Tannin	84316-77-8	633.08	301.01	634.0806	[M-H]-	5097.25785	6220.95764	3804.25985	22261.6594	16545.0294	11720.4504	11627.5596	14629.2568	17116.5867

* represents the presence of an isomer of the compound.