

Table. S2. The detail data for 182 differential 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	2-Hydroxycinnamic acid*	C9H8O3	Phenolic acids	Phenolic acids	583-17-5	163.04	119.05	164.0473	[M-H]-	11702959.91	10889151.07	10546548.99	10235525.01	10080350.25	10128075.34	14582851.41	14189657.67	13865588.72
2	o-Hydroxycinnamic Acid*	C9H8O3	Phenolic acids	Phenolic acids	5801-57-0	163.0401	119.0502	164.0473	[M-H]-	11484080.06	11357105.46	11321427.88	10374426.49	10119731.41	10238949.74	13246908.51	14873876.26	14013284.83
3	3-Hydroxycinnamic Acid*	C9H8O3	Phenolic acids	Phenolic acids	14755-02-3	163.04	119.05	164.0473	[M-H]-	10174947.87	11073831.66	10269587.45	9745958.583	9401503.949	9845393.457	13637118.31	14054314.88	14139235.02
4	4-O-Methylgallic Acid	C8H8O5	Phenolic acids	Phenolic acids	4319-02-2	183.03	124.02	184.0372	[M-H]-	1908573.421	2230906.264	2075349.382	5283832.107	4507638.312	5285518.212	9004367.925	9663017.166	11061022.2
5	Apigenin-6-C-glucoside (Isovitexin)*	C21H20O10	Flavonoids	Flavones	38953-85-4	431.1	311.05	432.1056	[M-H]-	5836585.113	5792391.388	5209346.866	6884193.757	6177770.945	6488187.084	8853498.122	7226531.136	11557314.4
6	Methyl gallate	C8H8O5	Phenolic acids	Phenolic acids	99-24-1	183.03	124.02	184.0372	[M-H]-	1639766.932	1845745.969	1861219.299	4596875.122	4004415.44	4460316.516	7442354.241	7909577.23	9224934.066
7	3-O-p-Coumaroylquinic acid	C16H18O8	Phenolic acids	Phenolic acids	87099-71-6	337.09	191.06	338.1002	[M-H]-	6870805.247	7136648.591	7047089.743	7362037.142	6657524.436	7202262.834	7223062.972	7745198.68	7798558.153
8	Vitexin-2"-O-rhamnoside	C27H30O14	Flavonoids	Flavones	64820-99-1	579.17	433.11	578.1636	[M+H]+	6478980.529	6523577.615	6053909.258	5453621.916	5644332.482	6335858.898	7182740.918	6940084.904	7422218.681
9	4-(3,4,5-Trihydroxybenzoyl)benzoic acid	C14H10O7	Phenolic acids	Phenolic acids	-	289.04	137.02	290.0427	[M-H]-	7082310.227	6764209.511	5080971.72	5453492.898	4743469.838	5147226.727	6505821.728	4972151.239	7055673.611
10	Apigenin-8-C-Glucoside (Vitexin)*	C21H20O10	Flavonoids	Flavones	3681-93-4	433.11	313.07	432.1056	[M+H]+	3794268.406	3481811.68	3517331.347	4316052.214	4284778.885	4492679.192	5491907.581	5786141.901	6810794.544
11	Ferulic acid*	C10H10O4	Phenolic acids	Phenolic acids	537-98-4	193.05	134.04	194.0579	[M-H]-	4534444.843	4191517.323	4261634.129	4844286.077	4437516.706	4424536.866	5229883.196	5090616.607	5126196.415
12	Quercetin-3-O-glucoside (Isoquercitrin)*	C21H20O12	Flavonoids	Flavonols	482-35-9	463.09	300.03	464.0955	[M-H]-	421057.3125	446645.4701	263769.876	1212120.92	1032665.445	1402252.605	3713237.528	3512582.88	4708750.8
13	4-Hydroxybenzoic acid	C7H6O3	Phenolic acids	Phenolic acids	99-96-7	137.02	93.03	138.0317	[M-H]-	3058025.608	3159386.159	2923961.223	3072831.121	3158008.416	3072402.471	3833794.247	3770062.884	3722624.21
14	Kaempferol-3-O-robinobioside(Biorobin)	C27H30O15	Flavonoids	Flavonols	17297-56-2	593.15	285.04	594.1585	[M-H]-	1860308.542	1763558.848	1254703.279	2294989.148	2186037.007	1879017.57	2982260.307	3097500.8	3858842.346
15	Quercetin-4"-O-glucoside (Spiraeoside)*	C21H20O12	Flavonoids	Flavonols	20229-56-5	463.09	301.04	464.0955	[M-H]-	450519.0918	426162.9262	320578.5502	1018447.344	1006256.02	1102172.195	2888189.869	2889136.475	4055777.684
16	Hesperetin-5-O-glucoside	C22H24O11	Flavonoids	Flavanones	69651-80-5	463.12	301.07	464.1319	[M-H]-	455748.5305	529312.3465	341796.5481	1028142.431	1008044.133	1111913.27	2688568.486	2834596.685	3880118.995
17	2,5-Dihydroxybenzaldehyde	C7H6O3	Phenolic acids	Phenolic acids	1194-98-5	137.02	93.03	138.0317	[M-H]-	2413115.606	2532170.59	2251703.092	2452020.852	2471300.128	2458317.07	2925034.734	3097795.715	2946586.781
18	Isoferulic Acid*	C10H10O4	Phenolic acids	Phenolic acids	25522-33-2	193.0506	134.0374	194.0579	[M-H]-	2701623.193	2461465.16	2555785.234	2578774.794	2637701.7	2733818.271	3075105.33	3018062.222	2821667.402
19	Quercetin-7-O-glucoside*	C21H20O12	Flavonoids	Flavonols	491-50-9	463.09	301.04	464.0955	[M-H]-	452057.8223	445017.2715	272312.8923	892933.8428	826908.1242	1180745.701	2491273.464	2507147.374	3691012.633
20	Quercetin 3-xylosyl-(1->6)-glucoside	C26H28O16	Flavonoids	Flavones	-	595.14	134.05	596.1377351	[M-H]-	1371754.409	1081944.862	1340157.665	1415160.404	1304481.213	1440066.331	2511555.3	2572278.209	2210860.429
21	2-(Formylamino)benzoic acid	C8H7NO3	Phenolic acids	Phenolic acids	3342-77-6	164.04	120.05	165.0426	[M-H]-	1971785.84	1763745.506	1824241.347	1692164.878	1685718.672	1604513.065	2198784.789	2211278.273	2126756.075
22	Gallocatechin 3-O-gallate*	C22H18O11	Flavonoids	Flavanols	5127-64-0	457.08	169.01	458.0849	[M-H]-	1341849.05	803428.1356	888131.1664	2267294.219	1977962.238	2014408.232	1943235.249	2155624.372	2045512.915
23	Kaempferol-7-O-glucoside*	C21H20O11	Flavonoids	Flavonols	16290-07-6	447.09	285.04	448.1006	[M-H]-	303188.1763	305734.892	247274.8191	698574.8005	638674.174	732649.0023	1596767.784	1743625.479	2301864.763
24	Kaempferol-3-O-galactoside (Trifolin)*	C21H20O11	Flavonoids	Flavonols	23627-87-4	447.09	285.04	448.1006	[M-H]-	321004.4791	305908.5747	213722.3932	686313.4164	615340.7377	761976.3922	1627863.714	1528297.638	2264533.452
25	Quercetin-3-O-robinobioside	C27H30O16	Flavonoids	Flavonols	52525-35-6	609.15	300.03	610.1534	[M-H]-	678256.8762	726892.2116	541386.5697	840664.0607	779403.8788	916269.3724	1397347.771	1415233.339	1511621.386
26	Kaempferol-3-O-glucoside (Astragalin)*	C21H20O11	Flavonoids	Flavonols	480-10-4	449.1078	287.0553	448.1006	[M+H]+	927220.2704	840695.1677	751285.0061	840198.244	837901.1097	872426.2122	633001.8379	1456413.655	1918861.665
27	Quercetin-3-O-rutinoside (Rutin)	C27H30O16	Flavonoids	Flavonols	153-18-4	609.15	301.04	610.1534	[M-H]-	572950.0118	490353.2117	391357.2034	771459.5191	645255.7237	602315.4626	1041467.817	1008284.223	1302361.866
28	Methyl cumalate*	C7H6O4	Phenolic acids	Phenolic acids	6018-41-3	153.02	109.03	154.0266	[M-H]-	1445859.237	1231188.111	1251315.113	1250822.75	1216791.509	1318675.715	1096351.338	1144797.722	1103544.467
29	Taxifolin-3"-O-glucoside*	C21H22O12	Flavonoids	Flavanonols	31106-05-5	465.13	303.05	466.1111	[M-H]-	633476.852	542042.6919	537202.3553	672062.5945	651898.2326	760872.7293	1017922.157	997527.9226	1114865.465
30	1,8-dihydroxy-4,5-dimethoxy-3-[[[(2s,3r,4s,5r,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]-	566317.3735	593562.0845	564520.9546	741938.24	660482.9319	633920.9775	999574.5407	807933.5974	1154453.699
31	Isovitexin-2"-O-rhamnoside	C27H30O14	Flavonoids	Flavones	-	579.17	313.07	578.1636	[M+H]+	866414.1311	898738.2216	1010474.562	850749.4656	953400.3837	884558.0493	968164.9556	981412.8825	961340.8445
32	Quercetin-5-O-β-D-glucoside*	C21H20O12	Flavonoids	Flavonols	-	465.1	303.05	464.0955	[M+H]+	45547.11298	223357.7463	52420.86542	51853.607	261755.79	119535.9766	1223228.621	462232.8572	1005375.811
33	3,4,2',4',6'-Pentahydroxychalcone	C15H12O6	Flavonoids	Chalcones	73692-51-0	289.07	163.04	288.0634	[M+H]+	1001597.456	873981.2431	636644.3722	501899.3685	555207.9968	602992.7323	923575.8825	829700.2517	855243.3493
34	Glucosyringic acid	C15H20O10	Phenolic acids	Phenolic acids	33228-65-8	359.1	197.05	361.1129	[M-H]-	381272.4814	400952.6625	418414.8091	541639.5343	641514.2469	581905.8677	871079.1118	879989.9231	842525.0614
35	4-Nitrophenol	C6H5NO3	Phenolic acids	Phenolic acids	100-02-7	140.03	98.96	139.0269	[M+H]+	13075656.93	12180580.03	12042611.08	1373444.527	1607729.138	1652747.624	739515.9023	697427.5453	1039870.076
36	Isoaonarin(Isovitexin-4"-O-glucoside)	C27H30O15	Flavonoids	Flavones	19416-87-6	595.17	313.07	594.1585	[M+H]+	711597.2055	694321.3	738377.3398	663937.0954	603569.8477	723885.3651	726034.9156	821342.2332	768824.3028
37	Phloroglucinol; 1,3,5-Benzenetriol	C6H6O3	Phenolic acids	Phenolic acids	108-73-6	127.04	81.03	126.0317	[M+H]+	714628.6371	627568.5981	787268.9673	594816.0202	433908.2055	609273.3534	604966.6307	642249.3541	888436.5116
38	Naringenin-4"-O-glucoside*	C21H22O10	Flavonoids	Flavanones	-	433.12	271.06	434.1213	[M-H]-	520345.8621	502233.9713	538413.5823	641616.5958	573160.3983	597089.0999	634969.7123	726860.1215	762040.6865
39	Quercetin-3-O-galactoside (Hypertin)*	C21H20O12	Flavonoids	Flavonols	482-36-0	465.1	303.06	464.0955	[M+H]+	47752.06767	87093.34587	103810.8887	97602.44124	187106.5171	341454.7604	570531.5	539067.6548	993533.2225
40	Isohyperoside*	C21H20O12	Flavonoids	Flavonols	35589-21-0	465.1019	303.0613	464.0955	[M+H]+	47752.06767	87093.34587	103810.8887	97602.44124	187106.5171	341454.7604	570531.5	539067.6548	993533.2225

41	Tricin-7-O-Glucoside*	C23H24O12	Flavonoids	Flavones	32769-01-0	493.13	331.08	492.1268	[M+H] ⁺	372456.8654	295201.5754	229996.4499	356320.8325	366148.6047	428503.2407	606027.9315	600641.8807	893746.1
42	Apigenin-6,8-di-C-arabinoside*	C25H26O13	Flavonoids	Flavones	-	535.14	499.12	534.1373	[M+H] ⁺	280789.0275	232218.0818	237742.0663	331725.1579	278345.8864	366898.8769	591020.4569	747719.4674	706862.4139
43	4-O-p-Coumaroylquinic acid	C16H18O8	Phenolic acids	Phenolic acids	32451-86-8	337.09	163.04	338.1002	[M-H] ⁻	594097.9453	595002.8565	529494.0693	568103.9602	549829.136	563676.0524	641283.8143	616842.4848	640149.225
44	Eugenol	C10H12O2	Phenolic acids	Phenolic acids	97-53-0	165.09	91.05	164.0837	[M+H] ⁺	702101.0474	555971.1372	881084.6121	492526.1095	385616.4785	519423.3071	581867.1022	706318.5705	586444.5111
45	2,6-Di-tert-butylphenol*	C14H22O	Phenolic acids	Phenolic acids	128-39-2	205.16	189.13	206.1671	[M-H] ⁻	589965.3892	724764.1943	799790.5017	726001.2772	740009.9893	793488.4455	639362.1297	681931.1389	519784.4175
46	Apigenin-6-C-arabinoside-8-C-xyloside*	C25H26O13	Flavonoids	Flavones	-	535.14	499.12	534.1373	[M+H] ⁺	233154.2938	200923.3562	142325.8556	318267.0608	297703.0438	291924.2174	558817.0455	544011.435	722476.6523
47	Sinapic acid	C11H12O5	Phenolic acids	Phenolic acids	530-59-6	223.06	193.02	224.0685	[M-H] ⁻	67682.48814	51625.14255	70575.75446	847206.3828	822014.4629	775020.9797	601498.424	571260.099	582672.9422
48	6-O-Caffeoyl-D-glucose*	C15H18O9	Phenolic acids	Phenolic acids	-	341.09	179.03	342.0951	[M-H] ⁻	426442.3233	483655.1852	468934.7944	530510.6715	496104.3698	470269.325	581614.9596	550035.345	607033.544
49	1-O-Sinapoyl-β-D-glucose	C17H22O10	Phenolic acids	Phenolic acids	-	385.11	223.06	386.1213	[M-H] ⁻	212109.3884	199120.1523	167958.93	441696.2147	403300.4113	361277.3475	531168.1501	568670.9248	598515.1257
50	Jacocidin-7-O-Glucoside*	C23H24O12	Flavonoids	Flavones	25474-11-7	493.14	331.08	492.1268	[M+H] ⁺	312085.0755	291704.1381	204325.9934	300853.5019	343062.7519	412460.939	525550.4974	458339.8474	705757.6328
51	Syringic acid	C9H10O5	Phenolic acids	Phenolic acids	530-57-4	197.05	123.01	198.0528	[M-H] ⁻	409717.7741	414310.7051	372650.6168	407886.454	423712.7145	433542.506	571926.813	584438.3885	509473.4454
52	Isoschaftoside	C26H28O14	Flavonoids	Flavones	52012-29-0	565.16	409.09	564.1479	[M+H] ⁺	530183.4033	465530.1378	385933.6461	456993.6718	464112.6494	504119.3885	495918.9314	530111.7263	622044.9718
53	4-O-Glucosyl-sinapate	C17H22O10	Phenolic acids	Phenolic acids	-	385.11	223.06	386.1213	[M-H] ⁻	233971.3922	217114.8681	158441.556	392183.1772	411381.0415	365319.0012	553757.6775	530453.5063	530171.0729
54	Dihydrokaempferide	C16H14O6	Flavonoids	Flavanols	137225-59-3	303.09	229.08	302.079	[M+H] ⁺	117396.4991	103089.2138	46845.31469	182132.7058	204947.1616	216551.2701	405379.4326	479405.1076	667434.7195
55	Chlorogenic acid (3-O-Caffeoylquinic acid)*	C16H18O9	Phenolic acids	Phenolic acids	327-97-9	353.09	191.06	354.0951	[M-H] ⁻	425723.4835	428685.6995	397611.491	435013.4195	454706.575	472680.784	524869.9	529585.91	485296.996
56	5-Glucosyloxy-2-Hydroxybenzoic acid methyl ester	C14H18O9	Phenolic acids	Phenolic acids	-	329.09	167.04	330.0951	[M-H] ⁻	399557.9571	509168.9866	530107.065	450931.7071	380126.0164	413365.0807	470831.7024	490936.8683	474591.3819
57	Chrysoeriol-5-O-glucoside	C22H22O11	Flavonoids	Flavones	-	461.11	299.1	462.1162	[M-H] ⁻	83106.05874	77629.90277	66624.51389	175186.7034	142297.0161	183497.4597	414026.9235	412310.0323	508464.3138
58	Methyl 4-hydroxybenzoate*	C8H8O3	Phenolic acids	Phenolic acids	99-76-3	151.04	136.02	152.0473	[M-H] ⁻	435647.5725	427823.4141	448080.7123	407686.8258	437846.544	406886.352	427137.7529	476159.3179	424049.1179
59	1,2,3,7,8-pentahydroxy-6-methylanthracene-9,10-dione	C15H10O7	Flavonoids	Other Flavonoids	-	303.05	229.05	302.0427	[M+H] ⁺	99831.91006	85280.92514	51441.51141	133382.1234	80641.88506	133614.9418	340836.461	355545.1554	609335.1946
60	1,2,4,5-tetrahydroxy-7-(hydroxymethyl)anthracene-9,10-dione	C15H10O7	Flavonoids	Other Flavonoids	-	303.05	229.05	302.0427	[M+H] ⁺	140537.6458	139785.9018	118658.3103	178106.8336	149577.533	192621.7641	364150.8113	338671.7384	540749.4435
61	5-O-Galloyl-D-hamamelose*	C13H16O10	Phenolic acids	Phenolic acids	-	331.07	169.02	332.0743	[M-H] ⁻	342493.7268	324260.7527	317027.4365	362328.6692	331714.9459	342211.3882	354761.7073	374990.155	397033.8967
62	1-O-Galloyl-β-D-glucose*	C13H16O10	Phenolic acids	Phenolic acids	58511-73-2	331.07	169.01	332.0743	[M-H] ⁻	326466.6362	336864.7696	340358.3545	332982.8666	314006.1704	332823.1574	347066.6183	386063.1996	375642.4875
63	6-O-Galloyl-β-D-glucose*	C13H16O10	Phenolic acids	Phenolic acids	13186-19-1	331.07	169.01	332.0743	[M-H] ⁻	326466.6362	336864.7696	340358.3545	332982.8666	314006.1704	332823.1574	347066.6183	386063.1996	375642.4875
64	Digalloylgucose*	C20H20O14	Phenolic acids	Phenolic acids	-	483.08	169.05	484.0853	[M-H] ⁻	317600.4884	235573.6248	252005.446	218704.1808	216840.6886	221537.9447	345324.2018	374360.009	357197.2231
65	Isochlorogenic acid B*	C25H24O12	Phenolic acids	Phenolic acids	14534-61-3	515.12	353.09	516.1268	[M-H] ⁻	124007.0436	134100.5654	56395.96743	192667.0454	206357.3074	161357.1011	357945.0131	307172.0016	408684.1907
66	Gallic Acid Ethyl Ester, Ethyl gallate	C9H10O5	Phenolic acids	Phenolic acids	831-61-8	197.05	124.02	198.0528	[M-H] ⁻	296431.1525	272613.6378	248213.8879	295796.2288	293622.8538	292308.5249	347889.4552	345646.182	379644.345
67	3,4-Methyleneoxy cinnamyl alcohol	C10H10O3	Lignans and Coumarins	Lignans	58095-76-4	177.06	117.04	178.063	[M-H] ⁻	125055.8528	126325.8994	103579.5228	197410.5203	174732.5869	218860.6685	326126.5222	357601.9761	386924.0239
68	4-Hydroxyphenylacetic acid*	C8H8O3	Phenolic acids	Phenolic acids	156-38-7	151.04	107.05	152.0473	[M-H] ⁻	296546.0393	287452.4274	271771.9685	239057.1158	300712.939	289455.069	270789.1663	392226.9154	376726.934
69	Dihydrochalcone-4'-O-glucoside	C21H24O10	Flavonoids	Chalcones	-	435.13	273.08	436.1369	[M-H] ⁻	137271.8177	183443.7869	160008.4037	228598.1918	200516.4637	187068.0024	313584.351	261320.753	390943.6986
70	Propyl 4-hydroxybenzoate	C10H12O3	Phenolic acids	Phenolic acids	94-13-3	179.07	92.03	180.0786	[M-H] ⁻	128036.0214	191142.7618	182271.8531	175293.7682	142987.4588	166710.1544	322799.9869	303607.1665	332747.6995
71	Phthalic acid	C8H6O4	Phenolic acids	Phenolic acids	88-99-3	165.02	77.04	166.0266	[M-H] ⁻	3513766.015	551707.2506	496446.6211	504460.4794	1402577.145	1339783.392	399007.3041	256740.8682	300455.9782
72	Apigenin-6-C-xyloside-8-C-arabinoside	C25H26O13	Flavonoids	Flavones	-	535.14	517.13	534.1373	[M+H] ⁺	243352.2643	327854.0223	161821.33	297092.5924	74768.54362	214703.3266	274032.5297	332926.7787	348482.9812
73	Myricetin-3-O-β-D-glucoside*	C21H20O13	Flavonoids	Flavonols	19833-12-6	481.1	319.04	480.0904	[M+H] ⁺	45864.23631	20217.00177	36986.91338	48819.50458	61128.61538	121946.4145	222404.1311	169910.0773	555107.598
74	Phloretin-2'-O-glucoside (Phlorizin)	C21H24O10	Flavonoids	Chalcones	60-81-1	435.13	167.04	436.1369	[M-H] ⁻	140831.342	158222.2356	136766.8901	204430.1751	188087.7133	204755.0875	322098.3197	280008.7623	328650.6
75	Sideretin (5,7,8-Trihydroxy-6-methoxycoumarin)	C10H8O6	Lignans and Coumarins	Coumarins	-	223.03	149.03	224.0321	[M-H] ⁻	34713.29687	21825.79021	39624.11524	371555.7966	482337.0147	357999.2904	263513.889	318065.9146	344403.1807
76	Vanillin acetate	C10H10O4	Phenolic acids	Phenolic acids	881-68-5	195.06	93.03	194.0579	[M+H] ⁺	414192.878	374190.6257	367965.7056	348951.7829	425854.8287	392873.2813	322035.13	300259.3823	301584.0172
77	5,7-Dihydroxy-1(3H)-isobenzofuranone	C8H6O4	Phenolic acids	Phenolic acids	27979-58-4	165.02	121.03	166.0266	[M-H] ⁻	1437920.024	380428.2158	384602.3163	363325.056	718302.7878	680936.6598	308320.4223	326658.7369	266560.3654
78	Anthramilate-1-O-Sophoroside	C19H27NO12	Phenolic acids	Phenolic acids	-	460.15	117.9	461.1533	[M-H] ⁻	124537.0126	105402.5234	100106.2648	157796.9363	96979.70624	89077.3583	211831.4653	396056.0334	286404.0197
79	1,4-Di-O-Galloyl-D-glucose	C20H20O14	Phenolic acids	Phenolic acids	-	483.08	169.01	484.0853	[M-H] ⁻	292582.1216	118251.6528	103792.3766	271386.3149	29100.24101	125217.515	452075.296	179199.1335	189935.0657
80	p-Coumaric acid methyl ester	C10H10O3	Phenolic acids	Phenolic acids	19367-38-5	177.06	145.03	178.063	[M-H] ⁻	82370.73427	91256.35214	68274.9224	154604.628	137868.4644	162926.4255	243090.9207	269990.5825	287048.618
81	1-O-Galloyl-6-O-p-Coumaroyl-β-D-glucose	C22H22O12	Phenolic acids	Phenolic acids	-	477.1	169.01	478.1111	[M-H] ⁻	198633.9054	221204.0623	153837.7465	189196.1395	160824.2538	185355.8688	225691.1897	200547.0486	307428.556
82	Apigenin-5-O-glucoside	C21H20O10	Flavonoids	Flavones	28757-27-9	433.11	271.06	432.1056	[M+H] ⁺	142250.6571	205073.5951	121645.7745	193535.3299	187499.3006	156103.74	312343.7417	244391.2488	235727.3679

83	2,6-dimethoxy-hydroquinone-4-O-β-D-glucopyranoside	C14H20O9	Phenolic acids	Phenolic acids	-	331.1	169.01	332.1107	[M-H]-	223545.8849	241042.1897	219062.2728	214669.5638	225094.1755	233459.6297	264850.7496	259350.1671	257990.2316
84	4,6-(S)-Hexahydroxydiphenyl-β-D-glucose	C20H18O14	Phenolic acids	Phenolic acids	36378-48-0	481.06	301	482.0697	[M-H]-	293089.1861	239349.2906	245331.8987	228786.8634	233872.5623	204473.9781	269837.7081	250902.1162	237347.809
85	Myricetin-3-O-galactoside*	C21H20O13	Flavonoids	Flavonols	15648-86-9	481.1	319.06	480.0904	[M+H]+	56549.4511	83095.09379	59535.1425	101139.214	74857.95554	149763.9929	193494.2519	219157.7166	338783.0247
86	2-Hydroxybenzaldehyde (Salicylaldehyde)	C7H6O2	Phenolic acids	Phenolic acids	90-02-8	121.03	77.04	122.0368	[M-H]-	2764194.206	436514.427	439629.6853	345807.1653	1071184.918	1123139.584	299817.5612	218150.9187	224687.6424
87	Brevifolin carboxylic acid	C13H8O8	Phenolic acids	Phenolic acids	18490-95-4	291.01	247.02	292.0219	[M-H]-	256936.9628	243751.9517	271571.7682	203855.541	236154.0545	206609.075	246284.3256	224261.5162	268190.2266
88	Apigenin-6,8-di-C-glucoside (Vicenin-2)	C27H30O15	Flavonoids	Flavones	23666-13-9	595.17	457.13	594.1585	[M+H]+	207100.2211	209770.5791	213172.595	177385.0922	174279.6529	235012.1927	223153.9738	220554.1009	240129.3974
89	1,6-Di-O-galloyl-β-D-glucose	C20H20O14	Phenolic acids	Phenolic acids	-	483.08	169.01	484.0853	[M-H]-	109686.4641	116668.7755	118412.8744	119600.2142	118909.685	28966.36509	218814.7638	215353.2731	249063.1014
90	3-Aminosalicylic acid	C7H7NO3	Phenolic acids	Phenolic acids	570-23-0	152.04	108.05	153.0426	[M-H]-	200063.9653	201924.5862	192330.2225	204845.3521	209217.0688	213041.04	227517.9026	215555.455	235440.4584
91	3-(4-Hydroxyphenyl)-propionic acid*	C9H10O3	Phenolic acids	Phenolic acids	501-97-3	165.06	119.05	166.063	[M-H]-	207570.1215	191151.987	208831.0221	186963.5646	196047.5343	202911.3131	221865.1895	233090.5712	212983.7107
92	Quercetin-7-O-rutinoside*	C27H30O16	Flavonoids	Flavonols	147714-62-3	611.1607	303.0499	610.1534	[M+H]+	91716.04376	85653.28401	81972.69814	137539.1518	91566.72582	128019.2857	196899.2404	243087.2175	213331.4455
93	Quercetagenin-7-O-glucoside(Quercetagenin)*	C21H20O13	Flavonoids	Flavonols	548-75-4	481.1	319.05	480.0904	[M+H]+	131275.1001	105591.3888	67338.11932	132081.4376	156735.3262	154318.7663	199203.4686	202883.4561	248545.4273
94	Vanillic acid	C8H8O4	Phenolic acids	Phenolic acids	121-34-6	167.03	108.02	168.0423	[M-H]-	188089.9738	180719.8586	190538.5676	122400.8616	145836.4029	127783.5854	195607.1284	218961.691	220248.67
95	Apigenin-8-C-Arabinoside	C20H18O9	Flavonoids	Flavones	-	403.1	367.08	402.0951	[M+H]+	166592.7818	132214.4983	85536.64409	157509.2632	137931.9831	61446.81692	152884.8764	278600.49	193832.6254
96	Galangin-7-O-glucoside*	C21H20O10	Flavonoids	Flavones	-	433.11	271.06	432.1056	[M+H]+	171821.2299	140057.6922	110986.6119	174601.9439	111519.9533	180409.4204	227286.3111	180786.0364	211064.5931
97	Apigenin-8-C-(2"-glucosyl)arabinoside	C26H28O14	Flavonoids	Flavones	-	565.16	457.11	564.1479	[M+H]+	213559.5527	145149.0975	143954.609	179008.2546	137104.8514	141929.5438	211773.3682	210031.9382	162093.227
98	Eriodictyol-3'-O-glucoside*	C21H22O11	Flavonoids	Flavanones	-	449.11	287.06	450.1162	[M-H]-	69223.56142	99956.41938	116992.6386	127147.955	104770.6046	105182.9686	188511.8077	176912.5361	216914.1823
99	3',5',5',7-Tetrahydroxy-4"-methoxyflavanone-3'-O-glucoside	C22H24O12	Flavonoids	Flavones	-	481.13	319.05	480.1268	[M+H]+	114247.1644	53326.8325	46812.56103	134634.8804	91223.30848	132293.5282	193731.2414	159080.0792	228011.9606
100	Protocatechuic aldehyde	C7H6O3	Phenolic acids	Phenolic acids	139-85-5	139.04	65.04	138.0317	[M+H]+	200642.8561	211684.7549	169493.1928	212249.136	191191.7143	209884.9226	155305.5601	200143.7822	182849.4645
101	Methyl-3-(3-hydroxyphenyl)Propionate	C10H12O3	Phenolic acids	Phenolic acids	61389-68-2	181.09	121.06	180.0786	[M+H]+	252726.4354	188618.9764	251663.4774	228240.235	257738.9632	263260.0794	195366.3801	153803.6919	187914.0326
102	2,6-Dimethoxybenzaldehyde*	C9H10O3	Phenolic acids	Phenolic acids	3392-97-0	165.06	119.05	166.063	[M-H]-	146685.7232	151785.4388	152634.2869	136907.4456	171535.031	140465.6892	161593.2698	165485.7676	197264.4549
103	7-Hydroxyflavanone	C15H12O3	Flavonoids	Flavanones	6515-36-2	239.07	207.04	240.0786443	[M-H]-	300403.3827	87211.52573	78277.49135	115661.6468	78907.12838	88319.38	106834.877	131268.2094	273073.0255
104	2,3-Di-O-Galloyl-β-D-Glucose*	C20H20O14	Phenolic acids	Phenolic acids	-	483.08	169.01	484.0853	[M-H]-	149092.4763	113137.2006	112015.8449	109134.5409	108509.5428	95634.59148	191148.5256	158249.3921	156771.234
105	Salicylic acid	C7H6O3	Phenolic acids	Phenolic acids	69-72-7	137.03	108.02	138.0317	[M-H]-	123418.5334	147573.1184	150087.117	142132.5439	137124.8333	142480.432	156885.8493	145888.0558	190007.671
106	β-Hydroxy-(3,4-dihydroxyphenylethanol)-glucoside	C14H20O9	Phenolic acids	Phenolic acids	-	331.1	151.04	332.111	[M-H]-	134299.5844	147654.422	143817.8821	148102.9062	151709.7227	148645.5717	159458.6082	158840.6036	172518.0449
107	Syringin	C17H24O9	Phenolic acids	Phenolic acids	118-34-3	371.13	209.08	372.142	[M-H]-	26181.1108	39617.50729	34101.98869	44592.31896	46416.41768	48345.9109	146821.55	159697.2409	164291.0794
108	kaempferol-3-p-coumaroyldiglucoiside	C36H36O18	Flavonoids	Flavonols	-	755.19	285.04	756.1902	[M-H]-	117268.5222	105668.4943	100560.4872	138508.3217	114224.6662	117403.2052	148034.4298	157017.8013	158452.8929
109	Ethyl phenylacetate	C10H12O2	Phenolic acids	Phenolic acids	101-97-3	165.09	91.05	164.0837	[M+H]+	102001.4156	141400.5365	92317.02888	74464.06481	85407.26482	122546.077	145673.8568	109817.5243	202893.7122
110	Quercetin-3-O-arabinoside	C20H18O11	Flavonoids	Flavonols	22255-13-6	433.08	300.03	434.0849	[M-H]-	3838.162701	17635.64785	9095.331049	34482.56256	26288.49176	34445.9846	136090.3168	121103.935	198967.0165
111	Delphinidin-3-O-galactoside	C21H21O12+	Flavonoids	Anthocyanidins	28500-00-7	465.1	303.05	465.1028	[M]+	97899.52411	97108.48518	78717.03576	101695.2139	113309.681	107411.8622	136035.243	134774.7583	140515.8389
112	Hispidulin-7-O-glucoside(Homoplantagin)*	C22H22O11	Flavonoids	Flavones	17680-84-1	463.13	301.09	462.1162	[M+H]+	74284.02947	28251.39652	53761.23333	59559.9335	53436.74239	58319.06904	111456.9641	122348.5945	157087.6327
113	Diomietin-7-O-glucoside*	C22H22O11	Flavonoids	Flavones	20126-59-4	463.12	301.07	462.1162	[M+H]+	52274.89487	39769.07955	48970.16663	70394.6035	59101.49483	77905.32993	95491.35827	121108.1469	162059.0189
114	Diomietin-7-O-galactoside*	C22H22O11	Flavonoids	Flavones	-	463.12	301.07	462.1162	[M+H]+	52274.89487	39769.07955	48970.16663	70394.6035	59101.49483	77905.32993	95491.35827	121108.1469	162059.0189
115	Diaceffoylschikimic acid	C25H22O11	Phenolic acids	Phenolic acids	-	499.13	163.04	498.1162	[M+H]+	71277.42491	66283.26115	63204.84292	69115.97055	85694.78324	99952.35326	111580.3078	115122.5286	145803.8756
116	Syringaldehyde; 4-Hydroxy-3,5-Dimethoxybenzaldehyde	C9H10O4	Phenolic acids	Phenolic acids	134-96-3	181.05	151	182.0579	[M-H]-	402237.8729	414834.8216	426257.5179	149769.6254	129218.2732	131697.4828	129340.9739	126155.3234	116874.2106
117	4-Hydroxyphenylacetic Acid*	C9H10O4	Phenolic acids	Phenolic acids	306-23-0	181.05	135.04	182.0579	[M-H]-	79294.52252	77103.61791	80490.51115	67591.72372	86282.34988	88390.16425	113052.0085	120304.5764	123481.1564
118	Luteolin-6-C-glucoside (Isoorientin)*	C21H20O11	Flavonoids	Flavones	4261-42-1	447.09	357.06	448.1006	[M-H]-	69377.47013	65111.5094	49727.03058	88072.9878	70554.73611	88068.68164	112204.0526	119074.8383	118337.5463
119	3-hydroxyphenylacetic acid*	C8H8O3	Phenolic acids	Phenolic acids	621-37-4	151.04	107.05	152.0473	[M-H]-	85988.93202	96179.1872	83606.0734	91559.77984	93239.23229	77221.06252	101953.4277	110374.9614	128263.9813
120	Methyl 2,4-dihydroxyphenylacetate*	C9H10O4	Phenolic acids	Phenolic acids	67828-42-6	181.05	135.04	182.0579	[M-H]-	71700.1836	69461.34	72721.56919	68251.64276	68696.79935	69002.80203	106171.1083	102100.2763	123815.8068
121	Hydroxyferulic acid glucoside	C16H20O10	Phenolic acids	Phenolic acids	-	371.1	209.05	372.1056	[M-H]-	21622.57325	17285.54888	24205.43922	31185.88604	35143.38544	28442.72397	78494.2591	101771.5555	105003.7883
122	Protocatechuic Acid Methyl Ester	C8H8O4	Phenolic acids	Phenolic acids	2150-43-8	167.04	108.02	168.0423	[M-H]-	36598.67629	40338.03776	38246.96609	55487.97392	52184.53665	60647.30024	91005.40906	97446.94941	91950.56571
123	Isovitexin-8-O-xyloside	C26H28O14	Flavonoids	Flavones	-	565.16	367.1	564.1479	[M+H]+	73595.84296	71995.86896	67995.26767	62900.89938	64095.42416	82123.57564	81603.18282	92553.88736	98964.82973
124	2-(3,4-dihydroxyphenyl)ethanediol 1-O-β-D-glucopyranoside*	C14H20O9	Phenolic acids	Phenolic acids	-	331.1	153.02	332.1107	[M-H]-	64701.78319	56496.476	67708.80036	63067.31069	56462.8977	69003.1084	90902.88918	92039.25469	84880.50111

125	Catechin gallate*	C22H18O10	Flavonoids	Flavanols	130405-40-2	443.1	139.04	442.09	[M+H] ⁺	30559.19797	35595.79722	56399.38133	21572.68009	77363.55318	50919.78792	67238.574	80449.95333	118719.0185
126	Tachioside*	C13H18O8	Phenolic acids	Phenolic acids	109194-60-7	301.09	123.01	302.1002	[M-H] ⁻	100533.5501	104298.4695	97381.28165	87164.90323	102806.2775	103616.1074	89239.60007	89207.75714	85928.54222
127	1-O-p-Coumaroyl-β-D-glucose*	C15H18O8	Phenolic acids	Phenolic acids	7139-64-2	325.09	163.04	326.1002	[M-H] ⁻	171136.5796	187270.5464	185622.8412	63895.76038	162287.2176	220614.1349	95816.98252	75298.02979	83094.58783
128	p-Coumaric acid-4-O-glucoside*	C15H18O8	Phenolic acids	Phenolic acids	117405-48-8	325.09	163.04	326.1002	[M-H] ⁻	171136.5796	187270.5464	185622.8412	63895.76038	162287.2176	220614.1349	95816.98252	75298.02979	83094.58783
129	Chrysoeriol-7-O-rutinoside	C28H32O15	Flavonoids	Flavones	-	607.17	299	608.1741	[M-H] ⁻	41223.01035	44567.6314	39992.08651	59658.09902	52114.7574	56040.93613	86453.45288	71329.26469	81526.51645
130	Furanofructosyl-α-D-(6-mustard acyl)glucoside*	C23H32O15	Phenolic acids	Phenolic acids	-	547.17	223.1	548.1741	[M-H] ⁻	19805.81321	25638.90808	26627.40115	60548.6177	59312.20228	62004.26918	65787.25128	60338.09821	95464.18308
131	Homovanilloylquinic acid	C16H20O9	Phenolic acids	Phenolic acids	-	355.1	121.03	356.1107	[M-H] ⁻	81097.96537	75015.94721	76700.01297	82707.78436	77907.414	87779.02312	72693.80724	74642.12144	73535.78307
132	4-Hydroxycoumarin	C9H6O3	Lignans and Coumarins	Coumarins	1076-38-6	161.02	117.03	162.0317	[M-H] ⁻	59594.67389	52766.47403	49260.99323	51125.9417	60487.1076	64637.29611	67608.30627	78079.70522	74298.47257
133	(S)-2-Hydroxy-3-(4-Hydroxyphenyl)Propanoic Acid	C9H10O4	Phenolic acids	Phenolic acids	23508-35-2	181.05	135.04	182.0579	[M-H] ⁻	48417.66378	50927.54805	38499.15897	45126.60674	47274.73027	43434.72103	73035.33603	67432.73222	77030.56523
134	2-Galloyl-6-O-Benzoyl Glucose*	C20H20O11	Phenolic acids	Phenolic acids	-	435.09	169.01	436.1006	[M-H] ⁻	80510.64933	40058.07051	39817.5775	54822.46297	44079.61558	54931.83537	61206.02416	65625.23147	85004.36991
135	6-O-Sinapoylsucrose*	C23H32O15	Phenolic acids	Phenolic acids	-	547.17	223.06	548.1741	[M-H] ⁻	32635.52799	26572.03669	33755.86831	68595.21307	71042.921	67245.73933	58601.83773	76037.22777	76128.57744
136	3-O-Methyl-epicatechin	C16H16O6	Flavonoids	Flavanols	76549-34-3	305.1	139.04	304.0947	[M+H] ⁺	47985.74287	51938.08143	49093.5358	49277.80924	38046.36066	38105.728	71690.59568	73930.84509	61142.41552
137	Isolaricresinol-9-O-glucoside*	C26H34O11	Lignans and Coumarins	Lignans	63358-12-3	521.2	359.15	522.2101	[M-H] ⁻	66742.11353	54634.40182	66657.66032	64453.83573	67918.04125	69004.06075	62295.52044	62155.67737	62001.6495
138	Procyanidin B1*	C30H26O12	Tannins	Proanthocyanidins	20315-25-7	577.14	425.09	578.1424	[M-H] ⁻	86689.69587	70753.03907	74523.5745	70469.12282	71321.41448	76719.33742	53583.18597	55881.79317	69285.43726
139	Phenylpropionic acid-O-β-D-glucopyranoside	C15H18O8	Phenolic acids	Phenolic acids	-	325.09	119.05	326.1002	[M-H] ⁻	85413.83125	85792.38969	77704.10475	80352.66641	76886.28754	74262.7137	67833.7657	46189.68135	62057.50858
140	Tyrosol; 4-Hydroxyphenylethanol	C8H10O2	Phenolic acids	Phenolic acids	501-94-0	139.08	55.02	138.0681	[M+H] ⁺	40712.94514	36194.51924	48488.25881	35184.17009	21606.36089	38887.66217	50912.60109	47870.28664	75926.2803
141	3',5',5',7'-Tetrahydroxyflavanone-7-O-glucoside*	C21H22O11	Flavonoids	Flavanones	-	451.12	289.07	450.1162	[M+H] ⁺	78069.42997	60969.10401	75578.93932	99712.76366	60306.0001	78026.5229	47894.48176	52302.05936	74217.1196
142	2-hydroxymethyl benzoic acid	C8H8O3	Phenolic acids	Phenolic acids	612-20-4	151.04	77.04	152.0473	[M-H] ⁻	38733.06339	37685.3384	39137.56	41770.29447	42301.82597	42839.8752	68827.08824	52479.94801	52598.24199
143	6-O-Feruloyl-D-sucrose	C22H30O14	Phenolic acids	Phenolic acids	118230-77-6	517.16	175.04	518.1636	[M-H] ⁻	130516.9075	101534.547	111348.0127	76860.27395	67249.36854	75092.97687	54266.135	58504.07897	54435.80588
144	Hydroxytyrosol	C8H10O3	Phenolic acids	Phenolic acids	10597-60-1	153.06	123.05	154.063	[M-H] ⁻	32896.49308	27563.49994	35414.62811	31756.64701	33560.65084	56404.89248	53532.24128	57392.59145	55356.46702
145	7-Methoxy-3-[1-(3-pyrrolyl)methylidene]-4-chromanone	C16H13NO3	Flavonoids	Other Flavonoids	-	268.103	136.0607	267.0895433	[M+H] ⁺	15637.53905	15567.45031	14743.6227	25278.36859	22253.22671	22519.6441	60399.64	52106.736	49885.01752
146	3,4-Dihydro-4-(4'-hydroxyphenyl)-5,7-dihydroxycoumarin glucoside*	C21H22O10	Lignans and Coumarins	Coumarins	-	435.13	273.08	434.1208	[M+H] ⁺	58356.52929	60707.80344	82184.79067	137703.7013	74944.86775	66869.51515	48984.92298	52310.78761	56328.3826
147	Skimmin (7-Hydroxycoumarin-7-O-glucoside)	C15H16O8	Lignans and Coumarins	Coumarins	93-39-0	325.09	163.04	324.0845	[M+H] ⁺	48858.49945	60032.72527	86980.53731	58797.30826	64693.20137	68121.09831	49756.09505	57947.35518	47188.99473
148	Kaempferol-7-O-rhamnoside*	C21H20O10	Flavonoids	Flavanols	20196-89-8	431.1	285.04	432.1056	[M-H] ⁻	6200.015834	5497.195461	5191.730566	12616.85725	12188.2078	19606.73356	45087.44125	50242.12647	59120.06652
149	2-Amino-3-methoxybenzoic acid	C8H9NO3	Phenolic acids	Phenolic acids	3177-80-8	168.06	94.06	167.0582	[M+H] ⁺	41358.86875	46777.52169	48698.75635	41157.15028	46092.16393	43873.86669	51270.9869	48079.15439	52764.81009
150	3-Hydroxy-4-methoxybenzoic acid; Isovanillic Acid	C8H8O4	Phenolic acids	Phenolic acids	645-08-9	169.05	65.04	168.0423	[M+H] ⁺	26302.97421	33552.92303	45903.28957	14973.40565	30487.97036	41552.56372	43973.27349	55330.69949	46629.45383
151	Kaempferol-3-O-rhamnoside (Afzelin)(Kaempferin)*	C21H20O10	Flavonoids	Flavanols	482-39-3	431.1	285.04	432.1056	[M-H] ⁻	2064.077162	2037.10358	5377.799179	16352.6692	13742.94334	14468.61102	34165.50058	44782.99844	61369.06853
152	Myricetin-3-(2"-galloyl)rhamnoside	C28H24O16	Flavonoids	Flavanols	-	617.11	471.06	616.1064347	[M+H] ⁺	74262.04936	14735.4005	11818.3397	16586.51195	24351.1354	16191.36247	50563.45848	37539.17107	37525.01822
153	Trans-5-O-(p-Coumaroyl)shikimate	C16H16O7	Phenolic acids	Phenolic acids	-	321.1	147.04	320.0896	[M+H] ⁺	53421.41567	43850.72076	64821.44396	96675.32125	100383.2361	65157.67693	41871.00931	30124.09555	50451.01215
154	Benzyl-(2"-O-xylosyl)glucoside	C18H26O10	Phenolic acids	Phenolic acids	-	401.14	269.1	402.1526	[M-H] ⁻	37228.78333	37044.61303	29357.72716	30805.09975	32803.48029	23077.16633	36542.66909	33253.3557	44544.64545
155	3,4-Digalloylshikimic acid	C21H18O13	Phenolic acids	Phenolic acids	-	477.06	169.01	478.0747	[M-H] ⁻	43542.93957	29308.84041	18180.80087	66464.68143	49753.405	68634.99049	44064.86476	36431.26736	31244.184
156	4-Hydroxypropiophenone	C9H10O2	Phenolic acids	Phenolic acids	70-70-2	149.07	92.03	150.0681	[M-H] ⁻	41930.66089	37876.26633	39133.27286	36896.55175	41325.46206	41872.50982	37354.58577	35673.61506	36859.65523
157	3-O-Methyltricetin-7-O-(6"-malonyl)glucoside*	C25H24O15	Flavonoids	Flavones	-	565.12	317.07	564.1115	[M+H] ⁺	164016.0261	140763.168	239354.5574	65283.2	136255.6031	87391.93543	14899.30256	47736.43793	43012.39466
158	Tamarixetin-3-O-(6"-malonyl)glucoside*	C25H24O15	Flavonoids	Flavanols	-	565.12	317.07	564.1115	[M+H] ⁺	164016.0261	140763.168	239354.5574	65283.2	136255.6031	87391.93543	14899.30256	47736.43793	43012.39466
159	1-O-Caffeoyl-4-O-galloyl-β-D-glucose	C22H22O13	Phenolic acids	Phenolic acids	-	493.1	169.01	494.106	[M-H] ⁻	35351.68628	29847.51144	28848.80668	21547.43476	27954.17979	19443.23162	31058.84726	23064.38535	43606.7867
160	p-Hydroxyphenyl-β-D-allopyranoside*	C12H16O7	Phenolic acids	Phenolic acids	-	271.08	108.02	272.0896	[M-H] ⁻	25611.3018	26103.12472	26433.03639	23189.16193	24962.44715	23287.53572	32027.78987	28590.30669	30556.70107
161	Gambirinin A1	C30H28O12	Tannins	Tannin	76250-49-2	581.17	139.04	580.1581	[M+H] ⁺	9	9	9	9	9	9	34956.77977	23536.80727	30023.79829
162	Apigenin-7-O-neohesperidoside (Rhoifolin)*	C27H30O14	Flavonoids	Flavones	17306-46-6	579.17	271.06	578.1636	[M+H] ⁺	31089.38516	8592.066485	15180.63178	8467.026928	13992.35087	19611.04954	18641.22668	26386.19891	41519.29951
163	3-Galloylshikimic acid	C14H14O9	Phenolic acids	Phenolic acids	110082-91-2	325.06	93.03	326.0638	[M-H] ⁻	13634.49915	18047.96402	12519.90925	18061.6049	18430.07772	19379.50877	26322.2701	31095.72311	26108.66957
164	Arbutin*	C12H16O7	Phenolic acids	Phenolic acids	497-76-7	271.08	108.02	272.0896	[M-H] ⁻	25312.16811	18803.66529	24410.58859	23433.70592	19183.55097	23261.68872	25108.79647	30088.03467	27247.46611
165	3-O-p-Coumaroylshikimic acid	C16H16O7	Phenolic acids	Phenolic acids	-	319.08	145.03	320.0896	[M-H] ⁻	170082.5972	154794.4399	177883.2782	87644.46788	95962.34106	58961.54806	35573.31903	22103.83752	20459.18982
166	Epicatechin-6-C-β-D-glucopyranoside*	C21H24O11	Flavonoids	Flavanols	-	451.1263	289.0729	452.1319	[M-H] ⁻	21396.44752	18733.11943	19658.51611	18794.91034	21220.39697	18616.23508	25366.54006	26001.25635	23635.15162

167	3,5-Dihydroxyacetophenone	C8H8O3	Phenolic acids	Phenolic acids	51863-60-6	151.04	65.04	152.0473	[M-H]-	24988.04435	22796.34668	24555.39861	24499.66269	8682.274697	17726.66438	17799.31725	28068.41968	28842.80221
168	5-O-Galloylshikimic acid	C14H14O9	Phenolic acids	Phenolic acids	-	325.06	169.02	326.0638	[M-H]-	32074.14987	33963.86587	38902.62981	41603.15989	35156.90981	40393.78776	42514.41768	7199.84156	14315.19964
169	catechin-4-β-D-galactopyranoside	C21H24O11	Flavonoids	Flavanols	-	451.12	289.07	452.1319	[M-H]-	18914.9285	21202.75968	23804.69135	13982.57766	15858.673	16207.00987	19690.43582	19307.59167	21878.86703
170	1-Hydroxypinoresinol-1-O-Glucoside	C26H32O12	Lignans and Coumarins	Lignans	81495-71-8	535.18	373.13	536.1894	[M-H]-	12693.9279	15181.14145	14686.30675	9950.314836	10028.93931	11729.03846	21161.64681	14872.95863	23426.06466
171	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]-	14549.43956	17460.10728	14728.69003	17629.50802	16191.89375	11363.36085	16871.66474	23972.25818	16700.47431
172	1-O-p-Cumaroylglycerol	C12H14O5	Phenolic acids	Phenolic acids	106055-11-2	237.08	163.04	238.0841	[M-H]-	8891.558851	9941.643596	5830.986642	8259.152987	15497.25307	8438.889993	14721.71895	17562.65049	16799.88516
173	Isocorilagin*	C27H22O18	Tannins	Tannin	-	633.07	301	634.0806	[M-H]-	4255.379068	3922.462355	3551.18054	9879.035385	14502.61146	8380.65647	11952.75542	14023.84394	17925.14209
174	Sanguin H4*	C27H22O18	Tannins	Tannin	84316-77-8	633.08	301.01	634.0806	[M-H]-	5097.257845	6220.957644	3804.259845	22261.6594	16545.0294	11720.45043	11627.55957	14629.25675	17116.58674
175	3-(3-Hydroxyphenyl)-3-hydroxypropanoic acid	C9H10O4	Phenolic acids	Phenolic acids	3247-75-4	181.05	121.03	182.0579	[M-H]-	28301.65975	30866.01823	36936.85763	17946.51687	13417.78029	15960.00784	16562.47683	9053.816982	11896.13514
176	Pinocembrin-7-O-neohesperidoside*	C27H32O13	Flavonoids	Flavanones	13241-31-1	563.18	255.07	564.1843	[M-H]-	8257.812347	8287.343137	8217.740443	1754.764047	6762.2251	7186.620445	8633.99445	8967.363563	11314.56684
177	Secoisolariciresinol-9-O-glucoside	C26H36O11	Lignans and Coumarins	Lignans	63320-67-2	523.22	475.2	524.2258	[M-H]-	11817.54601	9936.834648	10074.2947	15199.42677	11552.64467	11722.87336	10960.23143	11128.69669	4285.4874
178	Gallacetophenone	C8H8O4	Phenolic acids	Phenolic acids	528-21-2	169.05	65.03	168.0423	[M+H]+	9341.412364	5125.721072	13767.22021	9	9	9	8447.295011	6859.861217	10110.06366
179	Leomuride A	C14H20O9	Phenolic acids	Phenolic acids	121748-12-7	331.1	108.02	332.1107	[M-H]-	4088.685726	4807.088081	3929.989076	3593.345636	4186.77407	4397.67368	5706.535768	6142.858304	4825.747599
180	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]-	4310.652028	2766.714683	4364.264355	9	9	9	4681.536247	5491.301636	2562.079448
181	Kaempferol-6,8-di-C-glucoside	C27H30O16	Flavonoids	Flavanols	-	611.16	593.15	610.1539	[M+H]+	263774.1703	221704.5346	99418.10406	412537.0645	65935.80788	140895.93	9	9	9
182	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	390.0950823	[M+H]+	100372.1385	24482.33553	93096.80728	80652.95405	104218.7748	149761.6817	9	9	9

* represents the presence of an isomer of the compound.