

Compound	Subclass	Formula (DB)	Area	Height	Base Peak	End	Ions	Polarity	Mass	Score	m/z	RT
Cyanidin	Anthocyanins	C15 H11 O6	364140	60121	122,0812	9,485	2	Positive	287,0556	85,44	287,055	9,327
Cyanidin 3,5-O-diglucoside	Anthocyanins	C27 H31 O16	12380583	1997109	633,1433	9,842	9	Positive	611,1588	99,59	611,161	9,525
Cyanidin 3,5-O-diglucoside	Anthocyanins	C27 H31 O16	552908	63998	498,2603	9,386	5	Positive	611,1599	94,16	611,1605	9,267
Cyanidin 3-O-glucosyl-rutinoside	Anthocyanins	C33 H41 O20	15763531	2232682	498,2604	9,624	10	Positive	757,2184	98,02	757,2199	9,228
Cyanidin 3-O-sambubiosyl 5-O-glucoside	Anthocyanins	C32 H39 O20	819928	146538	122,0813	8,02	6	Positive	743,2008	98,12	743,2022	7,882
Cyanidin 3-O-xylosyl-rutinoside	Anthocyanins	C32 H39 O19	616059	104998	498,2602	9,248	6	Positive	727,2061	98,59	727,2078	9,129
Delphinidin 3-O-galactoside	Anthocyanins	C21 H21 O12	73741	19548	793,2173	9,366	3	Positive	465,1013	79,74	465,102	9,307
Malvidin 3-O-(6''-caffeoyl-glucoside)	Anthocyanins	C32 H31 O15	124325	20152	122,0814	12,871	2	Positive	655,1659	73,24	655,1654	12,752
Pelargonidin	Anthocyanins	C15 H11 O5	87330	15315	122,0813	15,424	2	Positive	271,061	75,96	271,0604	15,345
Pelargonidin 3,5-O-diglucoside	Anthocyanins	C27 H31 O15	464267	79017	512,276	10,792	5	Positive	595,1633	95,26	595,1655	10,633
Pelargonidin 3,5-O-diglucoside	Anthocyanins	C27 H31 O15	88740	13302	498,2603	9,228	2	Positive	595,1666	73,86	595,1659	9,109
Pelargonidin 3-O-(6''-malonyl-glucoside)	Anthocyanins	C24 H23 O13	4746437	653982	512,276	11,128	4	Positive	519,1116	88,4	501,1006	10,653
Peonidin	Anthocyanins	C16 H13 O6	100859	16029	122,0813	15,207	2	Positive	301,0713	85,16	301,0707	15,108
Petunidin 3-O-galactoside	Anthocyanins	C22 H23 O12	937456	145630	647,159	11,029	5	Positive	479,1183	99,74	479,1184	10,891

Petunidin 3-O-galactoside	Anthocyanins	C22 H23 O12	1159 225	208 814	633, 1433	9,78 2	4	Posi tive	479, 1187	99,3 3	479, 1182	9,52 5
Petunidin 3-O-rutinoside	Anthocyanins	C28 H33 O16	3293 453	418 411	498, 2604	9,40 6	4	Posi tive	625, 1769	99,7 9	625, 1765	9,20 8
Dihydromyricetin 3-O-rhamnoside	Dihydroflavon ols	C21 H22 O12	1563 20	217 89	122, 0814	10,3 56	3	Posi tive	466, 1108	78,7 3	471, 0896	10,1 98
Dihydroquercetin	Dihydroflavon ols	C15 H12 O7	3641 40	601 21	122, 0812	9,48 5	3	Posi tive	304, 058	85,4 4	287, 055	9,32 7
Dihydroquercetin 3-O-rhamnoside	Dihydroflavon ols	C21 H22 O11	1326 91	205 53	122, 0813	3,58 5	3	Posi tive	450, 118	88,2 4	473, 1075	3,48 6
(-)-Epigallocatechin 3-O-gallate	Flavanols	C22 H18 O11	1048 77	190 21	104, 1081	1,28 9	5	Posi tive	458, 0849	96,8 7	463, 0635	1,09 1
Eriodictyol	Flavanones	C15 H12 O6	8480 4	145 65	122, 0813	15,4 24	2	Posi tive	288, 0637	75,9 6	271, 0604	15,3 25
Hesperetin	Flavanones	C16 H14 O6	5496 54	941 56	122, 0813	17,7 21	3	Posi tive	302, 0791	99,1 9	285, 0757	17,5 23
Naringin 4'-O-glucoside	Flavanones	C33 H42 O19	2014 34	428 47	379, 1002	5,24 8	4	Posi tive	742, 232	74,1 6	765, 2201	5,14 9
6-Hydroxyluteolin	Flavones	C15 H10 O7	3065 53	231 70	498, 2603	9,40 6	3	Posi tive	302, 0426	81,5 3	303, 0499	9,30 7
6-Hydroxyluteolin	Flavones	C15 H10 O7	6314 12	481 77	122, 0813	8,23 8	2	Posi tive	302, 0425	81,9 2	303, 0498	8
7,3',4'-Trihydroxyflavone	Flavones	C15 H10 O5	8480 4	145 65	122, 0813	15,4 24	2	Posi tive	270, 0531	75,9 6	271, 0604	15,3 25
Apigenin 6-C-glucoside	Flavones	C21 H20 O10	1867 59	299 02	122, 0814	11,6 03	2	Posi tive	432, 1054	81,6 1	455, 0947	11,4 65
Apigenin 7-O-(6"-malonyl-aposyl-glucoside)	Flavones	C29 H30 O17	2737 5926	416 505 3	633, 1433	9,86 1	5	Posi tive	650, 1465	93,8 4	633, 1433	9,52 5
Chrysoeriol 7-O-(6"-malonyl-aposyl-glucoside)	Flavones	C30 H32 O18	1558 868	257 956	122, 0814	8,91 1	4	Posi tive	680, 1561	89,0 6	663, 1529	8,69 3

Apigenin 6,8-di-C-glucoside	Flavones	C27 H30 O15	1025 83	180 14	122, 0814	11,1 88	3	Posi tive	594, 1579	75,2 7	617, 1474	11,0 69
Apigenin 6,8-di-C-glucoside	Flavones	C27 H30 O15	1216 583	195 444	512, 276	10,8 51	6	Posi tive	594, 1583	99,2 9	617, 1476	10,6 33
Apigenin 6,8-di-C-glucoside	Flavones	C27 H30 O15	2118 70	362 69	122, 0814	10,2 37	4	Posi tive	594, 1583	95,2 4	617, 1473	10,0 99
Apigenin 6,8-di-C-glucoside	Flavones	C27 H30 O15	1094 96	156 54	498, 2603	9,22 8	3	Posi tive	594, 1586	73,8 6	595, 1659	9,14 9
Cirsilineol	Flavones	C18 H16 O7	1688 492	150 284	104, 1072	1,60 6	5	Posi tive	344, 0906	74,4 9	326, 08	1,24 9
Cirsimaritin	Flavones	C17 H14 O6	1171 96	175 11	122, 0813	17,8 2	3	Posi tive	314, 0794	80,0 1	297, 076	17,6 22
Diosmin	Flavones	C28 H32 O15	2140 45	341 93	122, 0813	7,84 2	3	Posi tive	608, 174	93,8 7	631, 163	7,72 3
Biochanin A	Isoflavonoids	C16 H12 O5	5496 54	941 56	122, 0813	17,7 21	3	Posi tive	284, 0685	99,1 9	285, 0757	17,5 23
Luteolin 7-O-(2-aposyl-glucoside)	Flavones	C26 H28 O15	9438 7	173 24	512, 276	10,7 13	3	Posi tive	580, 1422	73,9 1	603, 1315	10,6 14
Luteolin 7-O-(2-aposyl-glucoside)	Flavones	C26 H28 O15	1650 130	274 386	122, 0813	9,52 5	6	Posi tive	580, 1427	99,8 1	603, 132	9,32 7
3,7-Dimethylquercetin	Flavonols	C17 H14 O7	3808 22	531 20	122, 0813	3,07 1	4	Posi tive	330, 074	82,8 8	353, 0634	2,97 2
6,8-Dihydroxykaempferol	Flavonols	C15 H12 O8	1789 52	231 70	498, 2603	9,40 6	3	Posi tive	320, 0532	85,3 2	303, 0498	9,30 7
Isorhamnetin	Flavonols	C16 H12 O7	3770 503	597 412	647, 159	11,1 88	4	Posi tive	316, 0585	99,4 1	317, 0658	10,8 91
Isorhamnetin	Flavonols	C16 H12 O7	8459 500	102 623 4	498, 2604	9,42 6	4	Posi tive	316, 0587	99,1 2	317, 066	9,20 8
Isorhamnetin 3-O-galactoside	Flavonols	C22 H22 O12	5143 059	614 144	512, 276	11,1 28	7	Posi tive	478, 1112	99,6 7	479, 1185	10,6 53

Isorhamnetin 3-O-galactoside	Flavonols	C22 H22 O12	1012 507	170 007	633, 1433	9,78 2	4	Posi tive	478, 1109	99,3 3	479, 1182	9,52 5
Isorhamnetin 3-O-galactoside	Flavonols	C22 H22 O12	6719 38	893 24	498, 2604	9,40 6	3	Posi tive	478, 1107	96,9 3	479, 118	9,20 8
Isorhamnetin 3-O-glucoside 7-O-rhamnoside	Flavonols	C28 H32 O16	2406 153	412 039	512, 2761	10,7 72	7	Posi tive	624, 169	99,6 2	647, 1585	10,7 13
Isorhamnetin 3-O-glucoside 7-O-rhamnoside	Flavonols	C28 H32 O16	3122 074	395 386	498, 2604	9,40 6	4	Posi tive	624, 1691	99,7 9	625, 1765	9,20 8
Kaempferide	Flavonols	C16 H12 O6	9832 7	160 29	122, 0813	15,2 07	2	Posi tive	300, 0635	85,1 6	301, 0707	15,1 08
Kaempferol	Flavonols	C15 H10 O6	1411 30	215 11	512, 276	10,7 72	2	Posi tive	286, 0477	83,7 7	287, 055	10,6 33
Kaempferol	Flavonols	C15 H10 O6	3641 40	601 21	122, 0812	9,48 5	2	Posi tive	286, 0478	85,4 4	287, 055	9,32 7
Kaempferol	Flavonols	C15 H10 O6	3735 48	437 59	498, 2603	9,22 8	2	Posi tive	286, 0477	84,9	287, 0549	9,10 9
Kaempferol 3-O-(2''-rhamnosyl-6''-acetyl-galactoside) 7-O-rhamnoside	Flavonols	C35 H42 O20	2781 67	474 65	122, 0814	12,6 53	3	Posi tive	782, 2289	94,0 3	787, 2076	12,5 34
Kaempferol 3-O-(2''-rhamnosyl-galactoside) 7-O-rhamnoside	Flavonols	C33 H40 O19	4755 53	810 65	498, 2603	9,22 8	6	Posi tive	740, 2149	92,8 3	741, 2238	9,08 9
Kaempferol 3-O-(2''-rhamnosyl-galactoside) 7-O-rhamnoside	Flavonols	C33 H40 O19	5629 99	968 55	122, 0813	9,03	5	Posi tive	740, 2151	81,3 4	763, 2053	8,93 1
6-Hydroxyluteolin 7-O-rhamnoside	Flavones	C21 H20 O11	2087 14	249 43	512, 276	10,8 51	3	Posi tive	448, 1003	71,7 9	471, 0895	10,6 14
6-Hydroxyluteolin 7-O-rhamnoside	Flavones	C21 H20 O11	1563 20	217 89	122, 0814	10,3 56	3	Posi tive	448, 1003	78,7 3	471, 0896	10,1 98
Kaempferol 3-O-glucosyl-rhamnosyl-galactoside	Flavonols	C33 H40 O20	2524 6677	342 672 8	498, 2604	9,56 4	10	Posi tive	756, 2124	98,1 1	757, 2198	9,22 8
Kaempferol 3-O-glucosyl-rhamnosyl-galactoside	Flavonols	C33 H40 O20	4233 66	748 60	122, 0813	8,23 8	5	Posi tive	756, 2107	93,6 8	757, 2184	8,09 9

Kaempferol 3-O-glucosyl-rhamnosyl-galactoside	Flavonols	C33 H40 O20	4070 55	721 84	122, 0813	8,02	5	Posi tive	756, 2104	92,3 7	779, 2001	7,92 1
Kaempferol 3,7-O-diglucoside	Flavonols	C27 H30 O16	3180 9807	494 540 2	633, 1433	9,84 2	9	Posi tive	610, 1539	99,7 2	611, 1608	9,52 5
Kaempferol 3,7-O-diglucoside	Flavonols	C27 H30 O16	7851 39	106 755	498, 2603	9,38 6	6	Posi tive	610, 1532	98,6 9	633, 1421	9,26 7
Kaempferol 3-O-xylosyl-rutinoside	Flavonols	C32 H38 O19	1168 338	203 048	498, 2602	9,28 7	7	Posi tive	726, 2005	99,6 7	749, 1898	9,12 9
Myricetin 3-O-rhamnoside	Flavonols	C21 H20 O12	2399 79	342 58	122, 0812	9,50 5	4	Posi tive	464, 0949	80,3 5	487, 0842	9,30 7
Myricetin 3-O-rhamnoside	Flavonols	C21 H20 O12	7102 05	119 061	498, 2603	9,22 8	5	Posi tive	464, 0951	99,1 9	487, 0843	9,06 9
Myricetin 3-O-rutinoside	Flavonols	C27 H30 O17	8620 7	161 55	122, 0813	6,53 5	2	Posi tive	626, 1472	70,2 9	649, 1364	6,43 6
Quercetin 3-O-arabinoside	Flavonols	C20 H18 O11	3731 61	618 63	122, 0813	8,95 1	3	Posi tive	434, 0843	81,6 7	439, 0634	8,81 2
Quercetin 3-O-glucosyl-xyloside	Flavonols	C26 H28 O11	1160 82	128 51	122, 0812	3,03 1	3	Posi tive	516, 1626	74,3 5	521, 1416	2,91 2
Quercetin 3-O-xylosyl-rutinoside	Flavonols	C32 H38 O20	1514 109	258 241	122, 0813	8,06	7	Posi tive	742, 1952	99,1 6	765, 1846	7,88 2
Quercetin 4'-O-glucoside	Flavonols	C21 H20 O7	1318 19	184 00	498, 2603	9,21 5	3	Posi tive	384, 1199	96,7 4	366, 1088	9,14 9
Quercetin 7,4'-O-diglucoside	Flavonols	C27 H30 O12	2186 74	147 16	122, 0813	3,46 7	4	Posi tive	546, 173	74,0 7	551, 1524	3,13
6''-O-Acetyldaidzin	Isoflavonoids	C23 H22 O10	7083 6	127 14	122, 0814	8,71 3	3	Posi tive	458, 1218	87,0 8	481, 111	8,61 4
6''-O-Acetylgenistin	Isoflavonoids	C23 H22 O11	1161 92	206 90	122, 0812	6,06	4	Posi tive	474, 1158	98,7	497, 1052	5,96 1
6''-O-Acetylglycitin	Isoflavonoids	C24 H24 O11	8084 0	135 19	633, 1433	9,64 4	2	Posi tive	488, 1299	70,6 8	489, 1369	9,54 5

6''-O-Malonylgenistin	Isoflavonoids	C24 H22 O13	4036 996	653 982	512, 276	10,7 72	4	Posi tive	518, 1038	88,6 2	501, 1006	10,6 53
1-Acetoxy-pinoreosinol	Lignans	C22 H24 O8	4305 95	397 55	104, 1079	1,42 8	7	Posi tive	416, 1469	88,8 5	399, 143	1,15
Cyclolariciresinol	Lignans	C20 H24 O6	1889 23	139 56	293, 2116	21,0 87	2	Posi tive	360, 1568	83,6 6	343, 1535	20,9 48
Dimethylmatairesinol	Lignans	C22 H26 O6	2942 311	510 004	122, 0809	17,4 04	9	Posi tive	386, 1727	99,1 8	387, 18	17,1 67
Medioresinol	Lignans	C21 H24 O7	1459 49	282 60	349, 0897	4,91 2	4	Posi tive	388, 1521	78,1 1	371, 1474	4,85 3
Syringaresinol	Lignans	C22 H26 O8	3628 35	637 82	122, 0813	8,21 4	7	Posi tive	418, 1629	99,0 2	401, 1598	8,09 9
4-Vinylsyringol	Alkylmethoxyphenols	C10 H12 O3	7859 20	559 08	365, 106	21,2 79	2	Posi tive	180, 0786	87,7 2	163, 0753	20,9 48
4-Vinylsyringol	Alkylmethoxyphenols	C10 H12 O3	1646 50	261 50	122, 0813	3,10 4	2	Posi tive	180, 0785	73,5 4	181, 0862	2,99 2
3-Methylcatechol	Alkylphenols	C7 H8 O2	1440 489	233 037	263, 053	5,30 1	3	Posi tive	124, 0523	97,6 1	107, 0489	5,03 1
3-Methylcatechol	Alkylphenols	C7 H8 O2	7305 79	945 71	365, 1059	2,46 9	4	Posi tive	124, 0525	87,3 8	107, 0492	2,37 8
3-Methylcatechol	Alkylphenols	C7 H8 O2	9332 60	381 41	268, 1044	2,21 9	4	Posi tive	124, 0523	96,4 3	107, 0491	2,16
4-Ethylphenol	Alkylphenols	C8 H10 O	2939 994	483 571	122, 0814	3,56 6	3	Posi tive	122, 0734	97,9 7	105, 07	3,20 9
4-Vinylphenol	Alkylphenols	C8 H8 O	1702 360	356 392	166, 0866	2,47 7	3	Posi tive	120, 0575	87,7 8	103, 0543	2,41 7
5-Heneicosylresorcinol	Alkylphenols	C27 H48 O2	1574 244	278 40	738, 664	32,6 68	2	Posi tive	404, 3649	79,9 5	409, 3435	31,2 43
5-Nonadecenylresorcinol	Alkylphenols	C25 H42 O2	2523 718	178 31	738, 6639	33,8 16	6	Posi tive	374, 3185	87,6 9	357, 3149	30,8 86
p-Anisaldehyde	Hydroxybenzaldehydes	C8 H8 O2	8053 28	999 42	349, 0897	5,20 9	2	Posi tive	136, 0523	87,6 8	119, 049	4,85 3

Vanillin	Hydroxybenzaldehydes	C8 H8 O3	108027	22960	122,0813	6,903	4	Positive	152,0474	72,47	153,0548	6,813
2,3-Dihydroxy-1-guaiacylpropanone	Hydroxybenzoketones	C10 H12 O5	775731	135804	379,1002	5,347	3	Positive	212,0684	99,1	195,0651	5,169
3-Methoxyacetophenone	Hydroxybenzoketones	C9 H10 O2	1346476	140358	122,0813	2,477	4	Positive	150,068	96,09	151,0753	2,239
3-Methoxyacetophenone	Hydroxybenzoketones	C9 H10 O2	9001446	891711	268,1043	2,101	4	Positive	150,0678	99,48	151,0751	1,863
Sinapaldehyde	Hydroxycinnamaldehydes	C11 H12 O4	698443	95713	122,0813	7,208	3	Positive	208,0737	86,67	191,0703	6,852
Sinapaldehyde	Hydroxycinnamaldehydes	C11 H12 O4	226644	41466	122,0813	5,774	3	Positive	208,0736	86,97	191,0702	5,644
4-Hydroxycoumarin	Hydroxycoumarins	C9 H6 O3	1762692	173388	738,6634	29,758	3	Positive	162,0317	99,76	163,039	29,204
4-Hydroxycoumarin	Hydroxycoumarins	C9 H6 O3	1641060	259200	149,0237	21,482	3	Positive	162,0318	99,57	163,039	21,324
Esculin	Hydroxycoumarins	C15 H16 O9	948160	39878	268,1046	2,396	3	Positive	340,0794	83,21	363,0685	1,982
Mellein	Hydroxycoumarins	C10 H10 O3	883110	148494	263,053	5,169	4	Positive	178,0626	89,06	161,0594	5,031
1,4-Naphtoquinone	Naphtoquinones	C10 H6 O2	30329	6362	263,053	5,09	2	Positive	158,037	77,59	159,0438	5,031
3,4-Dihydroxyphenylglycol	Other polyphenols	C8 H10 O4	114150	20879	122,0813	6,892	3	Positive	170,0576	72,99	153,0548	6,813
Arbutin	Other polyphenols	C12 H16 O7	341707	62275	122,0814	7,365	3	Positive	272,0898	85,75	277,0685	7,268
Phlorin	Other polyphenols	C12 H16 O8	8534401	1179792	104,1081	1,566	7	Positive	288,0848	79,83	289,0921	1,091
Pyrogallol	Other polyphenols	C6 H6 O3	2532029	400225	104,1078	1,467	7	Positive	126,0321	97,23	127,0386	1,091

Carnosol	Phenolic terpenes	C20 H26 O4	204898	24092	365,106	20,79	2	Positive	330,1823	81,69	331,1896	20,671
Carvacrol	Phenolic terpenes	C10 H14 O	3470223	26102	738,6638	32,629	5	Positive	150,1047	85,7	133,1011	30,075
Hydroxytyrosol 4-O-glucoside	Tyrosols	C14 H20 O9	1645214	273179	122,0813	6,971	3	Positive	332,1111	92,33	337,0895	6,813
Ligstroside-aglycone	Tyrosols	C19 H21 O7	131819	18400	498,2603	9,215	3	Positive	361,1301	93,61	366,1088	9,149
Oleoside 11-methylester	Tyrosols	C17 H24 O11	1489223	212409	122,0813	6,753	4	Positive	404,1318	99,79	409,1105	6,496
Oleoside dimethylester	Tyrosols	C18 H26 O11	412480	72989	122,0812	6,039	5	Positive	418,1472	98,57	441,1361	5,941
2-Hydroxybenzoic acid	Hydroxybenzoic acids	C7 H6 O3	236325	35274	738,6632	29,544	3	Positive	138,0318	82,11	121,0285	29,204
2-Hydroxybenzoic acid	Hydroxybenzoic acids	C7 H6 O3	462447	61457	149,0237	21,733	2	Positive	138,0318	84,99	121,0285	21,562
2-Hydroxybenzoic acid	Hydroxybenzoic acids	C7 H6 O3	633511	96943	149,0237	21,463	2	Positive	138,0318	87,76	121,0285	21,324
2-Hydroxybenzoic acid	Hydroxybenzoic acids	C7 H6 O3	144844	26252	122,0807	2,75	3	Positive	138,032	76,71	139,0391	2,714
4-Hydroxybenzoic acid 4-O-glucoside	Hydroxybenzoic acids	C13 H16 O8	1641933	218941	122,0808	3,071	5	Positive	300,084	98,61	323,0731	2,695
5-O-Galloylquinic acid	Hydroxybenzoic acids	C14 H16 O10	493536	62396	349,0897	5,011	3	Positive	344,0744	97,45	367,0638	4,853
Benzoic acid	Hydroxybenzoic acids	C7 H6 O2	456330	54919	122,0813	6,991	3	Positive	122,0368	86,89	105,0334	6,694
Gallic acid ethyl ester	Hydroxybenzoic acids	C9 H10 O5	520483	46148	365,106	22,096	2	Positive	198,053	83,88	181,0497	21,562
Gallic acid ethyl ester	Hydroxybenzoic acids	C9 H10 O5	482804	68102	149,0237	21,463	2	Positive	198,053	87,25	181,0497	21,324
Protocatechuic acid 4-O-glucoside	Hydroxybenzoic acids	C13 H16 O9	310722	58437	104,1075	1,289	2	Positive	316,0802	83,48	321,0589	1,15

1,2-Diferuloylgentiobiose	Hydroxycinnamic acids	C32 H38 O17	284397	52408	122,0813	9,505	3	Positive	694,2104	96,49	717,1994	9,406
24-Methylcholestanol ferulate	Hydroxycinnamic acids	C38 H58 O4	452427	71485	738,6619	27,362	7	Positive	578,435	91,48	601,4223	27,184
24-Methylcholesterol ferulate	Hydroxycinnamic acids	C38 H56 O4	177047	14777	365,106	22,294	5	Positive	576,4159	84,78	599,4082	21,958
3,4-Diferuloylquinic acid	Hydroxycinnamic acids	C27 H28 O12	5038532	103088	122,0812	4,457	3	Positive	544,1608	76,55	527,1575	2,338
1-Caffeoylquinic acid	Hydroxycinnamic acids	C16 H18 O9	227871	22945	122,0808	2,794	3	Positive	354,0947	70,61	355,102	2,497
3-Feruloylquinic acid	Hydroxycinnamic acids	C17 H20 O9	558182	73138	122,0813	6,238	3	Positive	368,1108	84,92	391,1003	5,922
3-Sinapoylquinic acid	Hydroxycinnamic acids	C18 H22 O10	92293	16210	122,0813	7,268	3	Positive	398,1227	82,99	421,1105	7,149
3-p-Coumaroylquinic acid	Hydroxycinnamic acids	C16 H18 O8	132718	17624	122,0814	12,633	2	Positive	338,1001	71,53	339,1074	12,376
3-p-Coumaroylquinic acid	Hydroxycinnamic acids	C16 H18 O8	605925	82068	513,1582	6,615	4	Positive	338,1001	98,36	339,1071	6,258
3-p-Coumaroylquinic acid	Hydroxycinnamic acids	C16 H18 O8	236166	29579	122,0812	5,585	2	Positive	338,1003	72,84	339,1076	5,169
3-p-Coumaroylquinic acid	Hydroxycinnamic acids	C16 H18 O8	834472	71675	104,1068	1,626	3	Positive	338,1002	80,94	321,0966	1,348
5-5'-Dehydrodiferulic acid	Hydroxycinnamic acids	C20 H18 O8	91198	16065	122,0813	3,625	3	Positive	386,0999	76,5	369,0968	3,526
Caffeoyl glucose	Hydroxycinnamic acids	C15 H18 O9	213106	36786	122,0812	4,485	4	Positive	342,0939	76,32	343,1008	4,338
Caffeoyl glucose	Hydroxycinnamic acids	C15 H18 O9	80787	18900	166,0866	2,475	2	Positive	342,0945	76,52	343,1022	2,457
Caffeoyl tartaric acid	Hydroxycinnamic acids	C13 H12 O9	171284	26117	104,1075	1,302	3	Positive	312,0486	75,73	335,0377	1,131
Cinnamic acid	Hydroxycinnamic acids	C9 H8 O2	212557	36964	122,0812	18,691	2	Positive	148,0518	82,09	149,0592	18,632

Feruloyl glucose	Hydroxycinnamic acids	C16 H20 O9	3262 812	459 509	122, 0813	6,08	6	Positive	356, 1107	99,7 4	379, 0999	5,76 3
Feruloyl glucose	Hydroxycinnamic acids	C16 H20 O9	1283 5893	203 885 4	379, 1002	5,54 5	7	Positive	356, 1108	99,2 2	379, 1002	5,18 9
Hydroxycaffeic acid	Hydroxycinnamic acids	C9 H8 O5	4373 739	583 664	104, 1082	1,66 5	3	Positive	196, 0373	77,3 7	219, 027	1,07 1
Isoferulic acid	Hydroxycinnamic acids	C10 H10 O4	1218 398	128 547	122, 0813	15,7 41	3	Positive	194, 058	99,5 9	177, 0547	15,2 46
Isoferulic acid	Hydroxycinnamic acids	C10 H10 O4	2970 860	405 949	263, 053	5,50 6	7	Positive	194, 0578	99,7 2	177, 0546	5,16 9
m-Coumaric acid	Hydroxycinnamic acids	C9 H8 O3	2924 05	353 26	104, 1069	1,48 7	4	Positive	164, 0471	72,8 8	147, 0439	1,32 9
p-Coumaric acid 4-O-glucoside	Hydroxycinnamic acids	C15 H18 O8	1981 4472	279 549 8	349, 0898	5,20 9	5	Positive	326, 1005	99,1 9	349, 0898	4,85 3
p-Coumaric acid 4-O-glucoside	Hydroxycinnamic acids	C15 H18 O8	3576 963	264 592	104, 1072	1,86 3	6	Positive	326, 1014	77,6 8	308, 0909	1,24 9
p-Coumaric acid ethyl ester	Hydroxycinnamic acids	C11 H12 O3	2292 56	441 57	263, 053	5,08 6	2	Positive	192, 0787	85,3 5	193, 0859	4,99 1
Rosmarinic acid	Hydroxycinnamic acids	C18 H16 O8	5605 913	726 375	349, 0898	5,07	5	Positive	360, 0847	80,4	365, 064	4,85 3
Sinapic acid	Hydroxycinnamic acids	C11 H12 O5	3424 37	440 26	122, 0813	6,67 8	3	Positive	224, 0684	87,1	207, 0651	6,47 6
Sitostanyl ferulate	Hydroxycinnamic acids	C39 H60 O5	2615 79	336 92	738, 6639	30,5 47	4	Positive	608, 4421	78,8	590, 4294	30,5 1
Stigmastanol ferulate	Hydroxycinnamic acids	C39 H60 O4	1183 30	117 64	738, 6629	28,2 93	3	Positive	592, 4514	73,4 9	615, 4405	28,2 14
3,4-dihydroxyphenyl-2-oxypropanoic acid	Hydroxyphenyl propanoic acids	C9 H8 O4	1100 938	163 922	738, 6632	29,4 94	4	Positive	180, 0423	99,7	163, 039	29,2 04

3,4-dihydroxyphenyl-2-oxypropanoic acid	Hydroxyphenyl propanoic acids	C9 H8 O4	2092705	324445	149,0237	21,482	5	Positive	180,0424	99,57	163,039	21,324
Dihydro-p-coumaric acid	Hydroxyphenyl propanoic acids	C9 H10 O3	212557	36964	122,0812	18,691	2	Positive	166,0623	82,09	149,0592	18,632
Dihydro-p-coumaric acid	Hydroxyphenyl propanoic acids	C9 H10 O3	179731	44575	166,0868	2,477	2	Positive	166,0627	77,02	149,0597	2,417
Dihydrocaffeic acid	Hydroxyphenyl propanoic acids	C9 H10 O4	524041	85100	349,0898	5,031	3	Positive	182,0579	87,53	165,0545	4,853
d-Viniferin	Stilbenes	C28 H22 O6	56780	10965	122,0813	8,772	2	Positive	454,1414	72,54	436,1294	8,693
Cyanidin	Anthocyanins	C15 H11 O6	267777	43667	498,2604	9,21	2	Positive	287,0555	85,85	287,0549	9,111
Cyanidin 3,5-O-diglucoside	Anthocyanins	C27 H31 O16	12405550	1990624	633,1435	9,883	8	Positive	611,1589	99,18	611,1612	9,507
Cyanidin 3,5-O-diglucoside	Anthocyanins	C27 H31 O16	585836	64811	498,2604	9,368	5	Positive	611,1601	93,6	611,1606	9,249
Cyanidin 3-O-(6''-acetyl-galactoside)	Anthocyanins	C23 H23 O12	148988	23662	122,0813	3,627	3	Positive	491,1184	82,09	473,1077	3,508
Cyanidin 3-O-glucosyl-rutinoside	Anthocyanins	C33 H41 O20	16207071	2365763	498,2603	9,606	10	Positive	757,2182	98,59	757,2196	9,21
Cyanidin 3-O-sambubiosyl 5-O-glucoside	Anthocyanins	C32 H39 O20	828128	141635	122,0813	8,002	6	Positive	743,2009	97,95	743,2022	7,863
Cyanidin 3-O-xylosyl-rutinoside	Anthocyanins	C32 H39 O19	614942	110475	498,2604	9,229	6	Positive	727,206	98,71	727,2076	9,111
Delphinidin 3-O-galactoside	Anthocyanins	C21 H21 O12	78941	14698	122,0813	7,23	3	Positive	465,1011	70,9	465,1003	7,131

Malvidin 3-O-(6''-caffeoyl-glucoside)	Anthocyanins	C32 H31 O15	1280 24	191 91	122, 0813	12,8 72	2	Posi tive	655, 1657	72,6 5	655, 1651	12,7 34
Pelargonidin 3,5-O-diglucoside	Anthocyanins	C27 H31 O15	8966 7	142 76	498, 2605	9,21	2	Posi tive	595, 1661	70,8 7	595, 1657	9,09 1
Pelargonidin 3-O-(6''-malonyl-glucoside)	Anthocyanins	C24 H23 O13	4620 250	621 294	512, 276	11,0 9	4	Posi tive	519, 1115	88,0 3	501, 1005	10,6 35
Pelargonidin 3-O-galactoside	Anthocyanins	C21 H21 O10	3095 05	296 68	268, 1047	1,82 5	3	Posi tive	433, 1118	75,5 5	415, 0997	1,60 7
Pelargonidin 3-O-galactoside	Anthocyanins	C21 H21 O10	1703 41	322 50	104, 1071	1,48 9	3	Posi tive	433, 1114	84,4 2	415, 1006	1,46 9
Peonidin	Anthocyanins	C16 H13 O6	9674 8	177 23	122, 0813	15,1 88	2	Posi tive	301, 0712	75,1 6	301, 0706	15,0 89
Petunidin 3-O-galactoside	Anthocyanins	C22 H23 O12	9293 39	142 040	647, 1592	11,0 11	5	Posi tive	479, 1181	99,7 3	479, 1184	10,8 53
Petunidin 3-O-galactoside	Anthocyanins	C22 H23 O12	1215 910	203 559	633, 1435	9,74 4	4	Posi tive	479, 1188	99,5 5	479, 1184	9,50 7
Petunidin 3-O-rutinoside	Anthocyanins	C28 H33 O16	3365 883	435 971	498, 2603	9,38 8	4	Posi tive	625, 1769	99,8 1	625, 1765	9,19
3-Hydroxyphloretin 2'-O-xylosyl-glucoside	Dihydrochalco nes	C26 H32 O15	5064 6	133 44	122, 0813	6,69 2	2	Posi tive	584, 1736	75,5 3	585, 1811	6,65 6
Dihydromyricetin 3-O-rhamnoside	Dihydroflavon ols	C21 H22 O12	1174 62	198 41	122, 0814	10,2 98	3	Posi tive	466, 1106	78,3 2	471, 0893	10,1 8
Dihydroquercetin	Dihydroflavon ols	C15 H12 O7	2420 36	415 00	498, 2604	9,21	3	Posi tive	304, 0579	85,8 5	287, 0549	9,11 1
Dihydroquercetin 3-O-rhamnoside	Dihydroflavon ols	C21 H22 O11	9988 7	188 03	122, 0813	3,58 3	3	Posi tive	450, 1178	81,9 8	473, 1073	3,52 8
(-)-Epigallocatechin 3-O-gallate	Flavanols	C22 H18 O11	7284 3	163 15	104, 1081	1,21 1	4	Posi tive	458, 0848	92,4 5	463, 0634	1,07 3
Hesperetin	Flavanones	C16 H14 O6	5079 79	862 17	122, 0813	17,7 42	3	Posi tive	302, 079	99,6 1	285, 0757	17,5 25
Naringin 4'-O-glucoside	Flavanones	C33 H42 O19	1994 21	439 18	379, 1002	5,23	4	Posi tive	742, 2323	75,5 4	765, 2205	5,15 1

6-Hydroxyluteolin	Flavones	C15 H10 O7	2595 22	209 89	498, 2604	9,39 5	3	Posi tive	302, 0427	84,8 3	303, 05	9,24 9
6-Hydroxyluteolin	Flavones	C15 H10 O7	5942 72	498 10	122, 0813	8,20 7	2	Posi tive	302, 0426	81,4	303, 0499	7,98 2
Apigenin 6-C-glucoside	Flavones	C21 H20 O10	1561 18	256 18	122, 0813	11,5 75	2	Posi tive	432, 1054	81,3 1	455, 0945	11,4 47
Apigenin 6-C-glucoside	Flavones	C21 H20 O10	6572 4	155 20	513, 1583	6,31 2	2	Posi tive	432, 107	77,7 1	455, 0962	6,24
Apigenin 6-C-glucoside	Flavones	C21 H20 O10	1169 82	307 33	104, 1071	1,48 8	3	Posi tive	432, 1035	81,9 3	415, 1005	1,46 9
Apigenin 7-O-(6''-malonyl-apiosyl-glucoside)	Flavones	C29 H30 O17	2810 0701	426 558 0	633, 1435	10,0 02	5	Posi tive	650, 1467	94,7 4	633, 1435	9,50 7
Apigenin 7-O-apiosyl-glucoside	Flavones	C26 H28 O14	8714 9	200 60	104, 1081	1,21 1	6	Posi tive	564, 1483	71,2 5	569, 1277	1,11 2
Apigenin 7-O-glucuronide	Flavones	C21 H18 O11	4862 1	105 29	122, 0813	7,14	2	Posi tive	446, 0847	70,8 4	451, 0633	7,05 2
Chrysoeriol 7-O-(6''-malonyl-apiosyl-glucoside)	Flavones	C30 H32 O18	1528 832	264 690	122, 0813	8,86 2	4	Posi tive	680, 1564	90,4 8	663, 1532	8,67 5
Apigenin 6,8-di-C-glucoside	Flavones	C27 H30 O15	7551 7	162 77	122, 0813	11,1 4	3	Posi tive	594, 1583	73,7 8	617, 1474	11,0 51
Apigenin 6,8-di-C-glucoside	Flavones	C27 H30 O15	1125 562	185 089	512, 276	10,8 03	6	Posi tive	594, 1582	99,1 8	617, 1475	10,6 15
Apigenin 6,8-di-C-glucoside	Flavones	C27 H30 O15	1814 61	312 13	122, 0814	10,1 94	4	Posi tive	594, 1581	92,3 2	617, 1472	10,1 01
Apigenin 6,8-di-C-glucoside	Flavones	C27 H30 O15	8753 8	135 99	498, 2605	9,20 5	3	Posi tive	594, 1583	70,8 7	595, 1657	9,13
Cirsimaritin	Flavones	C17 H14 O6	8548 7	153 74	122, 0813	17,8 09	3	Posi tive	314, 0793	84,9 5	297, 0759	17,6 24
Diosmin	Flavones	C28 H32 O15	1932 91	330 24	122, 0813	7,81 5	3	Posi tive	608, 174	94,7 5	631, 1631	7,70 5

Biochanin A	Isoflavonoids	C16 H12 O5	4776 87	847 01	122, 0813	17,7 29	3	Posi tive	284, 0684	99,6 4	285, 0757	17,5 25
Luteolin 7-O-(2-apiosyl-glucoside)	Flavones	C26 H28 O15	1693 375	281 585	122, 0813	9,49 6	6	Posi tive	580, 1426	99,3 5	603, 1318	9,30 9
3,7-Dimethylquercetin	Flavonols	C17 H14 O7	3972 14	534 04	122, 0813	3,09 2	4	Posi tive	330, 0742	83,3 5	353, 0636	2,99 3
6,8-Dihydroxykaempferol	Flavonols	C15 H12 O8	3004 37	225 05	498, 2604	9,40 8	3	Posi tive	320, 0533	85,1 1	303, 05	9,24 9
Isorhamnetin	Flavonols	C16 H12 O7	7320 005	123 756 0	633, 1435	9,84 3	4	Posi tive	316, 0587	98,7 4	317, 066	9,50 7
Isorhamnetin	Flavonols	C16 H12 O7	8186 513	991 745	498, 2603	9,40 8	4	Posi tive	316, 0586	99,1 5	317, 0659	9,19
Isorhamnetin 3-O-galactoside	Flavonols	C22 H22 O12	4990 032	581 451	512, 276	11,0 9	7	Posi tive	478, 1112	99,6 1	479, 1185	10,6 55
Isorhamnetin 3-O-galactoside	Flavonols	C22 H22 O12	9859 08	165 075	633, 1435	9,74 4	4	Posi tive	478, 111	99,5 5	479, 1184	9,50 7
Isorhamnetin 3-O-galactoside	Flavonols	C22 H22 O12	7003 26	873 13	498, 2603	9,38 8	3	Posi tive	478, 1108	96,7 6	479, 1182	9,19
Isorhamnetin 3-O-glucoside 7-O-rhamnoside	Flavonols	C28 H32 O16	2190 255	369 038	512, 276	10,7 54	7	Posi tive	624, 1689	99,5 4	647, 1583	10,6 94
Isorhamnetin 3-O-glucoside 7-O-rhamnoside	Flavonols	C28 H32 O16	3211 871	408 723	498, 2603	9,38 8	4	Posi tive	624, 1691	99,8 1	625, 1765	9,19
Kaempferide	Flavonols	C16 H12 O6	9674 8	177 23	122, 0813	15,1 88	2	Posi tive	300, 0634	75,1 6	301, 0706	15,0 89
Kaempferol	Flavonols	C15 H10 O6	3583 02	591 82	122, 0813	9,48 7	2	Posi tive	286, 0477	85,6 3	287, 0549	9,30 9
Kaempferol	Flavonols	C15 H10 O6	2677 77	436 67	498, 2604	9,21	2	Posi tive	286, 0477	85,8 5	287, 0549	9,11 1
Kaempferol	Flavonols	C15 H10 O6	1064 32	191 06	122, 0813	9,01 2	2	Posi tive	286, 0479	83,8 6	287, 0551	8,91 3

Kaempferol 3-O-(2''-rhamnosyl-6''-acetyl-galactoside) 7-O-rhamnoside	Flavonols	C35 H42 O20	4166 79	675 80	122, 0813	12,8 72	3	Posi tive	782, 2286	94,6 8	787, 2072	12,7 34
Kaempferol 3-O-(2''-rhamnosyl-galactoside) 7-O-rhamnoside	Flavonols	C33 H40 O19	4679 17	786 62	498, 2605	9,21	6	Posi tive	740, 2144	92,8 7	741, 223	9,07 1
Kaempferol 3-O-(2''-rhamnosyl-galactoside) 7-O-rhamnoside	Flavonols	C33 H40 O19	5576 26	990 14	122, 0813	9,01 2	6	Posi tive	740, 2151	82,0 3	763, 2053	8,91 3
Kaempferol 3-O-acetyl-glucoside	Flavonols	C23 H22 O12	1379 90	209 70	122, 0813	3,62 7	3	Posi tive	490, 1106	82,0 9	473, 1077	3,52 8
6-Hydroxyluteolin 7-O-rhamnoside	Flavones	C21 H20 O11	1878 19	217 39	512, 276	10,8 33	5	Posi tive	448, 1004	71,9 3	471, 0893	10,6 15
6-Hydroxyluteolin 7-O-rhamnoside	Flavones	C21 H20 O11	1562 36	220 08	122, 0813	10,3 78	3	Posi tive	448, 1	75,0 3	471, 0893	10,1 8
Kaempferol 3-O-glucosyl-rhamnosyl-galactoside	Flavonols	C33 H40 O20	2606 7602	364 186 5	498, 2603	9,54 6	10	Posi tive	756, 2122	98,5 9	757, 2196	9,21
Kaempferol 3-O-glucosyl-rhamnosyl-galactoside	Flavonols	C33 H40 O20	4270 36	774 28	122, 0813	8,24	5	Posi tive	756, 2109	86,4 3	757, 2186	8,08 1
Kaempferol 3-O-glucosyl-rhamnosyl-galactoside	Flavonols	C33 H40 O20	4093 51	747 20	122, 0813	8,00 2	5	Posi tive	756, 2106	96,4 3	779, 2001	7,90 3
Kaempferol 3,7-O-diglucoside	Flavonols	C27 H30 O16	3252 7093	502 327 4	633, 1435	10,0 02	9	Posi tive	610, 1541	99,3 3	611, 1611	9,50 7
Kaempferol 3,7-O-diglucoside	Flavonols	C27 H30 O16	8369 96	105 361	498, 2603	9,36 8	6	Posi tive	610, 1533	97,9 7	633, 1421	9,24 9
Kaempferol 3-O-xylosyl-rutinoside	Flavonols	C32 H38 O19	1175 877	204 281	498, 2604	9,26 9	7	Posi tive	726, 2004	99,1 9	749, 1897	9,11 1
Myricetin 3-O-rhamnoside	Flavonols	C21 H20 O12	2409 77	323 85	122, 0813	9,46 7	4	Posi tive	464, 0949	79,3 4	487, 084	9,28 9
Myricetin 3-O-rhamnoside	Flavonols	C21 H20 O12	6896 21	111 324	498, 2605	9,19	5	Posi tive	464, 095	99,1 1	487, 0843	9,05 1
Myricetin 3-O-rhamnoside	Flavonols	C21 H20 O12	7894 1	146 98	122, 0813	7,23	3	Posi tive	464, 0933	70,9	465, 1003	7,13 1

Myricetin 3-O-rutinoside	Flavonols	C27 H30 O17	8499 1	138 38	122, 0813	6,51 7	2	Posi tive	626, 1477	74,0 2	649, 137	6,41 8
Quercetin 3-O-arabinoside	Flavonols	C20 H18 O11	3856 07	612 63	122, 0813	8,95 2	3	Posi tive	434, 0842	82,6 1	439, 0632	8,81 4
Quercetin 3-O-glucosyl-xyloside	Flavonols	C26 H28 O11	1280 47	144 60	122, 0813	3,05 3	3	Posi tive	516, 1627	82,9 9	521, 1417	2,89 4
Quercetin 3-O-xylosyl-rutinoside	Flavonols	C32 H38 O20	1481 272	244 569	122, 0813	8,03 5	7	Posi tive	742, 1952	99,2 2	765, 1845	7,86 3
Quercetin 4'-O-glucoside	Flavonols	C21 H20 O7	4404 89	322 12	122, 0813	8,15 2	3	Posi tive	384, 1199	96,5 3	366, 1087	7,94 3
Rhamnetin	Flavonols	C16 H27 O7	3664 6	519 5	336, 2285	5,36 9	2	Posi tive	331, 1759	74,3 3	313, 1632	5,27
6''-O-Acetyldaidzin	Isoflavonoids	C23 H22 O10	6868 9	122 11	122, 0814	8,69 5	3	Posi tive	458, 1217	76,0 8	481, 1106	8,59 6
6''-O-Acetylgenistin	Isoflavonoids	C23 H22 O11	1275 57	222 98	122, 0813	10,0 61	3	Posi tive	474, 1156	94,6 6	497, 1051	9,96 2
6''-O-Malonylgenistin	Isoflavonoids	C24 H22 O13	3909 390	621 294	512, 276	10,7 54	4	Posi tive	518, 1037	88,1 9	501, 1006	10,6 35
Glycitin	Isoflavonoids	C22 H22 O10	5210 1	103 23	122, 0813	9,09 1	3	Posi tive	446, 122	70,1 5	451, 1001	9,01 2
1-Acetoxy-pinorezinol	Lignans	C22 H24 O8	4202 85	340 13	104, 1079	1,40 9	7	Posi tive	416, 1475	86,7 9	439, 1373	1,15 2
Cyclolariciresinol	Lignans	C20 H24 O6	1969 62	157 19	293, 2115	21,1 08	2	Posi tive	360, 1568	83,4	343, 1534	20,9 5
Dimethylmatairesinol	Lignans	C22 H26 O6	2946 071	513 546	122, 0809	17,3 86	9	Posi tive	386, 1726	98,5 6	387, 1798	17,1 68
Medioresinol	Lignans	C21 H24 O7	1677 10	299 90	349, 0898	4,93 3	3	Posi tive	388, 1517	79,4 2	371, 1468	4,85 4
Syringaresinol	Lignans	C22 H26 O8	3662 96	635 72	122, 0813	8,19 6	7	Posi tive	418, 1629	98,5 9	401, 1596	8,08 1
4-Vinylsyringol	Alkylmethoxyphenols	C10 H12 O3	8081 92	571 68	365, 106	21,2 22	2	Posi tive	180, 0786	87,4 8	163, 0753	20,9 3

3-Methylcatechol	Alkylphenols	C7 H8 O2	1304 091	212 286	263, 053	5,31 2	3	Posi tive	124, 0524	98,1 1	107, 049	5,03 2
3-Methylcatechol	Alkylphenols	C7 H8 O2	1193 045	226 91	122, 0813	4,22 1	4	Posi tive	124, 0526	95,2 7	107, 0491	3,29
3-Methylcatechol	Alkylphenols	C7 H8 O2	2441 73	821 76	365, 1059	2,39 5	5	Posi tive	124, 0525	94,4 7	107, 0491	2,37 9
4-Ethylphenol	Alkylphenols	C8 H10 O	2880 789	467 082	122, 0815	3,50 8	3	Posi tive	122, 0734	97,3	105, 0701	3,21 1
4-Vinylphenol	Alkylphenols	C8 H8 O	1388 753	370 654	166, 0864	2,47 8	3	Posi tive	120, 0573	87,6 1	103, 0541	2,43 9
5-Heneicosylresorcinol	Alkylphenols	C27 H48 O2	3840 82	198 59	738, 6643	31,7	2	Posi tive	404, 3656	81,1 3	409, 3443	31,3 04
5-Nonadecenylresorcinol	Alkylphenols	C25 H42 O2	2599 023	167 64	738, 6641	33,8 38	5	Posi tive	374, 3186	83,2	357, 315	31,2 64
Demethoxycurcumin	Curcuminoids	C20 H18 O5	1225 1	206 25	365, 1058	2,36	4	Posi tive	338, 1159	76,0 9	343, 0924	2,36
p-Anisaldehyde	Hydroxybenzaldehydes	C8 H8 O2	8080 80	107 481	349, 0898	5,17 1	2	Posi tive	136, 0523	87,8 6	119, 049	4,85 4
Vanillin	Hydroxybenzaldehydes	C8 H8 O3	1164 70	224 75	122, 0813	6,90 4	3	Posi tive	152, 0476	86,7 3	153, 0546	6,79 4
2,3-Dihydroxy-1-guaiacylpropanone	Hydroxybenzo ketones	C10 H12 O5	8662 11	140 583	263, 0531	5,32 4	4	Posi tive	212, 0684	99,5 7	195, 065	5,19 1
3-Methoxyacetophenone	Hydroxybenzo ketones	C9 H10 O2	7341 66	122 507	122, 0813	4,61 7	5	Posi tive	150, 068	97,5 6	151, 0754	4,45 8
3-Methoxyacetophenone	Hydroxybenzo ketones	C9 H10 O2	8982 132	908 860	268, 1044	2,10 2	4	Posi tive	150, 068	99,8	151, 0753	1,86 5
Sinapaldehyde	Hydroxycinnamaldehydes	C11 H12 O4	2325 70	318 01	149, 0236	21,4 84	4	Posi tive	208, 0741	97,6 4	209, 0812	21,3 26
Sinapaldehyde	Hydroxycinnamaldehydes	C11 H12 O4	2977 61	440 62	122, 0813	6,00 2	3	Posi tive	208, 0736	86,9	191, 0704	5,64 6
4-Hydroxycoumarin	Hydroxycoumarins	C9 H6 O3	1330 086	162 440	149, 0236	21,9	3	Posi tive	162, 0317	99,7 2	163, 0389	21,5 83

4-Hydroxycoumarin	Hydroxycoumarins	C9 H6 O3	1662054	246303	149,0236	21,484	3	Positive	162,0317	99,82	163,039	21,326
Esculin	Hydroxycoumarins	C15 H16 O9	927890	38826	268,1045	2,379	3	Positive	340,0795	82,85	363,0686	2,003
Mellein	Hydroxycoumarins	C10 H10 O3	804853	133386	263,053	5,171	4	Positive	178,0626	90,71	161,0594	5,032
Acetyl eugenol	Hydroxyphenylpropenes	C12 H14 O3	1909686	259560	104,1074	1,528	5	Positive	206,0934	84,11	229,0821	1,132
1,4-Naphtoquinone	Naphtoquinones	C10 H6 O2	31754	5755	263,053	5,112	2	Positive	158,0367	74,94	159,0436	5,032
3,4-Dihydroxyphenylglycol	Other polyphenols	C8 H10 O4	123980	22163	122,0813	6,913	3	Positive	170,0576	88,62	153,0546	6,814
Arbutin	Other polyphenols	C12 H16 O7	347370	59425	122,0813	7,385	2	Positive	272,0899	85,83	277,0686	7,269
Phlorin	Other polyphenols	C12 H16 O8	8598372	1174981	104,108	1,588	7	Positive	288,0848	78,88	293,0639	1,093
Pyrogallol	Other polyphenols	C6 H6 O3	565580	112036	365,1033	23,226	3	Positive	126,0319	97,47	149,0211	23,147
Carnosol	Phenolic terpenes	C20 H26 O4	187117	24228	365,106	20,791	2	Positive	330,1824	82,1	331,1895	20,672
Carvacrol	Phenolic terpenes	C10 H14 O	2857764	23649	738,6642	32,452	5	Positive	150,1046	85,56	133,1011	30,136
Hydroxytyrosol 4-O-glucoside	Tyrosols	C14 H20 O9	1627987	271848	122,0814	6,992	5	Positive	332,1112	92,01	337,0895	6,794
Ligstroside-aglycone	Tyrosols	C19 H21 O7	1099644	110483	263,053	5,205	3	Positive	361,1298	93,2	366,1087	5,072
Oleoside 11-methylester	Tyrosols	C17 H24 O11	1894329	313653	122,0813	7,818	5	Positive	404,1318	99,82	409,1104	7,626
Oleoside dimethylester	Tyrosols	C18 H26 O11	441908	69701	122,0813	6,042	4	Positive	418,1471	98,6	441,1362	5,943

2-Hydroxybenzoic acid	Hydroxybenzoic acids	C7 H6 O3	2211 17	334 96	738, 664	29,4 43	3	Positive	138, 0318	75,0 3	121, 0285	29,2 05
2-Hydroxybenzoic acid	Hydroxybenzoic acids	C7 H6 O3	5796 39	623 82	365, 106	21,9 5	2	Positive	138, 0319	84,6 7	121, 0286	21,5 63
2-Hydroxybenzoic acid	Hydroxybenzoic acids	C7 H6 O3	6647 28	977 87	149, 0236	21,4 64	2	Positive	138, 0318	86,8	121, 0285	21,3 26
2-Hydroxybenzoic acid	Hydroxybenzoic acids	C7 H6 O3	1740 77	275 69	122, 0809	2,83 8	3	Positive	138, 032	76,9	139, 0392	2,69 6
4-Hydroxybenzoic acid 4-O-glucoside	Hydroxybenzoic acids	C13 H16 O8	1612 055	217 556	122, 0807	3,07 2	4	Positive	300, 0841	99,0 3	323, 0733	2,71 6
5-O-Galloylquinic acid	Hydroxybenzoic acids	C14 H16 O10	4927 40	657 89	349, 0898	5,01 3	2	Positive	344, 0745	84,1 9	367, 0637	4,85 4
Benzoic acid	Hydroxybenzoic acids	C7 H6 O2	4377 13	505 18	122, 0813	6,99 2	3	Positive	122, 0368	86,8 2	105, 0334	6,69 5
Gallic acid ethyl ester	Hydroxybenzoic acids	C9 H10 O5	5845 23	483 13	365, 106	22,2 36	2	Positive	198, 053	84,1 2	181, 0497	21,5 63
Gallic acid ethyl ester	Hydroxybenzoic acids	C9 H10 O5	4562 99	647 93	149, 0236	21,4 64	2	Positive	198, 0529	87,1 5	181, 0496	21,3 26
Protocatechuic acid 4-O-glucoside	Hydroxybenzoic acids	C13 H16 O9	2810 21	542 34	104, 1075	1,27 1	2	Positive	316, 0801	80,2 4	321, 0587	1,15 2
1,2-Diferuloylgentiobiose	Hydroxycinnamic acids	C32 H38 O17	2080 55	346 88	633, 1435	9,72 4	3	Positive	694, 2103	96,7 3	717, 1997	9,56 6
1-Sinapoyl-2-feruloylgentiobiose	Hydroxycinnamic acids	C33 H40 O18	1532 49	264 77	122, 0813	8,45 7	3	Positive	724, 2185	78,4 7	707, 2151	8,35 8
2-S-Glutathionyl caftaric acid	Hydroxycinnamic acids	C23 H27 N3 O15 S	2496 7	927 5	104, 1081	1,13 2	3	Positive	617, 1177	81,1 5	599, 1084	1,07 3
24-Methylcholestanol ferulate	Hydroxycinnamic acids	C38 H58 O4	5194 89	782 53	738, 6619	27,4 83	6	Positive	578, 4346	87,6 1	583, 4142	27,1 86
24-Methylcholesterol ferulate	Hydroxycinnamic acids	C38 H56 O4	1700 70	132 83	365, 106	22,3 16	4	Positive	576, 4159	81,6 4	599, 4082	21,9 79

3,4-Diferuloylquinic acid	Hydroxycinnamic acids	C27 H28 O12	665159	27848	122,0813	4,399	3	Positive	544,1598	81,76	527,1568	4,062
1-Caffeoylquinic acid	Hydroxycinnamic acids	C16 H18 O9	173955	29925	122,0814	2,32	4	Positive	354,0956	79,76	359,0749	2,221
3-Feruloylquinic acid	Hydroxycinnamic acids	C17 H20 O9	171179	21061	122,0813	7,547	3	Positive	368,1119	71,72	373,0893	7,448
3-Feruloylquinic acid	Hydroxycinnamic acids	C17 H20 O9	578685	68526	122,0813	6,26	5	Positive	368,1124	83,13	391,1003	5,923
3-Sinapoylquinic acid	Hydroxycinnamic acids	C18 H22 O10	63446	15386	122,0813	7,235	2	Positive	398,1211	81,78	421,1102	7,151
3-Sinapoylquinic acid	Hydroxycinnamic acids	C18 H22 O10	242386	18689	268,1045	1,805	4	Positive	398,1212	78,71	399,1273	1,508
3-p-Coumaroylquinic acid	Hydroxycinnamic acids	C16 H18 O8	86727	15718	122,0813	12,467	2	Positive	338,1001	83,97	339,1074	12,357
3-p-Coumaroylquinic acid	Hydroxycinnamic acids	C16 H18 O8	573859	80409	513,1583	6,61	4	Positive	338,1002	98,79	339,1072	6,24
3-p-Coumaroylquinic acid	Hydroxycinnamic acids	C16 H18 O8	161105	30583	379,1002	5,369	2	Positive	338,1	81,2	339,1074	5,171
3-p-Coumaroylquinic acid	Hydroxycinnamic acids	C16 H18 O8	923491	74663	104,1069	1,586	3	Positive	338,1008	79,24	321,0972	1,33
Caffeoyl glucose	Hydroxycinnamic acids	C15 H18 O9	210036	36101	122,0813	4,474	5	Positive	342,0943	87,22	343,1009	4,359
Caffeoyl glucose	Hydroxycinnamic acids	C15 H18 O9	43140	18393	365,1058	2,574	2	Positive	342,094	71,55	343,1019	2,498
Caffeoyl tartaric acid	Hydroxycinnamic acids	C13 H12 O9	170139	26434	104,1075	1,305	3	Positive	312,0486	73,57	335,0378	1,132
Cinnamic acid	Hydroxycinnamic acids	C9 H8 O2	202112	38363	122,0812	18,673	2	Positive	148,0518	79,83	149,0592	18,613
Feruloyl glucose	Hydroxycinnamic acids	C16 H20 O9	632220	80884	122,0813	6,359	5	Positive	356,1107	99	339,1072	6,24

Feruloyl glucose	Hydroxycinnamic acids	C16 H20 O9	1293 9703	207 528 7	379, 1002	5,52 7	7	Positive	356, 1108	99,1 5	379, 1002	5,19 1
Hydroxycaffeic acid	Hydroxycinnamic acids	C9 H8 O5	4223 809	570 955	104, 1082	1,66 7	3	Positive	196, 0373	77,5 9	219, 0269	1,07 3
Isoferulic acid	Hydroxycinnamic acids	C10 H10 O4	1129 345	130 409	122, 0813	15,6 64	3	Positive	194, 0581	99,6 6	177, 0547	15,2 48
Isoferulic acid	Hydroxycinnamic acids	C10 H10 O4	2891 240	392 940	263, 0531	5,44 8	6	Positive	194, 0578	99,5 7	195, 065	5,19 1
m-Coumaric acid	Hydroxycinnamic acids	C9 H8 O3	3025 42	329 19	104, 1068	1,56 8	4	Positive	164, 0469	75,9 5	165, 0547	1,33
p-Coumaric acid 4-O-glucoside	Hydroxycinnamic acids	C15 H18 O8	2008 3070	288 425 8	349, 0898	5,21 1	5	Positive	326, 1006	98,9 4	349, 0898	4,85 4
p-Coumaric acid 4-O-glucoside	Hydroxycinnamic acids	C15 H18 O8	1610 79	271 96	122, 0812	4,65 6	2	Positive	326, 101	82,7 9	349, 0903	4,57 7
p-Coumaric acid ethyl ester	Hydroxycinnamic acids	C11 H12 O3	2418 48	440 00	263, 053	5,09 2	2	Positive	192, 0787	85,5 6	193, 086	4,99 3
Rosmarinic acid	Hydroxycinnamic acids	C18 H16 O8	5613 804	742 746	349, 0898	5,09 2	4	Positive	360, 0848	80,3 4	365, 064	4,85 4
Sinapic acid	Hydroxycinnamic acids	C11 H12 O5	5820 03	981 18	263, 0531	5,22 5	4	Positive	224, 0683	86,8 8	207, 065	5,09 2
Sitosterol ferulate	Hydroxycinnamic acids	C39 H58 O4	3201 62	909 27	738, 6639	29,3 43	6	Positive	590, 4363	71,2 5	590, 4329	29,3 24
Verbascoside	Hydroxycinnamic acids	C29 H36 O15	4058 76	270 53	122, 0813	3,25 1	3	Positive	624, 2027	76,5 1	625, 2096	3,13 2
3,4-dihydroxyphenyl-2-oxypropanoic acid	Hydroxyphenyl propanoic acids	C9 H8 O4	1730 606	204 908	149, 0236	21,9 99	5	Positive	180, 0423	99,7 2	163, 0389	21,5 63
3,4-dihydroxyphenyl-2-oxypropanoic acid	Hydroxyphenyl propanoic acids	C9 H8 O4	1960 890	300 597	149, 0236	21,4 84	5	Positive	180, 0423	99,8 2	163, 039	21,3 26

Dihydro-p-coumaric acid	Hydroxyphenyl propanoic acids	C9 H10 O3	2021 12	383 63	122, 0812	18,6 73	2	Posi tive	166, 0623	79,8 3	149, 0592	18,6 13
Dihydrocaffeic acid	Hydroxyphenyl propanoic acids	C9 H10 O4	5434 41	868 27	349, 0898	5,05 2	2	Posi tive	182, 0578	87,5 7	165, 0545	4,85 4
Dihydrocaffeic acid	Hydroxyphenyl propanoic acids	C9 H10 O4	2116 39	250 63	104, 107	1,46 9	2	Posi tive	182, 058	75,1 2	165, 0549	1,33
Cyanidin	Anthocyanins	C15 H11 O6	3616 66	624 62	122, 0813	9,48 8	2	Posi tive	287, 0555	85,8 5	287, 0549	9,31
Cyanidin 3,5-O-diglucoside	Anthocyanins	C27 H31 O16	1248 7732	202 969 2	633, 1434	9,84 5	8	Posi tive	611, 1589	99,3	611, 1611	9,52 8
Cyanidin 3,5-O-diglucoside	Anthocyanins	C27 H31 O16	5381 22	649 36	498, 2603	9,38 9	5	Posi tive	611, 1602	89,5 8	611, 1607	9,27 1
Cyanidin 3-O-glucosyl-rutinoside	Anthocyanins	C33 H41 O20	1576 4134	225 694 3	498, 2603	9,66 7	10	Posi tive	757, 2184	98,2 1	757, 2198	9,21 1
Cyanidin 3-O-sambubiosyl 5-O-glucoside	Anthocyanins	C32 H39 O20	8205 53	139 705	122, 0813	8,02 3	6	Posi tive	743, 201	98,4 6	743, 2026	7,88 5
Cyanidin 3-O-xylosyl-rutinoside	Anthocyanins	C32 H39 O19	6011 11	100 782	498, 2603	9,25 1	6	Posi tive	727, 2058	98,0 8	727, 2075	9,11 2
Delphinidin 3-O-galactoside	Anthocyanins	C21 H21 O12	9124 8	186 40	122, 0813	9,38 9	3	Posi tive	465, 1017	78,6 8	465, 1022	9,31
Malvidin 3-O-(6''-caffeoyl-glucoside)	Anthocyanins	C32 H31 O15	1235 84	208 92	122, 0813	12,8 54	2	Posi tive	655, 1657	72,4 4	655, 1652	12,7 35
Pelargonidin 3,5-O-diglucoside	Anthocyanins	C27 H31 O15	4427 75	754 28	512, 276	10,7 75	4	Posi tive	595, 1634	72,1	595, 1653	10,6 17
Pelargonidin 3,5-O-diglucoside	Anthocyanins	C27 H31 O15	8709 6	142 61	498, 2603	9,25 1	2	Posi tive	595, 1659	73,9 5	595, 1654	9,11 2

Pelargonidin 3-O-(6''-malonyl-glucoside)	Anthocyanins	C24 H23 O13	4680 108	667 036	512, 2759	10,9 93	4	Posi tive	519, 1116	88,8 4	501, 1006	10,6 56
Pelargonidin 3-O-galactoside	Anthocyanins	C21 H21 O10	5736 11	371 76	268, 1047	1,82 7	3	Posi tive	433, 1114	74,7 6	415, 0998	1,51
Peonidin	Anthocyanins	C16 H13 O6	1118 34	173 28	122, 0813	15,2 5	3	Posi tive	301, 0713	77,7 2	301, 0708	15,1 11
Petunidin 3-O-galactoside	Anthocyanins	C22 H23 O12	9418 59	151 461	647, 1589	11,0 33	5	Posi tive	479, 1183	99,7 3	479, 1184	10,8 74
Petunidin 3-O-galactoside	Anthocyanins	C22 H23 O12	1123 775	209 839	633, 1434	9,74 6	5	Posi tive	479, 1188	99,6 7	479, 1183	9,52 8
Petunidin 3-O-rutinoside	Anthocyanins	C28 H33 O16	3269 497	420 913	498, 2603	9,40 9	4	Posi tive	625, 177	99,8	625, 1765	9,21 1
3-Hydroxyphloretin 2'-O-xylosyl-glucoside	Dihydrochalco nes	C26 H32 O15	5032 3	123 27	379, 1001	5,21 2	2	Posi tive	584, 1744	75,3 5	585, 1817	5,13 3
Dihydromyricetin 3-O-rhamnoside	Dihydroflavon ols	C21 H22 O12	1908 67	224 44	512, 2759	10,8 35	3	Posi tive	466, 1107	74,4 3	471, 0893	10,6 17
Dihydroquercetin	Dihydroflavon ols	C15 H12 O7	3662 84	663 49	122, 0813	9,48 8	3	Posi tive	304, 0579	85,8 5	287, 0549	9,31
Dihydroquercetin 3-O-rhamnoside	Dihydroflavon ols	C21 H22 O11	1802 92	293 76	122, 0814	11,5 67	2	Posi tive	450, 1161	82,0 3	455, 0948	11,4 48
(-)-Epigallocatechin 3-O-gallate	Flavanols	C22 H18 O11	9717 1	200 48	104, 1081	1,25 3	4	Posi tive	458, 0846	99,0 7	463, 0635	1,07 4
Hesperetin	Flavanones	C16 H14 O6	5098 87	852 97	122, 0813	17,7 04	3	Posi tive	302, 0791	99,6 3	285, 0758	17,5 26
Naringin 4'-O-glucoside	Flavanones	C33 H42 O19	1976 68	422 09	379, 1001	5,25 2	4	Posi tive	742, 2322	73,7 1	765, 2205	5,15 3
Naringin 6'-malonate	Flavanones	C30 H34 O17	1071 04	264 02	263, 0531	5,13 3	4	Posi tive	666, 1765	79,0 8	649, 173	5,07 4
Pinocembrin	Flavanones	C15 H12 O4	1066 461	753 29	268, 1046	2,16 3	3	Posi tive	256, 073	70,4	261, 0522	1,55
6-Hydroxyluteolin	Flavones	C15 H10 O7	1317 68	203 50	498, 2603	9,40 3	3	Posi tive	302, 0427	79,4 8	303, 0499	9,27 1

6-Hydroxyluteolin	Flavones	C15 H10 O7	5639 85	461 41	122, 0813	8,20 6	2	Posi tive	302, 0426	81,4 5	303, 0499	8,00 4
Apigenin 6-C-glucoside	Flavones	C21 H20 O10	1501 05	270 05	122, 0814	11,5 59	2	Posi tive	432, 1056	82,0 3	455, 0948	11,4 48
Apigenin 6-C-glucoside	Flavones	C21 H20 O10	5264 0	129 99	513, 1584	6,29 6	2	Posi tive	432, 1066	79,0 7	455, 0959	6,24 2
Apigenin 7-O-(6''-malonyl-aposyl-glucoside)	Flavones	C29 H30 O17	2786 4214	424 353 8	633, 1433	9,82 5	5	Posi tive	650, 1465	93,7 3	633, 1433	9,52 8
Apigenin 7-O-aposyl-glucoside	Flavones	C26 H28 O14	8239 5	208 42	104, 1078	1,20 7	6	Posi tive	564, 1481	75,9 4	569, 1275	1,11 4
Chrysoeriol 7-O-(6''-malonyl-aposyl-glucoside)	Flavones	C30 H32 O18	1507 524	253 500	122, 0813	8,89 6	4	Posi tive	680, 1565	90,5 8	663, 1532	8,69 6
Apigenin 6,8-di-C-glucoside	Flavones	C27 H30 O15	7419 8	156 99	122, 0814	11,1 57	3	Posi tive	594, 1583	74,6 9	617, 1476	11,0 72
Apigenin 6,8-di-C-glucoside	Flavones	C27 H30 O15	1134 527	184 575	512, 276	10,8	5	Posi tive	594, 1583	99,3 9	617, 1476	10,6 17
Apigenin 6,8-di-C-glucoside	Flavones	C27 H30 O15	1820 56	338 97	122, 0814	10,2 05	4	Posi tive	594, 1582	92,3 4	617, 1474	10,1 22
Apigenin 6,8-di-C-glucoside	Flavones	C27 H30 O15	7802 2	118 90	498, 2603	9,22 9	3	Posi tive	594, 1582	75,5	595, 1654	9,11 2
Cirsimaritin	Flavones	C17 H14 O6	8117 5	150 83	122, 0813	17,8 01	3	Posi tive	314, 0795	73,8	297, 0761	17,6 45
Diosmin	Flavones	C28 H32 O15	1860 42	355 27	122, 0813	7,82 8	3	Posi tive	608, 1738	98,5 5	631, 1629	7,72 6
Biochanin A	Isoflavonoids	C16 H12 O5	4701 34	829 25	122, 0813	17,6 88	3	Posi tive	284, 0686	99,6 5	285, 0759	17,5 26
Luteolin 7-O-(2-aposyl-glucoside)	Flavones	C26 H28 O15	1665 473	277 699	122, 0813	9,51	7	Posi tive	580, 1427	99,6 4	603, 132	9,33
3,7-Dimethylquercetin	Flavonols	C17 H14 O7	3738 67	529 14	122, 0812	3,07 4	4	Posi tive	330, 0739	85,5 2	353, 0632	2,97 5

6,8-Dihydroxykaempferol	Flavonols	C15 H12 O8	6245 54	485 13	122, 0813	8,22 1	2	Posi tive	320, 0532	81,8 3	303, 0499	8,00 4
Isorhamnetin	Flavonols	C16 H12 O7	3696 820	586 968	647, 159	11,2 31	4	Posi tive	316, 0585	99,0 2	317, 0657	10,8 74
Isorhamnetin	Flavonols	C16 H12 O7	7288 231	124 706 6	633, 1434	9,86 5	4	Posi tive	316, 0587	98,7 8	317, 066	9,52 8
Isorhamnetin 3-O-galactoside	Flavonols	C22 H22 O12	5138 453	632 193	512, 2759	11,0 33	7	Posi tive	478, 1113	99,6 1	501, 1006	10,6 56
Isorhamnetin 3-O-galactoside	Flavonols	C22 H22 O12	9967 16	171 462	633, 1434	9,74 6	5	Posi tive	478, 111	99,6 7	479, 1183	9,52 8
Isorhamnetin 3-O-galactoside	Flavonols	C22 H22 O12	6672 82	850 34	498, 2603	9,40 9	3	Posi tive	478, 1108	96,9 1	479, 1181	9,21 1
Isorhamnetin 3-O-glucoside 7-O-rhamnoside	Flavonols	C28 H32 O16	2477 827	396 332	512, 2759	10,7 75	7	Posi tive	624, 169	99,5	647, 1583	10,6 96
Isorhamnetin 3-O-glucoside 7-O-rhamnoside	Flavonols	C28 H32 O16	3078 903	398 718	498, 2603	9,38 9	4	Posi tive	624, 1691	99,8	625, 1765	9,21 1
Kaempferide	Flavonols	C16 H12 O6	1084 59	167 74	122, 0813	15,2 5	3	Posi tive	300, 0635	77,7 2	301, 0708	15,0 71
Kaempferol	Flavonols	C15 H10 O6	1349 43	191 87	512, 276	10,7 75	2	Posi tive	286, 0479	84,4 2	287, 0551	10,6 17
Kaempferol	Flavonols	C15 H10 O6	3616 66	624 62	122, 0813	9,48 8	2	Posi tive	286, 0476	85,8 5	287, 0549	9,31
Kaempferol	Flavonols	C15 H10 O6	2721 04	406 84	498, 2603	9,23 1	2	Posi tive	286, 0476	84,9 2	287, 0548	9,11 2
Kaempferol 3-O-(2''-rhamnosyl-6''-acetyl-galactoside) 7-O-rhamnoside	Flavonols	C35 H42 O20	6889 54	731 03	122, 0813	12,8 74	3	Posi tive	782, 2287	93,7 8	787, 2074	12,7 35
Kaempferol 3-O-(2''-rhamnosyl-galactoside) 7-O-rhamnoside	Flavonols	C33 H40 O19	4561 69	810 22	498, 2602	9,21 1	6	Posi tive	740, 2144	87,7 5	741, 2234	9,09 2
Kaempferol 3-O-(2''-rhamnosyl-galactoside) 7-O-rhamnoside	Flavonols	C33 H40 O19	5594 50	996 36	122, 0813	9,03 3	5	Posi tive	740, 215	81,2 8	763, 2052	8,93 4

6-Hydroxyluteolin 7-O-rhamnoside	Flavones	C21 H20 O11	1908 67	224 44	512, 2759	10,8 35	3	Posi tive	448, 1001	74,4 3	471, 0893	10,6 17
6-Hydroxyluteolin 7-O-rhamnoside	Flavones	C21 H20 O11	1539 49	217 95	122, 0813	10,3 79	3	Posi tive	448, 1001	73,2 2	471, 0894	10,2 01
Kaempferol 3-O-glucosyl-rhamnosyl-galactoside	Flavonols	C33 H40 O20	2547 5968	347 936 0	498, 2603	9,66 7	10	Posi tive	756, 2123	98,2 6	757, 2198	9,21 1
Kaempferol 3-O-glucosyl-rhamnosyl-galactoside	Flavonols	C33 H40 O20	4259 05	717 21	122, 0813	8,24 1	5	Posi tive	756, 2111	95,1 9	757, 2185	8,10 3
Kaempferol 3-O-glucosyl-rhamnosyl-galactoside	Flavonols	C33 H40 O20	3934 01	708 14	122, 0813	8,02 3	5	Posi tive	756, 2109	96,6	779, 2003	7,92 4
Kaempferol 3,7-O-diglucoside	Flavonols	C27 H30 O16	3243 1359	503 656 8	633, 1433	9,82 5	9	Posi tive	610, 1539	99,4 6	611, 1607	9,52 8
Kaempferol 3,7-O-diglucoside	Flavonols	C27 H30 O16	7754 45	109 931	498, 2603	9,37	6	Posi tive	610, 1533	97,7 7	633, 142	9,27 1
Kaempferol 3-O-xylosyl-rutinoside	Flavonols	C32 H38 O19	1140 687	193 879	498, 2603	9,27 1	7	Posi tive	726, 2002	99,1 1	749, 1895	9,13 2
Myricetin 3-O-rhamnoside	Flavonols	C21 H20 O12	2214 38	312 02	122, 0813	9,48 8	4	Posi tive	464, 0951	80,2 1	487, 0842	9,31
Myricetin 3-O-rhamnoside	Flavonols	C21 H20 O12	6684 91	113 424	498, 2602	9,21 1	5	Posi tive	464, 095	99,1 3	487, 0843	9,07 3
Quercetin 3-O-(6	Flavonols	C30 H32 O15	1235 84	208 92	122, 0813	12,8 54	2	Posi tive	632, 1759	70,1 3	655, 1652	12,7 35
Quercetin 3-O-arabinoside	Flavonols	C20 H18 O11	3599 59	589 88	122, 0813	8,95 4	3	Posi tive	434, 0844	87,4 4	439, 0633	8,81 5
Quercetin 3-O-xylosyl-rutinoside	Flavonols	C32 H38 O20	1469 449	243 799	122, 0813	8,05 6	7	Posi tive	742, 1953	99,1 1	765, 1846	7,88 5
Quercetin 4'-O-glucoside	Flavonols	C21 H20 O7	1452 42	186 96	122, 0813	8,06 3	3	Posi tive	384, 1199	96,2 7	366, 1088	7,86 5
6"-O-Acetyldaidzin	Isoflavonoids	C23 H22 O10	6594 1	112 97	122, 0813	8,71 6	3	Posi tive	458, 1219	75,9 7	481, 1108	8,61 7

6''-O-Acetylgenistin	Isoflavonoids	C23 H22 O11	1055 85	198 89	122, 0812	6,06 3	4	Posi tive	474, 1158	88,7 1	497, 1054	5,94 5
6''-O-Malonylgenistin	Isoflavonoids	C24 H22 O13	4680 108	667 036	512, 2759	10,9 93	4	Posi tive	518, 1038	88,8 4	501, 1006	10,6 56
Glycitin	Isoflavonoids	C22 H22 O10	5078 3	953 1	122, 0813	9,09 2	2	Posi tive	446, 1215	72,7 5	451, 1002	9,03 3
1-Acetoxy-pinorezinol	Lignans	C22 H24 O8	4229 30	436 02	104, 1079	1,41 1	7	Posi tive	416, 1473	86,2	439, 1368	1,13 4
Cyclolariciresinol	Lignans	C20 H24 O6	2054 32	159 20	293, 2116	21,1 1	2	Posi tive	360, 1567	81,9 5	343, 1533	20,9 31
Dimethylmatairesinol	Lignans	C22 H26 O6	2909 087	494 502	122, 081	17,4 07	9	Posi tive	386, 1728	98,7 4	387, 18	17,1 7
Syringaresinol	Lignans	C22 H26 O8	5405 1	109 85	122, 0813	7,98 4	3	Posi tive	418, 1645	85,1	423, 143	7,90 5
4-Vinylsyringol	Alkylmethoxyphenols	C10 H12 O3	8216 57	558 72	365, 1061	21,3 04	2	Posi tive	180, 0786	87,3 9	163, 0753	20,9 12
4-Vinylsyringol	Alkylmethoxyphenols	C10 H12 O3	1745 96	280 60	122, 0813	3,10 9	4	Posi tive	180, 0781	70,6 4	181, 0863	2,99 5
3-Methylcatechol	Alkylphenols	C7 H8 O2	1294 640	210 891	263, 0531	5,28 9	3	Posi tive	124, 0524	97,3 9	107, 049	5,03 4
3-Methylcatechol	Alkylphenols	C7 H8 O2	2647 29	896 67	365, 1057	2,39 7	5	Posi tive	124, 0524	93,1	107, 049	2,38 1
3-Methylcatechol	Alkylphenols	C7 H8 O2	4663 37	197 15	122, 0814	0,97 6	3	Posi tive	124, 0526	97,7 5	107, 0493	0,81 7
4-Ethylphenol	Alkylphenols	C8 H10 O	8238 433	391 46	738, 6626	33,3 44	3	Posi tive	122, 0733	97,8 5	105, 07	30,3 95
4-Vinylphenol	Alkylphenols	C8 H8 O	1165 060	356 557	166, 0868	2,48	3	Posi tive	120, 0577	87,7 4	103, 0544	2,42 1
5-Heneicosylresorcinol	Alkylphenols	C27 H48 O2	2478 7	178 09	871, 5751	32,9 49	2	Posi tive	404, 3639	76,9 4	409, 3426	32,9 29
5-Nonadecenylresorcinol	Alkylphenols	C25 H42 O2	2349 102	155 00	738, 6626	33,7 01	5	Posi tive	374, 3188	80,4 9	357, 315	31,2 06

p-Anisaldehyde	Hydroxybenzaldehydes	C8 H8 O2	7844 43	102 399	349, 0897	5,19 2	3	Positive	136, 0523	87,7 4	119, 049	4,85 6
Vanillin	Hydroxybenzaldehydes	C8 H8 O3	1633 31	278 48	122, 0813	8,93	3	Positive	152, 0476	87,5	153, 0547	8,81 5
Vanillin	Hydroxybenzaldehydes	C8 H8 O3	1115 22	177 49	122, 0812	6,90 6	4	Positive	152, 0475	85,4 8	153, 0548	6,81 6
2,3-Dihydroxy-1-guaiacylpropanone	Hydroxybenzoketones	C10 H12 O5	7842 85	142 757	379, 1002	5,36 2	3	Positive	212, 0684	99,2 3	195, 065	5,19 2
3-Methoxyacetophenone	Hydroxybenzoketones	C9 H10 O2	5865 013	393 83	738, 6626	33,1 86	2	Positive	150, 068	86,4 1	151, 0754	31,0 88
3-Methoxyacetophenone	Hydroxybenzoketones	C9 H10 O2	8904 589	895 192	268, 1041	2,10 4	4	Positive	150, 0678	99,3	151, 0751	1,86 6
Sinapaldehyde	Hydroxycinnamaldehydes	C11 H12 O4	6950 38	964 50	122, 0813	7,11 3	3	Positive	208, 0736	87,1 9	191, 0703	6,85 5
Sinapaldehyde	Hydroxycinnamaldehydes	C11 H12 O4	2683 08	425 98	122, 0812	5,82 6	3	Positive	208, 0736	87,0 2	191, 0704	5,64 8
4-Hydroxycoumarin	Hydroxycoumarins	C9 H6 O3	1706 508	187 661	738, 6627	29,6 03	3	Positive	162, 0316	99,7 8	163, 0389	29,2 07
4-Hydroxycoumarin	Hydroxycoumarins	C9 H6 O3	1543 451	240 382	149, 0237	21,4 86	3	Positive	162, 0318	99,8	163, 039	21,3 27
Esculin	Hydroxycoumarins	C15 H16 O9	5649 55	371 96	122, 0813	2,39	2	Positive	340, 0796	83,4 6	363, 0687	2,04 5
Mellein	Hydroxycoumarins	C10 H10 O3	8261 28	130 509	263, 0531	5,23 2	4	Positive	178, 0626	89,0 5	161, 0594	5,03 4
1,4-Naphtoquinone	Naphtoquinones	C10 H6 O2	3724 6	603 4	263, 0531	5,13 3	2	Positive	158, 037	75,4	159, 0439	5,05 4
3,4-Dihydroxyphenylglycol	Other polyphenols	C8 H10 O4	1730 88	292 84	122, 0813	8,93 4	2	Positive	170, 0579	87,5	153, 0547	8,81 5
Arbutin	Other polyphenols	C12 H16 O7	3503 49	598 17	122, 0813	7,45 9	2	Positive	272, 0899	86,0 2	277, 0686	7,27 1

Phlorin	Other polyphenols	C12 H16 O8	8595 582	117 446 3	104, 108	1,58 9	7	Posi tive	288, 0848	80,3 9	289, 0922	1,09 4
Pyrogallol	Other polyphenols	C6 H6 O3	7234 94	116 259	365, 103	23,4 06	3	Posi tive	126, 0315	97,6	149, 0206	23,0 7
Carnosol	Phenolic terpenes	C20 H26 O4	1611 92	231 61	365, 106	20,7 93	2	Posi tive	330, 1827	83,5 7	331, 1901	20,6 74
Carvacrol	Phenolic terpenes	C10 H14 O	2778 783	242 93	738, 6628	32,2 75	5	Posi tive	150, 1046	85,2 3	133, 1011	30,5 73
Hydroxytyrosol 4-O-glucoside	Tyrosols	C14 H20 O9	1591 286	268 888	122, 0812	6,95 4	5	Posi tive	332, 1112	91,2 1	337, 0894	6,81 6
Ligstroside-aglycone	Tyrosols	C19 H21 O7	1825 788	984 86	122, 0813	3,56 9	3	Posi tive	361, 1297	92,7 7	366, 1087	3,35 1
Oleoside 11-methylester	Tyrosols	C17 H24 O11	1814 111	315 177	122, 0813	7,83 8	4	Posi tive	404, 1319	99,7 6	409, 1106	7,62 7
Oleoside dimethylester	Tyrosols	C18 H26 O11	4453 97	693 51	122, 0812	6,08 3	5	Posi tive	418, 1472	98,5 5	441, 1361	5,94 5
2-Hydroxybenzoic acid	Hydroxybenzoic acids	C7 H6 O3	2388 39	354 84	738, 6626	29,4 44	3	Posi tive	138, 0318	84,2 4	121, 0285	29,2 07
2-Hydroxybenzoic acid	Hydroxybenzoic acids	C7 H6 O3	5209 52	635 20	149, 0236	21,9 32	3	Posi tive	138, 0319	86,0 7	121, 0286	21,5 65
2-Hydroxybenzoic acid	Hydroxybenzoic acids	C7 H6 O3	6964 51	979 75	149, 0237	21,4 86	2	Posi tive	138, 0318	87,6 9	121, 0285	21,3 27
2-Hydroxybenzoic acid	Hydroxybenzoic acids	C7 H6 O3	1584 43	268 51	122, 081	3,01 5	3	Posi tive	138, 032	82,5 3	139, 0394	2,69 8
4-Hydroxybenzoic acid 4-O-glucoside	Hydroxybenzoic acids	C13 H16 O8	1618 702	225 388	122, 0811	3,05 4	4	Posi tive	300, 0844	99,6 4	323, 0736	2,69 8
5-O-Galloylquinic acid	Hydroxybenzoic acids	C14 H16 O10	5007 44	618 91	349, 0897	5,03 4	2	Posi tive	344, 0744	83,7 6	367, 0637	4,83 6
Benzoic acid	Hydroxybenzoic acids	C7 H6 O2	1244 54	222 88	122, 0813	6,99 4	2	Posi tive	122, 0366	77,0 9	105, 0333	6,89 5

Benzoic acid	Hydroxybenzoic acids	C7 H6 O2	315859	53503	122,0812	6,816	3	Positive	122,0366	87,59	105,0333	6,717
Gallic acid	Hydroxybenzoic acids	C7 H6 O5	217358	16068	104,1073	1,47	2	Positive	170,0215	73,52	171,0288	1,272
Gallic acid ethyl ester	Hydroxybenzoic acids	C9 H10 O5	533269	45536	365,106	22,179	2	Positive	198,053	85,01	181,0497	21,585
Gallic acid ethyl ester	Hydroxybenzoic acids	C9 H10 O5	478286	64698	149,0237	21,486	2	Positive	198,0529	87,08	181,0496	21,327
Protocatechuic acid 4-O-glucoside	Hydroxybenzoic acids	C13 H16 O9	300649	54379	104,1075	1,272	2	Positive	316,0801	83,73	321,0586	1,154
1,2-Diferuloylgentiobiose	Hydroxycinnamic acids	C32 H38 O17	198112	33987	633,1433	9,706	3	Positive	694,2103	98,01	717,1994	9,568
1-Sinapoyl-2-feruloylgentiobiose	Hydroxycinnamic acids	C33 H40 O18	162403	24835	122,0813	8,499	3	Positive	724,2187	81,38	707,2152	8,4
24-Methylcholestanol ferulate	Hydroxycinnamic acids	C38 H58 O4	543449	78197	738,6615	27,484	6	Positive	578,4342	90,16	601,4213	27,187
24-Methylenecholestanol ferulate	Hydroxycinnamic acids	C38 H57 O4	439417	70289	738,6615	27,405	4	Positive	577,4278	71,24	600,4164	27,168
3,4-Diferuloylquinic acid	Hydroxycinnamic acids	C27 H28 O12	1652900	86873	122,0811	3,173	3	Positive	544,1607	75,84	527,1576	2,361
3-Feruloylquinic acid	Hydroxycinnamic acids	C17 H20 O9	308701	20867	122,0813	7,568	3	Positive	368,1125	73,63	373,0895	7,469
3-Feruloylquinic acid	Hydroxycinnamic acids	C17 H20 O9	543490	67676	122,0812	6,242	4	Positive	368,1114	83,03	391,1003	5,925
3-Sinapoylquinic acid	Hydroxycinnamic acids	C18 H22 O10	63063	15646	122,0813	7,246	3	Positive	398,1225	81,49	421,1101	7,192
3-Sinapoylquinic acid	Hydroxycinnamic acids	C18 H22 O10	240949	18106	268,1048	1,807	4	Positive	398,1209	89,42	399,1275	1,609
3-p-Coumaroylquinic acid	Hydroxycinnamic acids	C16 H18 O8	63904	13737	122,0813	12,458	2	Positive	338,1004	81,37	339,1076	12,359
3-p-Coumaroylquinic acid	Hydroxycinnamic acids	C16 H18 O8	517581	78710	513,1584	6,499	4	Positive	338,1002	98,45	339,1072	6,242

3-p-Coumaroylquinic acid	Hydroxycinnamic acids	C16 H18 O8	121913	24947	379,1002	5,291	3	Positive	338,1009	80,03	339,1072	5,173
3-p-Coumaroylquinic acid	Hydroxycinnamic acids	C16 H18 O8	826277	72836	104,1071	1,585	3	Positive	338,101	80,85	321,0975	1,352
5-5'-Dehydrodiferulic acid	Hydroxycinnamic acids	C20 H18 O8	55860	11114	122,0812	3,601	3	Positive	386,1011	70,03	369,098	3,549
Caffeoyl glucose	Hydroxycinnamic acids	C15 H18 O9	62723	16749	122,0812	5,526	2	Positive	342,0942	75,14	343,1016	5,47
Caffeoyl glucose	Hydroxycinnamic acids	C15 H18 O9	218373	36346	122,0813	4,46	4	Positive	342,0941	79,92	343,1012	4,341
Caffeoyl tartaric acid	Hydroxycinnamic acids	C13 H12 O9	172110	25158	104,1075	1,343	3	Positive	312,0484	74,95	335,0376	1,134
Cinnamic acid	Hydroxycinnamic acids	C9 H8 O2	214935	39350	122,0813	18,694	2	Positive	148,0519	85,96	149,0592	18,615
Feruloyl glucose	Hydroxycinnamic acids	C16 H20 O9	3122869	440757	122,0812	6,063	7	Positive	356,1107	99,21	379,1	5,766
Feruloyl glucose	Hydroxycinnamic acids	C16 H20 O9	12850133	2045760	379,1002	5,529	7	Positive	356,1108	99,22	379,1002	5,192
Hydroxycaffeic acid	Hydroxycinnamic acids	C9 H8 O5	4303096	590865	104,1083	1,728	3	Positive	196,0373	77,85	219,0269	1,055
Isoferulic acid	Hydroxycinnamic acids	C10 H10 O4	1958208	265525	513,1584	6,598	4	Positive	194,058	99,65	177,0547	6,242
Isoferulic acid	Hydroxycinnamic acids	C10 H10 O4	2895790	395843	263,053	5,45	7	Positive	194,0579	99,65	177,0546	5,192
m-Coumaric acid	Hydroxycinnamic acids	C9 H8 O3	315389	34550	104,1071	1,55	4	Positive	164,0471	78,06	165,0549	1,332
p-Coumaric acid 4-O-glucoside	Hydroxycinnamic acids	C15 H18 O8	20232278	2817227	349,0897	5,212	5	Positive	326,1005	99,17	349,0897	4,856
p-Coumaric acid 4-O-glucoside	Hydroxycinnamic acids	C15 H18 O8	3495023	294741	104,1072	1,589	6	Positive	326,1015	78,42	308,091	1,272

p-Coumaric acid ethyl ester	Hydroxycinnamic acids	C11 H12 O3	234903	46120	263,0531	5,074	2	Positive	192,0786	87,01	193,0859	4,994
Rosmarinic acid	Hydroxycinnamic acids	C18 H16 O8	5683658	722999	349,0897	5,093	4	Positive	360,0847	80,97	365,0639	4,856
Sinapic acid	Hydroxycinnamic acids	C11 H12 O5	349724	46324	122,0813	6,666	5	Positive	224,0685	87,14	207,0652	6,499
Sitostanyl ferulate	Hydroxycinnamic acids	C39 H60 O5	190325	44944	738,6626	29,324	5	Positive	608,4413	71,71	590,4298	29,266
Verbascoside	Hydroxycinnamic acids	C29 H36 O15	415528	28272	122,0812	3,232	3	Positive	624,2028	78,25	625,2098	3,133
3,4-dihydroxyphenyl-2-oxypropanoic acid	Hydroxyphenyl propanoic acids	C9 H8 O4	1417574	187769	738,6626	29,543	4	Positive	180,0423	99,78	163,0389	29,207
3,4-dihydroxyphenyl-2-oxypropanoic acid	Hydroxyphenyl propanoic acids	C9 H8 O4	2040071	306557	149,0237	21,486	5	Positive	180,0424	99,8	163,039	21,327
Dihydro-p-coumaric acid	Hydroxyphenyl propanoic acids	C9 H10 O3	214935	39350	122,0813	18,694	2	Positive	166,0625	85,96	149,0592	18,615
Dihydro-p-coumaric acid	Hydroxyphenyl propanoic acids	C9 H10 O3	139446	41751	166,0868	2,48	2	Positive	166,0627	71,41	149,0598	2,441
Dihydrocaffeic acid	Hydroxyphenyl propanoic acids	C9 H10 O4	508422	78425	349,0897	5,014	3	Positive	182,0579	87,2	165,0545	4,856
Dihydrocaffeic acid	Hydroxyphenyl propanoic acids	C9 H10 O4	248074	27450	104,1071	1,51	2	Positive	182,0578	78,06	165,0549	1,332
d-Viniferin	Stilbenes	C28 H22 O6	87419	12275	122,0812	6,935	2	Positive	454,1403	75,9	454,1399	6,836