

**Table S1. All metabolites obtained by UPLC-MS/MS.**

NAME_EN	CLASS_EN	KERNE1	KERNE2	KERNE3	KERNE4	KERNE5	KERNE6	PEEL-1	PEEL-2	PEEL-3	PEEL-4	PEEL-5	PEEL-6
1,5-Anhydro-D-glucitol	Alcohols and polyol	47750	61031	43254	34976	68812	144686	2457.4	3882	1962.5	1907	1932.7	2450.1
D-Sorbitol	Alcohols and polyol	15564	19993	1342.5	23072	10644	8944	16305	604.69	0	14281	9490.5	21783
3-Dehydroquinate	Alcohols and polyol	6957.5	11908	8998.1	10085	11859	10544	7571.1	12662	6471.2	10845	23815	10176
Trigonelline	Alkaloids	9E+06	9E+06	1E+07	1E+07	4E+06	4E+06	9E+06	8E+06	6E+06	1E+07	5E+06	6E+06
Sarracine	Alkaloids	5E+06	2E+06	2E+06	4E+06	4E+06	3E+06	3E+06	3E+06	2E+06	273080	484412	3E+06
3alpha,6beta-Ditigloyloxy	Alkaloids	5E+06	2E+06	2E+06	4E+06	4E+06	3E+06	3E+06	3E+06	2E+06	273080	484412	3E+06
O-Acetyethanolamine	Alkaloids	2E+06	2E+06	3E+06	2E+06	3E+06	3E+06	2E+06	3E+06	2E+06	3E+06	4E+06	4E+06
Indole	Alkaloids	2E+06	1E+06	1E+06	2E+06	2E+06	1E+06	1E+06	1E+06	1E+06	1E+06	1E+06	1E+06
Phyllalbine	Alkaloids	686386	538578	586926	325654	490321	1E+06	5722.3	22927	0	3508.6	3187.6	16261
DL-Alanine	Alkaloids	951522	308884	329991	543582	353390	131238	54459	82835	46356	60515	50897	88558
DL-Tyrosine	Alkaloids	504655	537855	450472	378885	323340	50624	25483	136594	87473	173180	85005	56867
Crotonoside	Alkaloids	265485	340742	399768	687952	441241	62656	505376	692575	376093	556585	850357	521688
D-Serine	Alkaloids	452872	332154	358753	371911	278112	322405	117074	135937	126240	123872	124897	146724
D-Aspartic acid	Alkaloids	393568	289522	204193	324747	171700	235535	208135	202027	150701	330728	193796	247421
Methyl anthranilate	Alkaloids	1859.1	229919	369010	3219.4	322992	2696.4	340529	536082	2943.5	317853	824499	361460
Betaine	Alkaloids	176443	246291	42219	63429	62852	53913	414872	181830	54563	116277	86268	111437
Cevadine	Alkaloids	108729	5697.8	93751	5906.7	143801	2760.6	122604	269989	48871	156367	196859	6022.1
Isoquinoline	Alkaloids	40798	44877	85471	59076	54284	31656	80417	91096	46762	33470	62288	43592
Nicotinamide	Alkaloids	42972	52002	39635	32950	61768	50512	23415	32420	58733	43226	41533	10822
(-)-Cinchonidine	Alkaloids	66405	27394	30852	39177	47999	42714	688285	3E+06	560477	1E+06	3E+06	512727
Amabiline	Alkaloids	26119	9028.7	25745	55709	44906	30586	45072	53739	17151	20564	32423	17781
Agrocybenine	Alkaloids	25590	18876	25003	22468	14856	74720	12368	9573.1	2601.3	16067	15911	3703
Calystegine A6	Alkaloids	10445	73415	44920	28122	4697.4	9081.1	31782	54102	39409	33663	13632	18444
3-Methylindole	Alkaloids	58026	16800	18242	25071	34445	13145	9452.5	7372.3	9791.4	23263	6112.3	5299.7
(2S,3R,4E)-2-Amino-4-he	Alkaloids	30000	15159	18637	30522	22334	27183	28755	16738	39961	31043	21747	31136
Dhuririn	Alkaloids	32079	17096	22705	33245	22482	11178	37063	49653	17987	19495	29844	16570
8-Azabicyclo-3.2.1-octan-	Alkaloids	14357	16966	15083	30579	12272	37785	11387	12636	17824	22894	20387	9950.5
Denudatine	Alkaloids	22707	27757	21165	16307	21252	17429	12360	16754	12099	21207	14346	39858

Vasicine	Alkaloids	51646	10247	13396	18726	19767	7226.6	4855.1	8878.5	4491.1	13940	5034.5	3329.7
Cinchonine	Alkaloids	10929	13510	26485	22709	25610	10497	557458	1E+06	335410	617942	1E+06	513824
Kynurenic acid	Alkaloids	17592	13754	15900	14515	36016	11033	9304.7	13947	25321	35630	13025	16016
Arecaidine	Alkaloids	18558	6394.4	6640.8	31057	21929	23170	4608.8	17534	18937	15105	17754	9714.2
Synephrine	Alkaloids	14143	35618	10575	11541	10765	24850	11457	21912	15847	13336	8081.1	11384
Talatisamine	Alkaloids	9736.5	13038	21426	12861	14737	24215	11977	24964	12320	20770	10547	13759
L-Nicotine	Alkaloids	21993	15692	9263.1	11805	14915	5828.6	43603	9604.2	12285	11408	34300	12849
Nordihydrocapsaicin	Alkaloids	20737	3803.1	12601	16408	11384	13993	17982	9339.2	5197.8	16743	20904	8129.3
Pseudotropine	Alkaloids	28417	18163	9919.2	2672	10308	7086.7	12982	5671.8	11424	4315.2	5564.1	29675
Methylisopelletierine	Alkaloids	16966	10452	6680.6	19948	11023	11213	13485	8018.7	9017.5	9812.9	7157.5	9842.6
3-Methyl-1-butylamine	Alkaloids	4976.9	6410	10036	7847.4	13982	11207	18518	13947	11455	16319	8539.7	10010
3-(Carboxymethylamino)p indolin-2-one	Alkaloids	5923.1	6232.4	6400.4	11565	13405	7104.6	2453.3	12467	7959.2	8785.1	3513.2	2057.2
Hordenine	Alkaloids	6831.6	5504	18605	5673.8	7146.6	6455	3914.9	5799.1	13627	8815.4	7707.2	4621.4
Tacrolimus	Alkaloids	5520.2	3378.9	9388.4	10565	14630	6566.7	5510.5	6413.3	11214	8213	6090	9624.6
Cochlearine	Alkaloids	10057	6648.3	6004	7764.2	9750.8	9396.3	13086	20651	7822.3	4084	19878	712.45
Solasodine	Alkaloids	10672	4858.8	6450.4	10637	13000	3421.5	23353	13920	8177.1	7193.1	7399.5	4334.8
3-Hydroxy-2-methylpyridi	Alkaloids	10523	3580.7	12400	3876.6	12985	5529.4	9510	10792	11953	6228.2	11809	5576.7
Norepinephrine	Alkaloids	8307.7	12685	9461.7	4868.5	3723.7	9598.8	3437.7	4457.6	5076.8	4142.2	4301.3	4285.2
N-p-Coumaroyloctopamin	Alkaloids	3067.4	6331.9	11259	10248	11720	4729.4	10646	5473.1	6408.4	9592.6	2843.7	6568.1
Gramine	Alkaloids	7553.1	11286	9143.2	4323.4	4932.9	6442.8	13306	11342	11297	7704.2	11072	8974.7
Dihydrocapsaicin	Alkaloids	4931.6	6853.5	4523.5	11086	8852.5	5360.7	12363	13072	10409	7270.9	7280.6	5456.3
Pilocarpine	Alkaloids	8542.3	4010.3	3037.2	5495.9	10140	10293	11732	4695.2	3900.5	8393.5	6714.6	2335.5
Theobromine	Alkaloids	3147.8	5664.3	13209	4082.7	5005	8616.3	1877.2	13275	4746.3	3155.1	10251	5323.3
Knightinol	Alkaloids	5062.6	6672.6	6152.7	5377.7	6835.2	7970.8	9071.4	15339	6391	8342.2	8876.1	12337
Piperidine	Alkaloids	12207	3470.1	2897.4	6020	4321	6927.4	2091.5	428.74	0	0	0	1879.5
Bellendine	Alkaloids	7205.6	3672.7	4360.5	5431.6	5305.5	6111.7	2088.7	2540.1	2819.5	5494.6	1444.9	3508.7
2-Hydroxypyridine	Alkaloids	12646	2911.9	2658.8	5038.4	5353.5	3106.3	4152.6	8315.3	4569.2	4355.8	3167.9	4000.6
Tropine acetate	Alkaloids	7513.2	6597.2	3653.8	5484.2	4374.8	3911.4	2601.8	7382.5	5543.1	3512.6	6031.8	4031.8
Gentioflavin	Alkaloids	5119.8	3842.4	4177.9	5618	4217.2	8202.4	4609.1	2619.6	2647.1	3766.3	3836	3182.8
Angustifoline	Alkaloids	0	4457.4	4500.1	7072.7	5477.3	8952.5	8118.6	4030.3	4486.3	643.7	3789.2	4645.4
5-Hydroxytryptophan	Alkaloids	1211.3	6622.6	6486.9	6611.6	4504.2	3796.2	3113.1	3510	2973.9	3018	4889.4	4208.7
		6277.9	7490.3	5058.3	2430.4	3421.6	4079.1	2792.5	4788.6	6264.7	4083.9	2401.4	2463.4

Melatonin	Alkaloids	6160.7	5728.7	2998	0	10404	1557.1	4180.7	3800	3079.4	3099.9	1684.8	4107.5
Theophylline	Alkaloids	6006	4660.4	3985.4	2709.6	3461.7	4300	6301.2	5568.4	5155.8	6532	6443.6	4830.6
Bufotenine	Alkaloids	5655.7	5761.5	5117.7	3717.6	1829	2317.4	3322.8	3753.9	5624.8	2409.4	1832	3020.8
Protoveratrine A	Alkaloids	7004.7	8823.2	0	3266.5	1570.5	3424.9	9503.8	8489	19990	4929.5	3046.3	0
Lumichrome	Alkaloids	2615.2	5872.8	5517.6	1770.4	863.1	6852.2	10648	3376.4	13540	7536.1	10572	862.21
Dictamnine	Alkaloids	2769.6	2238.8	4828.1	4648.1	2775.7	5650.3	3471.6	9078.3	5706.3	3629.7	5130.1	8055.9
6-(Furfurylamino)purine	Alkaloids	2073.2	3397.4	3600.5	2610.7	3292.6	4985.7	1557.5	4458.1	1913.6	617.22	4460.4	1902.4
Acetylcholine chloride	Alkaloids	2221.3	6594.6	3338.1	1992.4	1779.7	3735.2	1170.8	2933.7	4974.4	2335.9	2740.4	5504.2
Mitraphylline	Alkaloids	1983	1068.2	1041.1	3868	6781.7	4862.4	5901.4	3545	2927.3	5303.3	7492.8	3225.3
(-)-Huperzine A	Alkaloids	4646.1	1249.3	1917.5	7060.9	594.74	3814.5	7867.5	585.25	4119.3	643.52	1824.5	1194.6
Abrine	Alkaloids	3858.2	1931.3	3835	5233.7	2462.1	1873.5	5092.3	8162.1	5681.8	6180.7	5144	1768.5
Allocryptopine	Alkaloids	963.38	1189.6	2415.8	7808.6	3035.6	2058.1	4157.5	3450.2	2323.1	2401.8	6259.3	653.71
Tryptophan	Alkaloids	0	7208.7	0	0	4301.3	5579.5	1942.9	1794.6	2301	5860.4	1910.2	0
Oxoglaucine	Alkaloids	4504.5	1102.1	482.35	3786.5	4173.7	1310.6	3842.3	6754.3	3257.8	1578	11696	1824.8
Harman	Alkaloids	2327	3453.1	1776.2	2288.9	1941.3	3228.8	10958	5422.7	7499	4039.5	7078.3	5108
Cytisine	Alkaloids	5946.4	887.04	3593	0	2393.8	1435.4	867.1	2085.7	1930.7	1489.2	873.65	653.65
Yohimbic acid monohydra	Alkaloids	5041.3	462.54	831.27	2177.6	5400.4	266.07	3615.3	8297.5	2001.3	1761.8	1858.3	1295.8
Riddelline	Alkaloids	2309.7	1108.1	1086.9	3030.6	4626.6	1974.2	3928.4	5655.6	4001.6	4966.5	2398.8	1777.3
8-Amino-7-oxononanoic a	Alkaloids	3359.8	673.23	2262.5	2562.8	2120.4	2445.9	1651.1	3834	648.62	998.09	1603	4740.2
Tombozine	Alkaloids	2524.6	955.71	2195.9	4108.8	1387.7	1983.8	994.45	2959	670.11	656.25	664.86	4380.6
Grossamide	Alkaloids	5348	335.87	1005.3	2029.5	0	4032.1	2557.9	2715.8	1009.4	3434.2	3332.6	1452.4
Harmaline	Alkaloids	1383	1055.8	848.67	3271.3	4454	1296.5	1719.8	4724.5	3997.8	2203.9	4133.7	3539.9
Oxymatrine	Alkaloids	1833.3	3080	1406.9	1992.6	2817.3	761.95	1814.8	1469.8	1431.1	1401.1	2395.3	2675.5
Benzoyltropein	Alkaloids	1788	4248.5	1202.3	2518.3	1138.5	615.05	8739.2	0	2359.1	1859.5	4337	4303.2
(-)-Anonaine	Alkaloids	683	713.16	2395.4	2146.1	3514.8	1424.1	1341.8	686.07	1705.8	447.58	1578.8	777.52
Otonecine	Alkaloids	2195.6	1502.5	1775	1886.2	2049.2	908.97	1591.9	2882.1	2795.1	2629.5	1650.9	1469.5
Rivularine	Alkaloids	2998.9	2230.4	909.87	1872.8	756.37	1037.4	2107.3	1756.1	1931.3	736.88	1250.1	2500.3
Desoxypeganine	Alkaloids	4654.2	717.09	670.41	665.68	748.89	1600.3	1464.7	2966.2	3598.7	5448.7	709.2	1752.8
1H-Indole-3-carboxylic ac	Alkaloids	1789.4	982.9	1629.2	2237	1205.9	1096.6	2987.5	4246.8	4837.4	3728.9	2713.9	5665.6
Matrine	Alkaloids	424	1810.8	1403	2196.8	1364.9	1708.4	633.59	2907.3	846.17	2495.1	1245.7	3286.7
Huperzine B	Alkaloids	500.48	1779.5	0	3448.9	1006.1	988.85	1022.6	1808.8	2626.4	3006.5	2252.5	723.45
Narciclasine	Alkaloids	1570.1	696	1131.4	1155.3	1130.7	1980.3	4116.9	2555.6	221.69	1592.1	902.25	1119.5

Calystegine B2	Alkaloids	612.37	2138.4	872.74	1227.7	900.38	1890.2	1230.3	2205	612.37	4291.1	3331	748.99
(-)-Sedamine	Alkaloids	0	0	3024.1	0	3031.4	693.47	5397	6628.3	1190.6	564.6	3966.4	1779
Astrocasine	Alkaloids	1418	621.85	565.29	1534.9	1232.1	711.22	1103	697.71	1172.6	886.51	1408.2	1567.8
Anacrotine	Alkaloids	622.35	2580.9	597.73	909.33	785.76	0	393.79	1713.2	1706.8	216.81	2667	1365.5
4-Aminoantipyrine	Alkaloids	1451	796.97	349.22	847.94	1303.9	431.97	2289.9	1594.4	1577.1	719.11	1404.5	527.01
Platyphylline	Alkaloids	227.77	2386	472.46	245.48	956.97	685.01	2022.7	1194.7	1820	2737.6	2140.6	2161
Perakine	Alkaloids	759.57	0	0	263	3060.1	776.9	503.42	8043.9	2500	1029	1013	0
Tabersonine	Alkaloids	0	419.05	420.88	0	0	1345.1	4705.4	5187.8	3712.9	3618.7	3693.5	3938.2
Arecoline	Alkaloids	3E+07	3E+07	4E+07	4E+07	4E+07	4E+07	1E+07	1E+07	2E+07	8E+06	2E+07	1E+07
L-Arginine	Amino acid and deri	1E+08	1E+08	1E+08	1E+08	2E+08	9E+06	1E+07	8E+07	1E+07	3E+07	2E+07	2E+07
L-Phenylalanine	Amino acid and deri	3E+07	9E+07	5E+07	1E+08	1E+07	930611	537288	1E+06	648865	800532	620732	512844
Proline	Amino acid and deri	1E+07	1E+07	1E+07	1E+07	8E+06	2E+06	1E+06	5E+06	1E+06	4E+06	6E+06	3E+06
L-Citruline	Amino acid and deri	1E+07	4E+06	7E+06	1E+07	8E+06	2E+06	3E+06	2E+07	5E+06	9E+06	9E+06	7E+06
L-Lysine	Amino acid and deri	1E+07	3E+06	4E+06	9E+06	3E+06	5E+06	2E+06	4E+06	1E+06	2E+06	5E+06	4E+06
L-Glutamic acid	Amino acid and deri	5E+06	4E+06	5E+06	5E+06	5E+06	6E+06	2E+06	2E+06	2E+06	3E+06	2E+06	2E+06
L-Pipecolic acid	Amino acid and deri	4E+06	3E+06	5E+06	4E+06	3E+06	3E+06	1E+06	3E+06	1E+06	2E+06	3E+06	3E+06
L-Histidine	Amino acid and deri	1E+06	1E+06	957248	1E+06	707937	421712	236643	609844	341724	313747	461384	336685
L-Serine	Amino acid and deri	452872	332154	358753	371911	278112	322405	117074	135937	126240	123872	124897	146724
5-Aminovaleric acid	Amino acid and deri	453765	604133	249203	431604	156532	61035	21648	51253	24504	41187	44637	50974
L-Aspartic acid	Amino acid and deri	393568	289522	204193	324747	171700	314406	208135	254310	150701	330728	193796	247421
2-Aminoisobutyric acid	Amino acid and deri	265671	296774	112240	282838	426675	224150	101218	496017	106174	455847	550055	447237
N6-Acetyl-L-lysine	Amino acid and deri	224316	348716	222470	381397	157222	65439	175266	543727	199275	494466	59317	319407
L-Glutamine	Amino acid and deri	158513	194139	170743	391769	103306	304461	113214	249742	100672	88205	513628	405889
L-Homoglutamic acid	Amino acid and deri	290032	250916	198801	257896	144720	70559	14393	15563	7971.6	4391.6	6703.4	16060
CYS-GLY	Amino acid and deri	21640	1693.4	2592.5	616901	409685	1047.4	63422	86408	142235	364698	97968	123399
N,N-Dimethylglycine	Amino acid and deri	265671	296774	112240	54968	86203	146188	101218	304005	106174	93026	133796	447237
L-Homoserine	Amino acid and deri	173399	156943	134051	81911	141671	63840	44408	78845	66586	54298	53661	56668
L-Methionine	Amino acid and deri	178854	148829	63898	160538	90924	23473	11266	8386.3	6779.1	5717.7	11928	12181
L-Threonine	Amino acid and deri	173399	132638	109744	81911	87397	53391	43100	78845	66586	39915	53661	56668
5-oxoproline	Amino acid and deri	82035	59171	58363	77581	47669	52263	118902	203310	136437	161847	173443	177451
trans-4-Hydroxy-L-proline	Amino acid and deri	60406	56824	67878	94072	24577	54415	15302	43391	21650	15793	16216	30994
L-Isoleucine	Amino acid and deri	29426	92036	49299	49921	48360	10332	15823	32810	18261	22281	28946	18920

Isoleucine	Amino acid and deri	29426	92036	49299	49921	48360	5520.2	15823	32810	18261	22281	28946	18920
L-Norleucine	Amino acid and deri	29426	92036	49299	49921	46467	5520.2	8300.1	42517	18261	22281	19438	18920
L-Asparagine	Amino acid and deri	26446	19510	26745	29920	26972	35068	48809	112810	32327	41989	110356	70307
S-Adenosylmethionine	Amino acid and deri	33119	19491	22586	26502	33948	16723	9137.6	20818	0	55733	16880	0
Allysine(6-Oxo DL-Norleu	Amino acid and deri	41510	23870	33575	19956	16797	14078	35797	33397	29302	29008	30933	29818
N-Acetyl-L-phenylalanine	Amino acid and deri	0	0	0	125098	392.98	0	0	22295	0	24361	21556	18276
N-formylmethionine	Amino acid and deri	6265.3	13224	5492.5	3321.3	7512.8	26465	9752.4	8347	2052.9	10632	7313.8	14174
L-Theanine	Amino acid and deri	1861.6	25578	6950.8	4626	16943	3265.5	55206	3211.4	42832	9970.8	73296	38088
D-Alanyl-D-Alanine	Amino acid and deri	9367	9258.7	5689.8	4770.9	7799.2	5984.7	7128.9	4883.4	4283.5	5919	7582.9	11943
N-Acetyl-L-glutamic acid	Amino acid and deri	4811	5943.9	3339.7	7562.7	3678.7	12849	6318	4268.8	3879	6924.6	6993.9	8382.2
L-Homocitrulline	Amino acid and deri	7949.5	4792.6	4572	5736.8	9285	2242.1	10246	6103.1	22732	3479.2	14419	5894
N-Acetyl-l-leucine	Amino acid and deri	4513.7	7419.3	5506.8	4744.8	8458	3177.5	8314.8	6496.2	3566.7	3714.4	6773	6266.4
L-Ornithine	Amino acid and deri	3233.9	3751.8	9610.9	5826.5	2613.1	4607.8	6030.4	3688.8	4644.1	7615.9	5133.5	3705.9
Phenylacetylglycine	Amino acid and deri	5885.3	4422.4	3818.9	5481.1	6102.6	1262.6	5983.9	3457.3	4468.6	2875	9111.5	6064.5
Glutathione	Amino acid and deri	2422.7	0	2860.7	7917	6380.2	4941.7	7178.3	6124.1	2825.9	6472	11057	4384
Phenylacetyl-L-glutamine	Amino acid and deri	3030.6	1215.3	2983.5	5765.4	6837.6	3321.9	7003.9	4141.8	6979.7	6157.6	3042.6	4982.4
3-Aminoisobutanoic acid	Amino acid and deri	13089	1803.1	1641.8	3154.6	1646.4	1166.7	18357	778.4	1155.9	15778	2197.3	29847
Tyramine	Amino acid and deri	5333.6	2791.3	4003.6	1777.3	2689.2	4889.5	5976.9	2166.5	2395.7	4250.4	2756.7	3961.7
N'-Formylkynurenine	Amino acid and deri	1391.2	2145.2	2521.2	6027.3	4878.8	2170	5153.2	2441.8	3959.4	3592.4	5676	4053.8
Levodopa	Amino acid and deri	1292	1970.5	1393.1	2954.7	1925.9	1183.9	2237.7	2094.6	3207.8	1475.6	2760.6	961.71
(5-L-Glutamyl)-L-amino a	Amino acid and its d	16479	8365.8	6937.3	37573	9995	6336.1	5103.1	10368	7637	5230.1	9399.5	6743
L-Tyrosine	amino acids	504655	537855	450472	378885	323340	4512	2947.1	136594	87473	173180	85005	2155.3
3-Methy-L-histidine	amino acids	163275	90804	113492	66970	35116	33585	50295	83041	54380	66111	72807	64010
beta-Alanine	amino acids	93994	115942	93355	78442	42233	51909	119644	44320	42376	58946	29077	88368
1-Methy-L-histidine	amino acids	44742	24095	35187	46091	10945	16629	12365	20600	27928	12774	20361	22817
4-Aminobutyric acid	amino acids	22065	0	19275	29074	17864	19480	124389	95061	65868	55773	159609	135793
5-Hydroxylysine	amino acids	3378.6	3522.6	6532.4	3319.2	3698.3	4302.1	1867.3	5000.2	4540.3	3022.9	2740.7	2467.3
Questinol	Anthraquinones	22022	15317	10531	26572	16338	11858	19822	25878	19183	24047	8352.8	28333
Aurantio-obtusin	Anthraquinones	21527	16899	8453.6	12920	19435	22083	11491	10768	13498	20361	12382	15323
Aloeemodin	Anthraquinones	2859.8	3388.8	1617	15320	6488.3	25977	1524.6	4720.8	7899.9	1534	5585.2	2231.9
Lucidin	Anthraquinones	2231.6	3388.8	1679.9	15320	6488.3	25977	1524.6	4304.1	3213.1	1137	5585.2	2125.9
Anthraquinone	Anthraquinones	5475	3801.5	3400.2	7544.1	4186.8	1685.4	5488.1	8738.3	5405.9	6897.6	6367.9	6430.3

Chrysophanol	Anthraquinones	1783.8	2893.9	2179.7	2931.1	3644	5774.2	1778.7	5292.4	1770.7	3143	3028.9	1320.2
Citreorosein	Anthraquinones	898.87	2949.5	2691.4	4584.1	1975.2	1292.7	2744.2	1532.2	915.09	1639.7	1509.6	2718.5
Alizarin 2-methyl ether	Anthraquinones	2220.7	2130.7	3566.6	1845	1924.9	1387.4	2147.6	971.72	929.09	452.25	1174.7	2760.2
Glucofrangulin B	Anthraquinones	509.5	2867.6	0	0	0	3781.9	0	0	1008.7	8540.1	0	8326.1
Urocanic acid	Azoles	80626	2E+06	3E+06	3E+06	2E+06	3E+06	25557	8547.6	37442	21160	36045	27795
Tricyclazole	Azoles	15253	9612.5	13985	18561	26794	9379.3	14020	24557	17869	4560.2	12203	11052
Benzocaine	Benzene and substit	3E+07	9E+07	5E+07	1E+08	1E+07	930611	6726.6	1E+06	5136.4	7211.5	17106	8050.1
4-Methylbenzaldehyde	Benzene and substit	994971	1E+06	5E+06	1E+06	3E+06	1E+06	1E+06	2E+06	3E+06	968879	1E+06	2E+06
Enol-phenylpyruvate	Benzene and substit	517818	553544	509746	340015	523599	1E+06	16895	31398	23389	23486	27090	35561
Phenethylamine	Benzene and substit	126177	293365	168315	451738	26945	9857.3	5916.6	10766	3984.3	12242	6242.2	5174.1
2-(Methylamino)benzoic a	Benzene and substit	4888	50109	55500	82022	62777	87468	20173	5164.4	22995	35146	9679.1	9632.9
Formylanthranilic acid	Benzene and substit	16743	27618	42634	13609	25880	92140	4908.1	12556	11101	20665	9987.6	10339
Ephedrine	Benzene and substit	6036.1	25833	23167	10521	20116	29845	3172.5	10651	5792.5	2222.4	4355	8513.5
4-Hydroxyphenylacetalde	Benzene and substit	7099.6	17907	12637	19494	13098	10344	8753.2	9703.3	12687	10177	33273	10912
2-Phenylacetamide	Benzene and substit	11654	14659	11474	23817	7305.8	4722.3	379321	11807	665945	329269	900408	8727
2-Hydroxy-3-(4-hydroxyl	Benzene and substit	11403	7040.5	9376.8	7536	7605.7	7643.5	8325.2	12564	6367.2	7665.1	16934	11937
Xylometazoline	Benzene and substit	9445.9	10506	6317	4004.9	5332.6	7129.2	3697.3	5899.3	8683.5	5496.4	9042.6	3357.3
5-Phenyl-1,3-oxazinane-2,	Benzene and substit	4936.4	8375.5	10498	5095.1	1029.9	2094.5	1067.7	3170.6	3302.4	1720	334.15	1415.4
N-Acetylarylamine	Benzene and substit	859.74	5161.3	5541.9	4137.7	0	0	0	25557	0	16832	24987	0
N1-(alpha-D-ribosyl)-5,6-(	Benzimidazole ribon	12102	9033.3	8001.5	6167.4	6679.9	7046.3	87355	112571	74249	40280	89438	29291
Dimethylbenzimidazole	Benzimidazoles	10210	10578	6482.4	11797	8416.8	7833.6	10568	15669	4120.1	11239	15828	17546
Carbendazim	Benzimidazoles	3068.2	694.7	1865.2	1146.4	1642.7	908.95	3732.8	1834.2	2815.9	3517.4	2690.8	1365.3
Safrole	Benzodioxoles	125045	36745	70051	107300	147254	66690	143143	134445	137349	47430	136982	76579
p-Aminobenzoate	Benzoic acid derivat	2E+06	1E+06	2E+06	3E+06	740887	677018	2E+06	1E+06	2E+06	2E+06	1E+06	1E+06
6-Methoxymellein	Benzopyrans	2714	8920	2322.1	3031.6	1714.9	1038.5	3551.6	6601	2258.3	2801	2117.6	3947.1
2(3H)-Benzothiazolethion	Benzothiazoles	5378.8	3926.1	5000.4	1645.1	3596.9	2020.6	5215.1	11114	3725.4	10172	4349.4	7337.6
(R)-2-Hydroxy-2H-1,4-ber	Benzoxazines	8793.7	16173	11462	18522	17346	11077	13400	15440	13353	16858	9915	12361
Sucrose	Carbohydrates	1E+07	1E+07	1E+07	4E+06	2E+07	9E+06	7E+06	7E+06	5E+06	1E+07	6E+06	1E+07
D-Maltose	Carbohydrates	1E+07	9E+06	8E+06	1E+07	1E+07	5E+06	1E+07	8E+06	8E+06	7E+06	9E+06	1E+07
D-Glucose 6-phosphate	Carbohydrates	873896	1E+06	2E+06	1E+06	1E+06	1E+06	289162	269012	278083	477754	288763	458990
Gluconic acid	Carbohydrates	350051	697979	480331	1E+06	358958	406562	306385	661283	311217	982933	286550	343016
alpha-D-Glucose	Carbohydrates	181913	96424	107530	171775	167181	99451	179758	50047	105358	126256	125247	188720

D-glucuronic acid	Carbohydrates	74241	132842	76664	88200	52967	65073	86158	100941	81922	76920	53813	94529
beta-Lactose	Carbohydrates	5507.9	204366	5205.6	201762	12070	11442	2923.6	3906.8	4209.9	939.95	841.84	989.89
Maltotetraose	Carbohydrates	29162	23943	16330	54121	31290	28769	12099	10032	0	13089	6393.9	4248.3
D-Ribose	Carbohydrates	20397	30914	27152	32529	6700.6	7925.4	24700	17081	11043	10792	11302	21192
Gluconolactone	Carbohydrates	23095	16459	15095	28548	9606.2	4511.3	17464	15534	6410.4	14067	12374	13567
2-Deoxyribose 5'-phosphate	Carbohydrates	14828	9366.5	23421	11290	13218	12309	7813.4	36671	22901	21192	7314.6	9865.4
D-Xylulose	Carbohydrates	13071	13373	9635.4	15620	9450.3	4609.3	10773	11721	6040.8	9901.5	6486	9899.3
L-Gulose	Carbohydrates	6554.6	3118.3	2466	6002	3013	5614	5195.5	11108	11233	3607.1	4980.1	5571.2
Palmitoylethanolamide	Carboximidic acids and derivatives	54602	0	38240	57587	0	0	0	42737	42096	38914	52023	61960
D-Proline	Carboxylic acids and derivatives	1E+07	1E+07	1E+07	1E+07	4E+06	2E+06	1E+06	5E+06	1E+06	4E+06	6E+06	3E+06
D-alpha-Aminobutyric acid	Carboxylic acids and derivatives	4E+06	1E+07	6E+06	5E+06	1E+07	7E+06	9E+06	1E+07	7E+06	1E+07	1E+07	1E+07
D-Glutamine	Carboxylic acids and derivatives	1E+07	5E+06	4E+06	9E+06	3E+06	5E+06	2E+06	4E+06	1E+06	2E+06	5E+06	4E+06
Pyrrolidonecarboxylic acid	Carboxylic acids and derivatives	4E+06	3E+06	5E+06	4E+06	3E+06	3E+06	1E+06	3E+06	1E+06	2E+06	3E+06	3E+06
Hydroxypropanedioic acid	Carboxylic acids and derivatives	716244	1E+06	619855	2E+06	310419	242626	353267	139822	150421	62168	179116	257992
Proline betaine	Carboxylic acids and derivatives	201226	335876	184862	53014	132301	78218	162235	286403	135554	143723	181494	124574
NG,NG-Dimethylarginine	Carboxylic acids and derivatives	109141	116258	86338	212974	80971	0	70246	173122	34198	97418	192473	57846
(S)-2,3,4,5-tetrahydropyridine	Carboxylic acids and derivatives	33722	28202	14323	38265	39457	35315	7405.7	5564.5	6453.9	10239	7138.3	5386.1
2-Aminomuconate semialdehyde	Carboxylic acids and derivatives	18821	24030	16675	27599	6423.2	11060	6355.3	20721	25848	23257	16059	23069
N-Acetyl-L-glutamate 5-semialdehyde	Carboxylic acids and derivatives	18626	17410	14226	13327	13206	27256	7103.2	7737.1	1241.9	5636.1	4550.4	3869.4
Lincomycin	Carboxylic acids and derivatives	22686	3937.4	9172.7	8934	34149	6203	9427.2	6030	0	3561.2	13860	14468
Beta-Tyrosine	Carboxylic acids and derivatives	4195.2	21733	4008.9	28790	3673.3	5528.9	3283.7	10589	2868.1	6398.6	5219.4	5356.1
L-Hypoglycin A	Carboxylic acids and derivatives	6881.5	12812	1305.9	8818.6	6432.2	11978	10437	19214	13673	23454	8478.2	15972
Ergothioneine	Carboxylic acids and derivatives	6028.9	8543.4	8899.7	6571.5	4561.3	6062.3	9007	16385	6610	13308	8122.3	9994.1
Clavulanate	Carboxylic acids and derivatives	7538.8	7352.5	4111.6	7069.8	4769.9	3382.2	5544.8	5822.6	4963.6	7791.9	2986.9	4614
Maleic acid	Carboxylic acids and derivatives	8427.7	6220.3	2907.5	5540.4	7076.5	2947.9	5978.9	9038.3	4466.3	4095.9	9710.7	8540.7
Asp-Phe methyl ester	Carboxylic acids and derivatives	3319.7	3763	8691.8	7087	2221.4	2517.7	42119	97479	60580	83497	93970	41777
Isocitrate	Carboxylic acids and derivatives	1918.1	5982.5	6172	2795.9	3133.4	6164.4	1934.2	2177.6	3703.3	8368.3	5158.7	6411.5
p-Hydroxyphenylacetylglutamate	Carboxylic acids and derivatives	4371.9	6032	5316.3	1399.5	5982.7	2528.4	6538.8	3561.5	5231.2	5815.7	4411.6	10352
cis-2-Methylnaconitate	Carboxylic acids and derivatives	2647.5	4680.1	3717.2	4063.4	5412.6	4747	4409.4	3354.6	6364.5	3835.7	2610.2	3986.1
Tricholomic acid	Carboxylic acids and derivatives	2049.6	5706.2	2227	3425.9	3027.9	4114	5662	3827.9	2761.2	4729.8	3359.3	2639
N-Acetyl-L-histidine	Carboxylic acids and derivatives	5359.2	2511.5	1099	2796.9	1670.2	0	2842.3	10783	4189.9	4809.8	0	4026.1
S-Lactoylglutathione	Carboxylic acids and derivatives	1310.9	2260.1	2265.7	1657.7	1606.8	4006.6	1346.1	1137.3	989.04	221.71	0	230.56

L-Targinine	Carboxylic acids and	2413.5	743.92	271.88	2248.2	1798.2	1538.9	3195.9	2459.8	2475.8	1238.9	1320.4	1624.4
Okanin	Chalcones	4E+06	4E+06	4E+06	3E+06	4E+06	4E+06	16724	22333	19222	11960	12558	17039
Hydroxysafflor yellow A	Chalcones	257489	16166	210063	280519	8762.5	290213	237753	286626	484698	15957	16144	214964
Asebogenin	Chalcones	18983	28832	27268	13458	20838	22565	7187	7464.8	6169.2	4938.4	5311	7371.5
Phlorizin	Chalcones	23875	8332.1	42972	10370	13113	12015	0	0	0	555.61	0	0
Safflor Yellow A	Chalcones	11539	2143.5	3480.7	2165.5	4970.9	3455.1	2239.5	15279	9486.9	0	4081.6	15789
Butein	Chalcones	5599.5	2093.7	4610	1150.5	8678.3	3332.7	1895	3327.8	2779.5	4414.8	4636.8	3883.4
2',6'-Dihydroxy 4'-methoxy	Chalcones	5397.8	5408	4089.7	3396.6	3909.1	2355.2	3622	9954.7	14430	8293.6	19137	5186.7
Neosperidin dihydrochalcone	Chalcones	0	0	0	0	0	0	0	10164	37912	0	0	2606
Phosphorylcholine	Cholines	866139	464183	644183	509231	646946	2E+06	337002	187513	222135	434079	209778	322326
O-Phosphocholine	Cholines	1736.2	1557.6	2409.9	11025	6778.1	2957.2	3617.6	9650.6	5425.5	7830.2	3976.8	5047.7
Glycerophosphocholine	Cholines	3256.6	6545.1	4311	0	0	0	0	9246.9	1340.5	5116.6	0	4291
Ethyl trans-p-methoxycinnamate	Cinnamic acids and	88436	50133	61875	34482	97985	89049	26040	53658	88238	25919	53016	38999
3-(3,4-Dihydroxy-5-methoxyphenyl)propanoic acid	Cinnamic acids and	6721	16560	4493.7	3509.2	5619.1	3073.9	5277.2	4068	6705.4	3849.4	5426.8	2990.6
Carbofuran	Coumarans	6740.7	9602.8	8729.2	7353	4078.6	5210.2	1360.9	3392.4	1038.1	1842.6	1916.8	1943.3
8-Geranyloxypsoralen	Coumarins	1E+06	717131	604796	639672	618169	469215	700449	599957	374489	45472	144422	489376
Micromelin	Coumarins	46003	41704	79294	196968	22665	79919	1271.3	3753.2	642.02	0	634.03	7102
Psoralidin	Coumarins	40801	16367	22762	18931	31767	38648	80064	119872	43984	55740	37167	56901
Scoparone	Coumarins	12120	14941	29873	10726	15253	20629	23827	27035	15712	20296	14374	9438.9
Lansiumarin A	Coumarins	15054	3570.2	2405.7	16084	15014	43352	11645	21182	6918.8	21993	12538	25660
Alloimperatorin	Coumarins	14854	14469	32216	11055	15762	7035.3	8714.5	7513.5	11093	7379.5	16148	9094.4
Luvangetin	Coumarins	17304	16893	11507	14193	5928	18476	3334.6	2718.6	2051.3	1812.4	2880.3	1571.7
8-Hydroxybergapten	Coumarins	33673	7764.6	1193.3	1838.5	19654	4663.2	610.89	8346.4	14261	14878	12500	1798
Bergamotone	Coumarins	10345	5591.6	2901.7	20353	5799	11273	22849	6737.6	3053.9	6427.1	10881	10870
Daphnoretin	Coumarins	12112	7011.4	4572.3	12963	684.15	18602	11734	24025	14992	2144.5	20354	4198
Herniarin	Coumarins	6556.6	3828.4	7657.5	7633.2	9428.9	13933	16405	18693	4735.1	17250	28071	6128.3
Fraxetin	Coumarins	4631.9	4128.2	5914.9	5249.3	12084	10158	10661	1612.8	4716	9303.9	6317.8	2897.2
4-Methylumbelliferyl acetate	Coumarins	10467	6179.3	3775.7	9264.8	3888.9	4486.1	5313.9	8388.4	5156.9	8511.4	9600.4	15983
Neoglycyrol	Coumarins	4772.9	1143.1	8628.8	2288.8	19283	1855.9	3379.1	10172	7532.6	3596.5	12376	15204
Decursin	Coumarins	8842.3	3690.4	2924.1	5872.3	8224.2	2944.6	6082.5	10018	2809.9	6161.1	17258	1702.3
Notopterol	Coumarins	10930	0	6151.9	2359	1565.1	5808.3	4369.1	13779	6116.8	3478.9	8198.5	5807.5
4-Methylumbelliferone	Coumarins	2806.1	6912.9	3489.9	4905.7	4454	3352	3655.1	10701	5989.4	4734.9	1765.8	3426.1



Mellein	Coumarins	2252.7	4910.9	2229.9	4914.7	2610.9	6411.5	8775.5	4377.8	4529.8	5198.7	3288.9	3605.1
Esculin	Coumarins	3128.5	4016.9	3400.1	5114	2506	4499.3	2317.7	8401	4524.8	6575.5	12360	363.33
Bergapten	Coumarins	1940	1921.7	5964	5123.7	4775.3	2911.4	4259	8670	1362	693.47	5535.3	6452.6
Dalbergin	Coumarins	736.83	1339	3628.8	3985.7	9821	1324.2	2209.3	2637.6	520.77	2305.2	4028.9	2081.4
Isobergapten	Coumarins	2408.1	3173.7	3386.6	2302	2431.2	4227.8	5674	2530.6	1783.7	1481.2	1500.7	3087.7
Nodakenin	Coumarins	1297.3	6034.5	3548.7	1388.4	1428	710.62	4617	4571	10487	2284	3649.6	1544.9
Bergaptol	Coumarins	2069.9	1750.4	1976.8	1901.2	1526.4	3618.1	2785.9	3531.5	2993.3	6116.1	3134.8	2847.3
Warfarin	Coumarins and deriv	392.35	398.29	595.39	1159.1	401.32	847.5	3420.9	6759.6	2721.8	5381.8	2665.3	0
Miltirone	Diterpenoids	781511	590678	783016	2E+06	988052	949177	905493	1E+06	718095	578654	954398	732066
Kirenol	Diterpenoids	409532	220217	170483	350771	238069	182464	256377	217149	140871	17293	30808	186903
Kaurenoic acid	Diterpenoids	30157	47512	49420	39176	40610	51892	0	0	0	0	468.78	0
Bruceine D	Diterpenoids	5304.8	8356.2	16684	16252	10063	19290	0	0	1612.4	1609.9	1587.3	1036.3
Sterebin A	Diterpenoids	17370	6418.5	0	13880	8790.1	7447.8	263338	958065	403896	399382	773966	253714
6,7-Dehydroferruginol	Diterpenoids	5435.2	6172.5	10974	3735.1	5894.5	4171.1	6888.6	10097	10552	8955.7	10117	10369
Abietic acid	Diterpenoids	8048.8	2099.2	5380	3024.8	5169.8	6209.5	4296.1	3082.3	2428.4	2346.7	0	10281
Diosbulbin D	Diterpenoids	5513.9	684.48	2794.7	6444.1	4016.2	1358.9	3088.7	1063	1749.7	5581.9	1040.1	4236.2
Picrasin B	Diterpenoids	387.22	4107.8	1691.1	3429.6	3959.5	2737.4	1343.6	573.93	312.2	1117.4	1156.5	2576.4
Triptdiolide	Diterpenoids	3173	2300.8	1165	4888.4	3751	611.89	580.74	1372.6	594.74	2628.7	4105	1176.1
(+)-Glaucarubinone	Diterpenoids	2361.2	1291.1	0	2835.4	1930.2	5745.3	0	4223.1	934.73	3858.3	0	0
Mevastatin	Diterpenoids	4109.9	0	0	3924.4	2312	2252	15640	8649.1	0	0	6439.2	1414.1
Bromocriptine	Ergoline and derivat	7006.2	1517.1	46015	98491	139129	5578.9	81080	89673	3156.5	6219.4	15075	31639
Turanose	Fatty Acyls	1E+07	1E+07	6E+06	1E+07	1E+07	9E+06	7E+06	7E+06	1E+07	1E+07	6E+06	7E+06
Lubiprostone	Fatty Acyls	4E+06	3E+06	3E+06	4E+06	3E+06	2E+06	5E+06	4E+06	2E+06	2E+06	3E+06	3E+06
Oleamide	Fatty Acyls	3E+06	2E+06	14226	7E+06	6E+06	15067	3E+06	33980	5E+06	18547	35129	31613
Kojibiose	Fatty Acyls	2E+06	2E+06	2E+06	2E+06	3E+06	1E+06	802576	478709	881221	2E+06	2E+06	2E+06
Erucic acid	Fatty Acyls	1E+06	835754	663545	783990	885107	786204	1E+06	988323	427342	50101	146137	689298
L(-)-Malic acid	Fatty Acyls	1E+06	867319	491683	680570	426138	113180	656148	739382	702381	374039	1E+06	1E+06
8,9-DiHETrE	Fatty Acyls	1E+06	654441	597130	88847	48396	70878	943421	198219	46665	37127	85268	84563
Oleic acid	Fatty Acyls	612275	155331	170034	554254	544952	404795	667350	1E+06	385629	267555	468146	337449
Itaconic acid	Fatty Acyls	277374	4518.8	289881	331615	161534	321506	119203	4957.4	110131	134651	294185	235020
6-Aminocaproic acid	Fatty Acyls	112488	178400	90945	122521	77062	25048	25273	60975	42102	30823	40496	26357
Octadecanamide	Fatty Acyls	35465	21980	29887	74532	38363	49701	48987	57799	36554	20315	58268	36274

Pimelic acid	Fatty Acyls	39548	47900	35869	52337	31743	38751	83956	104151	106017	115130	95110	116234
Methyl hexadecanoic acid	Fatty Acyls	13827	16316	18444	30723	60915	35580	22200	22282	19610	24047	14055	42104
20-HETE	Fatty Acyls	28019	30565	15683	26505	29161	23864	19042	17560	13229	2980.3	4298.5	18336
L-2-Hydroxyglutaric acid	Fatty Acyls	5629.5	34205	19084	8886.1	16879	46000	4409.2	12652	35564	29235	13872	32900
L-Acetylcarnitine	Fatty Acyls	34584	20624	15821	8884.2	20126	12154	20279	11736	7422.7	39531	18177	27631
Colneleate	Fatty Acyls	21639	12867	14726	12072	19943	11454	127011	248326	68343	89908	134960	42152
Stearic Acid	Fatty Acyls	15838	13611	3826	17725	16059	9904.1	12470	15450	7546.4	6618.1	11729	10599
9,10-DHOME	Fatty Acyls	14442	13685	9167.5	17283	14342	3128.2	15245	4196	8806.6	5400.2	11836	6655.6
(10E,12Z)-(9S)-9-Hydroperoxy-10,12-octadecadienoic acid	Fatty Acyls	5478.2	4544.4	14288	14708	13754	16362	111343	242736	81203	269697	159489	77045
3-Isopropylmalate	Fatty Acyls	5512.1	8174.3	3673	7073.8	9103.4	6214.5	12372	9898.9	14697	18501	12227	5839.2
13(S)-HPOT	Fatty acyls	5552.8	2730	7932	13156	4882.5	3968.8	7924.4	17152	8525.1	9105	22651	15213
Methyl jasmonate	Fatty Acyls	7098.8	7080.8	6596.2	1900	10617	2486.3	4706.9	6351.4	9325.8	10039	9035.8	0
Traumatic acid	Fatty Acyls	5657.8	8828.9	4586.6	5720.3	5172.8	3738.7	3693.4	6470.2	3662	5508.7	5219.6	8214.4
12(13)-EpOME	Fatty Acyls	6256.8	1545.1	6972.3	4627.7	7048	2741.5	2405.7	11884	12995	6226.1	6351.1	4618.6
9-OxoODE	Fatty Acyls	0	4549	12168	8316.6	0	3122.6	61341	132786	52031	41185	170560	60367
Jasmonic acid	Fatty Acyls	2996.1	5903.9	8418	2969.3	4017.7	1696	2494.1	5949.1	5441.6	7270.4	5823.7	8745.5
8-Methylnonenoate	Fatty Acyls	4040.9	3238	3546.4	2896.1	5544.1	1783.1	2109.9	3326.7	677.13	3966.5	2091.1	1711.9
(13E)-11a-Hydroxy-9,15-cis-11-octadecadienoic acid	Fatty Acyls	5383.3	2730	2736	3485.7	1403	2702.7	4209.7	5519.4	2140	0	4209.8	1400
20-COOH-Leukotriene B4	Fatty Acyls	4037	2569.4	1016.3	1391.7	1336	0	2826.5	1380.4	2148	5775.4	9780.5	14850
5,6-DHET	Fatty Acyls	2764.3	2875.3	284.71	0	2738.2	716.34	1202.7	2364.9	11304	3629.5	4794.6	2202.6
9(S)-HPOT	Fatty acyls	835.69	645.96	521.25	1707.9	634.69	1075	2536.7	7440.5	3832.2	6697.9	4449.8	1677.4
Prostaglandin I2	Fatty Acyls	1006	1101.4	0	0	221.94	683.1	0	0	3450.2	12613	9500.4	6282
Xanthohumol	Flavanone	1850.3	3021.7	1871.7	3571.1	1349.3	1667.8	1833.9	2320.4	1912.1	2620.3	1410.4	1292.7
Cianidanol	flavonoids	2E+08	2E+08	1E+08	1E+08	1E+08	2E+08	253258	643033	221971	551768	169720	247570
Epicatechin	Flavonoids	1E+07	1E+07	9E+06	8E+06	9E+06	3E+07	67361	318974	191245	116874	100556	171563
Procyanidin B2	flavonoids	8E+06	7E+06	7E+06	6E+06	7E+06	2E+07	53888	233926	62006	49716	42556	79011
Procyanidin B1	flavonoids	7E+06	7E+06	8E+06	1E+07	6E+06	1E+07	11423	51033	7353.7	32377	8311.3	10697
Narcissoside	flavonoids	3E+06	2E+06	2E+06	3E+06	2E+06	4E+06	0	0	11222	17815	0	13282
L-Epicatechin	flavonoids	1E+06	1E+06	1E+06	770162	1E+06	3E+06	0	40772	15239	11430	17250	11293
Rutin	flavonoids	567351	583445	357298	565559	473391	776282	0	0	0	3837.8	0	466.78
Wighteone	Flavonoids	1E+06	717131	604796	14031	618169	3975.4	700449	41953	12666	14762	143709	28123
Cyanidin 3-rutinoside	Flavonoids	258745	430506	436315	451839	491356	964922	2883.7	14096	2918.6	8683.5	367998	109615

Maltol	Flavonoids	194639	378050	632851	214228	271636	297104	528614	148518	247553	272723	263565	100205
Vestitol	Flavonoids	210084	81083	298651	178857	428322	265446	7680.1	6088.3	2198.1	1342.3	4092.6	1736
Cynaroside	flavonoids	108572	187970	140644	201597	269260	326016	2E+06	423756	3E+06	498547	1E+07	5E+06
Peonidin-3-glucoside	Flavonoids	112287	149989	171088	113625	116872	371679	3E+06	1E+06	3E+06	846042	1E+07	5E+06
Kaempferol-3-O-rutinosid	flavonoids	65550	67547	114588	210520	192998	261972	5386.5	2312.8	2756.2	6801.3	5387.1	4525.1
Taxifolin	flavonoids	149596	67431	105333	164583	147888	208871	53469	34746	33219	41285	38882	31870
Dalbergioidin	Flavonoids	93670	74214	66764	73251	289570	229625	33540	46359	53285	189839	182235	104433
Karanjin	Flavonoids	266814	47769	84079	93867	84273	160599	65035	322795	198565	376151	190393	159060
Eriodictyol	flavonoids	59578	37079	56245	86280	111729	170553	14939	17336	22871	8058.2	62903	23331
Rhoifolin	flavonoids	23778	114516	40563	82275	107115	152029	22214	12154	6983	13024	54290	23584
Chalconaringenin	flavonoids	46884	43408	48915	86791	68469	113565	6641.6	7865.9	5838.5	7259	8501	7040.7
Glycinol	Flavonoids	81794	34725	33385	87664	47673	119415	7059.3	3606.1	4164.8	2998.8	3546.2	8257.9
Catechin	Flavonoids	76884	66200	36338	36478	44451	105550	2241.8	4432.9	515.32	2158.8	0	558.27
Delphinidin-3-O-glucoside	Flavonoids	68372	41474	77265	64068	56986	51479	1762.8	3366.6	1223	3473.3	2585.6	4646.2
Genistin	flavonoids	53135	111222	8712.5	56521	92446	30519	187827	25386	92122	5249	326144	215728
Naringenin	flavonoids	53686	54422	36842	86791	25409	83462	9071.7	3278.2	5236.9	7070.9	3355.1	3804.8
Tricetin	Flavonoids	18100	55633	65490	3828.3	7344.7	97589	0	791.7	788.9	600.54	689.01	582.58
Naringenin chalcone	Flavonoids	37721	18520	84015	26902	47864	31151	5924.3	14370	10145	26648	10895	8236.9
Blumeatin	Flavonoids	33790	25811	34554	34255	20109	61678	629.54	4991.3	2968.8	1170.3	1169.9	1217.6
Malvidin-3-O-galactoside	Flavonoids	6883.7	68215	39471	25691	29573	22214	949.65	2741.4	467.7	1218.9	478.04	233.55
Kazinol A	Flavonoids	38933	28275	21930	39376	34201	28197	36933	35353	13129	5985.7	11194	20924
Dihydromyricetin	flavonoids	25800	21545	36145	31878	20669	44167	5117.4	581.97	2868.3	1143.6	41436	3350.9
Morusin	Flavonoids	22686	25881	18726	82828	9443.5	14070	7990.8	70918	15841	17379	7545.4	21590
Brazilin	Flavonoids	19319	11752	20940	19008	23594	53876	4601	3545	1867.2	4512.9	7028.9	9751.6
Tricin	Flavonoids	19146	17476	23003	27776	18595	27776	14173	18538	13441	25055	37363	26450
Isoquercitrin	Flavonoids	11600	8196.6	5158	35201	8288.6	51479	2910.5	5240.6	5162	4485.8	2955.2	2746.5
Diosmin	flavonoids	0	42240	0	0	0	71807	21907	0	17054	34085	158075	89495
Neoastilbin	Flavonoids	29172	9852.6	20054	13914	7663.8	24389	1266	1268.9	880.7	4008	3081	628.85
Quercetagetin	Flavonoids	18340	20218	24531	0	17840	22728	11762	19786	21431	2808	0	28742
Isorhamnetin	flavonoids	6015.2	9301.5	18245	0	12671	54688	0	1982.9	0	3394.8	815.7	1503.4
Aromadendrin	Flavonoids	17901	8266	18061	20549	15321	11121	4582.7	14805	8711.8	7751.5	9627.1	4923.6
Hydrangenol	Flavonoids	10815	5140.7	15907	11836	29105	12412	10634	15381	4304.5	15351	12348	10845

Pelargonidin-3,5-O-digluc	Flavonoids	12485	20573	7486.2	13641	16619	8750.7	560100	735102	356218	442360	799663	571926
2',3,5,7-Tetrahydroxyflavo	Flavonoids	12232	4102.8	10082	6395.9	27065	18998	1360.4	4097.1	4955.7	7764.7	2657.9	1924.7
Tectorigenin	flavonoids	9892.2	4379.9	12357	7158.3	18640	26398	57989	108639	111936	92266	307148	165604
Deguelin	Flavonoids	17658	7789.3	6250.3	19995	9766.5	16235	13390	14408	10108	7077.9	10662	7255.9
Hyperoside	flavonoids	5489.1	12370	24763	4690.5	17022	10616	7291.5	5062.6	81798	1921.1	33176	1215.2
Luteolin-6-C-glucoside	Flavonoids	18050	20650	8267	7825.6	10756	8365.2	128667	134559	7095.2	71491	49501	165137
7-Hydroxyflavone	Flavonoids	14291	14675	9784.5	14027	4619.3	15200	16241	18070	24888	31850	32058	22647
Fustin	Flavonoids	18935	4924.8	9831.3	12508	8773.9	17417	2407	2175.8	2525.9	3900.1	1161.2	1710.8
Astilbin	Flavonoids	10468	17768	14264	4658.6	12046	11011	1907.8	2095	800.91	424.51	1637.4	427.28
3,8'-Biapigenin	Flavonoids	18687	10638	11538	11552	6230.1	9437	7179	12685	9217.2	7684.5	18977	6239.5
2,3-Dihydro-2-phenyl-4H-	Flavonoids	9877.8	4754.6	20528	8815.8	11370	11456	6206.8	15455	8473.2	4116.3	9479.2	6547.1
Hinokiflavone	Flavonoids	18687	8340.6	11538	11751	6230.1	9437	7179	12685	9217.2	7684.5	18977	6239.5
Norwogonin	Flavonoids	10547	15687	7921	14673	9503.9	6756.2	15110	10760	10869	6981.8	9903.8	7149.8
Genistein	flavonoids	10874	11158	12078	10111	5946.4	12218	8771.3	10199	1436.8	5238	4727.8	6045.9
Biochanin A	flavonoids	4861.9	16374	5313.4	12416	3853.7	13919	18470	23912	20046	12564	4278.6	8603.7
Procyanidin B4	Flavonoids	14816	771.23	4600.3	15700	11643	6982.2	7097.7	3539.7	0	3108.6	0	2141.7
Pedalitin	Flavonoids	10423	6799.5	5480.2	9604.7	12392	8502.3	8346.2	10697	7258.5	12444	5304.6	9215.1
Gallocatechin	flavonoids	9833.4	2911.1	8359.4	9021.9	7587.8	14282	3815.5	3278.9	1817.3	4222.9	3558.7	2549.9
Procyanidin A2	Flavonoids	5419.7	7348.1	5710.5	12685	4872.7	11742	698.82	1180.3	700.18	1531.5	760.6	6123.9
Homoorientin	flavonoids	18050	3100.8	2605.9	8605.1	5111.9	10216	128667	134559	5083.2	71491	361855	165137
Robinetin	Flavonoids	3347.2	8793.2	2556.1	3770.4	12246	13458	6875.3	11039	6972.1	14513	7129.2	8869.9
Isovitexin 2"-O-arabinosid	Flavonoids	2332.1	5746.1	0	2922.3	12751	19081	36765	43830	10405	60777	45763	57742
Isovitexin	Flavonoids	7979.7	6819.6	12639	1343.4	4224.4	9642.6	6660.2	10613	27413	8171.6	10123	2831.8
Daidzein-4',7-diglucoside	Flavonoids	3804.1	11504	6061.8	11609	905.77	8598.2	1880.7	1940.2	2313.5	5981.3	1198.1	1423
4',7-Isoflavandiol	Flavonoids	9077.3	7324	0	6951.4	10122	5984.7	5138	6565.1	4528.2	7348.7	8274.6	3420.7
3',4',7-Trihydroxyisoflavo	Flavonoids	7118.1	6746.6	4647.2	8155.3	8085.8	4680.7	5054.5	3337.9	5366	2857	5319.4	9929.1
Homoeriodictyol	Flavonoids	10141	4893.2	6042	5188.3	4773.4	7688.8	10803	6764.9	17399	10752	14597	17590
isoliquiritigenin	flavonoids	6434	9458.3	4675.2	6981.7	5633.2	4337.2	5855.4	7768.6	3730.9	6875.9	6242.3	6465.5
Swertiajaponin	Flavonoids	9704.5	5139.8	5516.3	9077.7	4849.8	1978.4	19952	59283	15533	19244	52838	17664
Demethoxycapillarisin	Flavonoids	3704	6972.6	7002.6	5235.8	8400.8	4834.6	876.69	2254.8	888.3	3813.3	4431.3	3680.2
Isosakuranetin	Flavonoids	1408.5	5436	908.28	1890.9	21896	4065.8	1989	1811.8	3971	2035	2894.8	4549.7
Vitexin	flavonoids	3233.9	1349.1	11011	1343.4	8502.8	9642.6	6660.2	10613	125136	8171.6	10123	5384.8

Diosmetin	flavonoids	2455	0	4659.8	5565.1	11967	10053	30320	65281	54285	69658	140318	118204
Fisetin	flavonoids	3815.7	4957.7	2318.1	1774.4	7672.4	13895	1199.8	881.72	1750	3448.7	601.65	1457.4
Chrysoeriol 7-apiosylgluc	Flavonoids	4031.5	8891	2425.3	6665.4	6117.6	5119.7	8606.9	5096	20273	5792.1	21725	4021.7
2'-Hydroxydaidzein	Flavonoids	4851.7	4714.1	8455.1	6851.6	6188.7	1782.3	4615.5	6613.2	7304.2	6457.4	5554	4064.7
Galangin	flavonoids	5147.2	3324.1	10977	8373.4	2123.4	2093.3	5049.9	5426.5	4829.3	6928.7	3041.4	1893
2'-Hydroxygenistein	Flavonoids	2268.4	2742.8	3165.3	17738	3783.1	2100.9	1250	3414	2517	2808.4	4382.7	3232.8
Irisflorentin	Flavonoids	963.26	0	2395.6	0	1001.2	26958	17682	52307	9341.3	57558	23189	15123
Morin	Flavonoids	902.93	3276.9	3231	7914.9	2236.3	13387	2467.8	1596.8	3453.9	2738	1868.3	4499
(+)-Afzelechin	Flavonoids	9292.8	4594.1	7627.9	4072	2291.4	2070.9	8242.3	3991.1	6762.6	9930.2	5231.8	7573.2
Methyl hesperidin	Flavonoids	1800.5	0	4133.6	9468.3	8756.7	5305.2	9449.8	25995	16593	6160.4	16506	6093
4',5,6,7-Tetramethoxyflav	Flavonoids	4070.6	8965.3	2737.5	7299.2	2003.5	4054.3	13760	7445.8	5743.9	4720	8701.8	7551.4
Saponarin	Flavonoids	5474.4	0	617.56	1707.2	3829.5	17374	91208	98673	91823	88909	214536	178844
Schaftoside	Flavonoids	4575.4	7925.5	1252	5037.1	3237.6	6578.5	10728	9858.8	2755.1	24075	13471	16097
Isorhamnetin-3-O-nehespe	flavonoids	2073.8	880.99	2573.4	4394.3	873.67	17431	2924	16180	0	10783	5146.4	8783.4
4'-Methoxyflavone	Flavonoids	4751.7	6024.5	6834.5	3481.7	3126.9	3901.2	8349.8	28366	5594	14548	10022	7827
3,9-Dihydroxypterocarpan	Flavonoids	6708.9	3107.7	4070.7	3818.2	3942	5953.9	3345.5	3297.2	7597.6	4670.8	3094	6007.3
Delphinidin	Flavonoids	3069	2239.6	7386.9	5514.9	3702.2	4881.5	7068.9	3255	1451.2	3006.2	369.1	1115.8
Daidzin	flavonoids	3056.4	1366.4	6328.2	1036.6	3028.4	11835	2731.1	2271.5	1522.5	1028.1	1008	4198.1
Liquiritigenin	Flavonoids	4388.1	4605.6	4330	3265.7	3307	6710.6	2800.1	2863	3157.8	2439.9	2636.1	2426.9
Plantagoside	Flavonoids	3489	1139.5	2148.9	2260.3	8765.2	8643	0	1905.5	371.79	1917.5	0	6435
Homopterocarpin	Flavonoids	9133.6	3188.9	3019.3	4717.7	3836.8	2501	2061.4	2834.8	4159.4	4439.4	3041.8	2754.2
4',5,7-Trimethoxyflavone	Flavonoids	4471.4	3009.6	4580.2	7345.9	4055.4	2001.8	5990.2	5796.2	3166.9	4627.7	9901.2	3394.7
Nobiletin	Flavonoids	5877	0	0	12005	0	7180	6908.7	8192.8	4121.1	0	3012.3	7922.5
Phloretin	flavonoids	7468	2007.7	1559	763.23	8415.6	4788	6533.7	12403	4694.3	8246	4949.5	6283
Sciadopitysin	Flavonoids	7524.8	2839.3	0	4678.8	3553.4	6082.8	7287.1	4829.7	3279.9	10129	12487	4659.1
Apigenin	Flavonoids	5161.9	2866.9	3234.6	6458.4	4522.4	2386.6	7427.9	6633	3480.9	10754	9096.1	3236
Apiin	Flavonoids	5786	6208.2	2617.3	924.36	5268.2	3557.8	0	433.82	0	0	0	0
Icariin	flavonoids	0	0	2026.3	0	985.1	21012	0	558.07	1610.9	340.9	0	842.46
Glycitein	Flavonoids	756.24	2933.3	1402.2	2585.2	15211	715.02	713.95	1289.3	1277.1	1200.2	1988.8	0
Flavone	Flavonoids	3118.8	2397.7	3047.8	9232.9	2568.3	3153.8	1242.7	3550	7420.4	2413.2	3132.8	3846.8
Glycitin	flavonoids	1407.9	986.38	0	2797.7	11276	5682.3	1996.4	1006.5	981.41	465.94	476.69	3783.2
Resokaempferol	Flavonoids	4571.9	3519.6	6186.6	3370.3	1952.9	2252.5	3967.5	2363.5	2212.4	2259.6	1664.2	4335.9

Butin	Flavonoids	3813.9	4505.1	1585.2	2661.7	4623.1	4653.4	13975	4053.4	4333.9	8473.3	4669.3	7615.7
Myricetin	flavonoids	2601.2	6994	3142.8	3226.7	1650.5	3711.5	2981.7	2901	1728.6	2399.2	2387.7	0
Chrysin	flavonoids	1189.9	7884.1	4736.2	1700.7	1763.5	3802.2	8982.9	2950.4	2392.9	2426.1	6943.1	2452.1
Meloside A	Flavonoids	5126.2	0	2236.7	1707.2	3829.5	8067.3	126499	98673	91823	100921	214536	201036
Vitexin 2"-glucoside	Flavonoids	5126.2	0	2236.7	1707.2	3829.5	8067.3	91208	98673	91823	88909	214536	201036
Dihydrorobinetin	Flavonoids	2843.1	631.04	4767	3764.7	3529.7	5074.3	4295.1	3776	1809.5	1275.3	1213.9	598.9
Pinobanksin	Flavonoids	1699.5	2354.7	1851.2	4370.6	2684.8	7579.3	4718.3	5014	3305.4	4953.4	4218.6	1788.3
Quercetin	flavonoids	2261.5	5233.9	2282	1103.6	1131.4	8263.7	379.05	392.74	376.37	193.17	187.47	562.52
Baicalein	Flavonoids	1198.6	1385	6145.7	5104.5	3767.2	2259.1	3498.5	4947.2	1723.4	4181.2	3804.2	3100
4',7-Dihydroxyflavone	Flavonoids	1031.8	3963.5	4506.1	2840.4	3515.1	3050.6	701.55	956.1	477.75	3496.3	1209.5	460.05
7,8-Dihydroxyflavone	Flavonoids	2447.8	1198.4	3903.9	2417.9	5560.7	3372.4	1348.3	5256.1	1021.8	2361.4	2657.3	4579.5
Silibinin	flavonoids	1470.2	1444.9	6651.6	2485.4	2051.7	3628.9	1988.2	2124.8	0	4028.7	1522.8	711.09
Isoscoparin	Flavonoids	1217.8	2955.3	772.38	1188.2	4705.9	3624.1	5152.8	8002.2	0	0	3230.5	2681.5
Kuwanon H	Flavonoids	6241.6	1516.8	0	3849	0	1597.1	7547.6	2372	0	0	3125.2	2846
Theaflavin	Flavonoids	5095.3	0	0	937.93	2363.1	3788.2	0	236.13	230.51	0	0	0
Poncirin	Flavonoids	874.13	891.89	1909.5	1471.9	5793.1	1203	3389.1	2237.3	2713.5	1883.7	2893.5	3287.9
Tectochrysin	flavonoids	0	1506.7	6616.7	0	2110	1495.7	0	3314.2	7708.2	0	5552.6	0
Homoferreirin	Flavonoids	278.34	3085.5	3434.7	2294.1	839.48	1729.4	2839.8	2349	858.64	1610.6	2600.1	2266.1
5,7-Dihydroxyisoflavone	Flavonoids	1231.8	1222	2039.8	4193.9	2263.4	589.22	767.9	1680.6	2967.3	1960.3	2274.8	2307.6
Scutellarein	Flavonoids	2134.6	1158.7	1393.5	1279.2	1062.5	4071.4	1338.2	5834	3410.7	1865.8	8759.7	3200.5
Hesperetin	Flavonoids	657.82	913.04	2051.2	1638.2	2128.5	3248.5	3557.5	2822.9	837.1	1247.7	1482.7	2017.9
Cyanidin-3-O-rutinoside c	Flavonoids	1558.3	1254.4	844.85	840.99	3251	1316	1919.1	2414.5	2055.5	1304.5	2849.9	1479.5
Glabridin	Flavonoids	1819.5	0	0	0	5493	1259	6952.8	0	6879.3	0	3594.1	1750.5
Ononin	Flavonoids	1019.3	1496.5	463.89	1190.6	708.43	3631.5	714.35	3427.6	486.92	1090	735.74	945.06
Luteolin	flavonoids	1324.4	270.06	1055.4	540.04	1399.7	2206.7	1071.3	1137.5	2166	1723.1	16438	6060.8
Liquiritin	Flavonoids	448.61	904.5	0	2905.9	1991.8	348.23	466.96	0	1381.8	0	473.61	4544.8
Cyanidin-3-O-rhamnoside	Flavonoids	464.65	244.73	0	1681.4	245.7	3459.1	469.43	746.34	2363.5	0	713.66	230.95
Tangeretin	flavonoids	0	1927.5	0	0	0	1424	5596.9	0	0	0	0	0
D-Glucurono-6,3-lactone	Furofurans	8218.7	28350	14080	9851.7	9481.6	15307	32924	15739	19456	23083	13752	16047
DG(16:0/16:0/0:0)	Glycerolipids	571302	30547	28397	23068	24119	9625.5	40199	1E+06	29505	22524	74027	518988
Malic acid	Hydroxy acids and d	1E+06	867319	491683	1E+06	426138	113180	656148	739382	702381	374039	1E+06	1E+06
Sinapyl alcohol	Hydroxycinnamoyl c	3488.1	1086.7	781.16	2420.7	1102.1	5306.3	2544.8	2965.6	1584.1	2983.3	1068.6	1252.2

AICAR	Imidazole ribonucle	396898	298999	301668	542961	318270	228694	292191	365732	239486	27170	54568	356290
7-Methylguanine	Imidazopyrimidines	3155.4	2953.9	5667.8	3157.4	4478	758.39	2160.9	661.5	1543.2	1309.9	1865.2	2529.8
Levamisole	Imidazothiazoles	32122	40638	40391	44925	36160	21866	32597	71402	21843	39176	36564	38567
3-Indoleacetonitrile	Indole derivatives	13347	4138.8	3548	4903.1	4298.5	4845.3	9343	7556.9	3240.7	4709.6	6729.8	9216.6
Leukoaminochrome	Indoles and derivativ	34781	34159	37976	66894	37512	21012	46693	48262	37729	54002	69654	49889
1H-Indole-2,3-dione	Indoles and derivativ	9133.1	28174	13430	15188	6159.5	6734.7	3713.6	11175	5051.4	7017.1	5309.8	5171.7
Leucodopachrome	Indoles and derivativ	5714.2	9923.6	21730	4500.2	10093	7779.9	12206	10525	27056	9371.6	18708	22389
Methoxyindoleacetic acid	Indoles and derivativ	12562	9109.8	11097	4522.9	10163	4593.7	5617.8	4312.4	5899.2	7012.5	6236.9	4060.5
5-Hydroxyindole-3-acetic	Indoles and derivativ	4836.5	7524.1	3001.3	4922.6	3658.8	7469.9	2415.2	602.23	1770.8	3582.7	3634	6033.6
Valechlorine	Iridoids	11184	2460.5	8659.8	6070.7	5137.7	386.3	8107.1	2073.1	3546.8	4564.2	1158.2	1174.1
Geniposide	Iridoids	1253.3	0	8453.9	0	4595.2	3184.8	0	4667.1	1239.6	1275.3	2426.1	3358.8
Pseudobaptigenin	Isoflavonoids	7977.5	3670	3976	8701.6	1237.3	7179.2	9094.9	2982.5	4203	6098.6	5695.9	2466.1
(S)-2-Acetolactate	Keto acids and deriv	101694	116437	97928	100545	66343	11219	5795.8	3092.2	3430.6	8300.2	10658	5611.5
2-Keto-6-acetamidocaproa	Keto acids and deriv	83176	39599	46551	36622	44480	97792	19597	26538	17809	19903	26623	9739.3
(S)-2-Aceto-2-hydroxybut	Keto acids and deriv	58806	38251	59660	33281	62753	68986	32021	41201	49893	91377	89653	39314
2-Isopropyl-3-oxosuccinat	Keto acids and deriv	8483.9	6675.1	4338.8	6718.9	7868.9	9801.9	4488.4	5704.5	6647.2	8272.7	6334.6	7152.7
Prephenate	Keto acids and deriv	681.23	1194.4	790.45	3630.1	1974.2	975.63	1874.5	707.57	2209.8	2097.3	669.21	2873.3
Neocnidilide	Lactones	4804.6	7089.4	2581.4	4999.4	10529	4692.1	10293	2563.3	4259.4	3537.3	5405.5	16730
Liriodendrin	Lignans	256072	58920	223399	327235	0	235334	181903	109564	0	0	2274	105443
Nordihydroguaiaretic acid	Lignans	13186	7134	9124.1	3165.2	16966	24577	2048	2245.2	2820.3	3508.7	1652.8	3475.8
Kadsurin A	Lignans	15405	2187.5	21430	3352.3	1269.3	4270	11785	3607.5	5688.3	2739.5	4659.9	13194
Butyl 4-Hydroxybenzoate	Lignans	5631.5	9415.3	10822	12520	3183.4	6204.7	8428.7	6433.7	3816.6	5274.4	11435	10459
Yatein	Lignans	3322	631.53	2762.2	4681	7695	7436.1	1605.8	4648.5	634.53	5015.6	3868.2	1829.5
Anwulignan	Lignans	3081.8	1308.7	3967.5	9000.1	1336	6306.2	5364.7	9468.5	3159.8	17501	4209.8	4772.2
gamma-Diasarone	Lignans	1293.1	8026.6	852.26	1742.4	443.35	1813.5	431.47	2303.9	1727.8	1770.7	3601.9	1273.2
Arctiin	Lignans	952.68	0	0	0	0	11898	7619.6	8569.5	3253.2	13532	3218.4	4432.5
Schisandrol A	Lignans	1388	2797.5	1383.4	3993.7	667.17	708.46	2764	3679.8	0	8605.8	10765	2802
Podophyllotoxin	Lignans	1689.2	409.34	201.53	2045	1477.1	1905.8	1276.3	1639.8	2296.6	2225.7	2556.7	2197.1
Acanthoside B	Lignans	0	0	0	3328.2	2643.9	0	11865	0	0	4172.8	29446	25195
Guaiacin	Lignans	224.35	0	0	0	1412	1378.7	1125.6	1846.8	222.05	5640.9	681.33	2001.8
Palmitic acid	Lipids	45418	50907	24053	73878	117906	94943	68338	107216	22994	25862	66961	105686
Myristoleic acid	Lipids	17473	11608	15165	6854	9248.1	14598	7934.3	12974	10142	3931.5	6016.7	16591

13-HPODE	Lipids	5478.2	4544.4	14288	14708	13754	16362	111343	242736	81203	269697	159489	77045
Chamazulene	lipids	7522.5	13960	6489.6	8910.4	11396	9373	4859.1	14767	3994.1	10062	5378.9	16397
alpha-Zearalenol	Macrolides and analogs	25800	543.45	36145	31878	1669.2	44167	5117.4	2259	1646	100113	26844	3350.9
Tiglic acid	Miscellaneous	983929	190825	263720	772887	1E+06	2E+06	161169	259835	666803	315668	594481	191100
Diallyl disulfide	Miscellaneous	218581	153802	522034	285630	297209	408491	185014	255078	268424	286427	327393	445309
2-Pentylfuran	Miscellaneous	144264	133402	130254	98531	122677	282427	160951	81546	265206	345592	85716	116743
Ethyl caproate	Miscellaneous	105018	202819	95123	206755	128090	123630	152027	170292	140914	150042	196656	203363
O-Phosphorylethanolamine	Miscellaneous	143220	86290	124589	70991	122183	0	0	0	30030	0	14824	0
D-Arabinose	Miscellaneous	20397	30914	27152	32529	12253	7925.4	24700	17081	11043	10792	11302	21192
Ethyl isovalerate	Miscellaneous	21710	29882	9115.9	22753	14067	11319	15201	17181	67053	18967	83871	25069
Pregabalin	Miscellaneous	11872	14083	14305	15591	16420	35262	19218	15776	10077	10366	35800	28377
1-Octacosanol	Miscellaneous	30295	10906	7057.1	19508	28264	9317.7	23326	18787	5295.7	1322.1	4501.8	8971
Furfuryl acetate	Miscellaneous	9258.9	14879	12328	17788	9383.3	23867	28590	21211	8681.4	13873	16328	17367
Methyl linoleate	Miscellaneous	5478.2	4544.4	14288	29071	13754	16362	209765	242736	127211	269697	588582	172768
Bakkenolide A	Miscellaneous	17150	9259.8	7342.8	22349	14757	11548	17483	25521	5689.1	5917.2	10722	16380
Panaxynol	Miscellaneous	7719.7	8067.5	17138	17280	15343	10386	8259.9	25259	6332	12530	12332	15368
Astaxanthin	Miscellaneous	8135.2	13322	6920.1	13012	27346	4645.2	12477	21503	8042.6	7539.6	17776	8943.8
Allicin	Miscellaneous	15716	10150	9889.8	12688	11122	10808	13283	5457	5027.5	6592.6	3670.8	7518.1
Undecanolactone	Miscellaneous	7588.1	9124.8	19149	9080.7	8563.9	13956	14339	11400	14437	16899	26340	21935
Alliin	Miscellaneous	18149	9949.6	2228.3	7863	6338.6	13405	5096.4	4290.4	2247.8	6122.9	4705.1	3458.8
(R)-Acetoin	Miscellaneous	11420	5748.7	11264	9827.9	7633.6	8529.1	24395	21096	9719.8	13687	19708	17749
Fingolimod hydrochloride	Miscellaneous	9224.5	12181	12458	10465	3774.2	1854.1	26716	15135	8535.8	10689	15604	3817.2
Sulforaphane	Miscellaneous	8552.7	7725.1	9027.5	8281	10584	2960.3	4251.6	33460	8303.4	7144.1	16514	9316.2
L-Quebrachitol	Miscellaneous	7682.9	4496.1	12363	4788.7	10860	3813.5	6755.7	2641.3	1754.8	4136.2	3128.4	2359.2
Homodihydrocapsaicin I	Miscellaneous	6187.2	5530.4	6125.6	8830.9	11288	5819.5	7572.2	7191.5	5510.5	3079.7	2729.1	5616
3-Butylidenephthalide	Miscellaneous	3354	17939	6207.1	7395	2813.2	3792.6	5375.7	6790.7	7494.8	8292.8	6673.5	3758.8
Pogostone	Miscellaneous	10741	5041.8	6532	5980	5646.4	6189.2	5392.4	7726	3935	9487.7	18055	6005.5
6(1H)-Azulenone, 2,3-dihydro	Miscellaneous	8345.8	549.62	5609.3	7995.8	4325.1	3886.3	2839.7	5866.2	1147.2	2252.1	4520.9	8076.2
Homobaldrinal	Miscellaneous	6711.3	3705.8	3176.3	3608.4	6238.5	6613.7	2503.1	1858.3	3040.7	7432.2	5016.2	3308
D-Pinitol	Miscellaneous	11723	5200.6	2142.9	5750.1	1976.1	2252.6	3686	2968.3	10099	3122.1	3925.8	3731.8
3-Nitro-L-tyrosine	Miscellaneous	1660.5	7805.3	1576	9225.8	5416.3	3023.8	4094.4	4836.6	5284.4	6753	9822.7	2882.2
Baldrinal	Miscellaneous	2330.9	4174.7	3899.6	1994.9	5871.8	5230.1	4325.9	4651.1	7956	4636.1	4976.7	3091.9



Lusianthridin	Miscellaneous	2353.6	2367.1	2329.9	4344.8	1721.1	1386.3	3092.5	6777.3	2731.8	1923.9	1470.3	2315.8
Agomelatine	Miscellaneous	2214.8	797.04	2805.8	1480.7	2743.8	1235.9	1690	1077.8	1384.4	1587.2	3939.1	1708
Cheilanthifoline	Miscellaneous	2232.3	2657.9	1110.1	2398.5	1052.6	1203.3	3493.9	1172	1465.9	937.33	1271.2	1135.3
Torachryson 8-O-glucoside	Miscellaneous	1470.7	1466.7	2131.3	1067.3	3735.7	710.62	5196.8	4571	10487	5590.5	5643.4	3205.8
Acitretin	Miscellaneous	435.43	460.6	2505.8	1121.3	4892.3	946.46	1115.2	927.07	1576.2	1444.6	1838.8	2028.2
Phytic acid	Miscellaneous	2525	2894.9	1674.7	845.43	0	582.98	1423.1	295.6	0	0	1241.6	0
Citronellyl acetate	Monoterpenoids	15817	37233	11492	13711	22861	25257	17767	18803	11693	10573	12167	9894.1
(+)-Carvone	Monoterpenoids	20215	34453	14019	33110	14573	7818.5	16690	28011	12116	19133	14356	17780
Cineole	Monoterpenoids	14351	17930	11924	20572	22103	15937	12363	15481	9019	19453	13970	17632
Cantharidin	Monoterpenoids	8288.8	14541	24835	6551.2	25023	18538	32296	15456	9637.8	13853	16168	14342
Carvacryl acetate	Monoterpenoids	9737.8	12278	16343	7105.3	18480	7968.1	11316	7529.8	23568	10966	9427.9	15623
Nerylacetate	Monoterpenoids	16963	10753	18523	11835	6751.5	6837.5	11074	10233	6662.8	14074	15744	4854.1
(-)-Carvone	Monoterpenoids	11685	13229	9903.3	8808.3	13785	11398	9627.4	12184	9250.4	32666	7528	10057
beta-Citronellol	Monoterpenoids	13658	5279.3	7117.2	6097.9	10540	10702	13158	9414	5966.1	7424.4	7851	5775.7
Bornyl acetate	Monoterpenoids	3895.9	8528.4	5002.2	7803.4	9225.5	5546.2	10804	6413	4537.8	14570	12744	6001.1
(1R)-(-)-Menthyl acetate	Monoterpenoids	3104.4	5808.2	1202.3	4314.9	1805.5	3483	1805	0	0	1789	4889.1	4843.5
Isopulegol	Monoterpenoids	8045.1	2433.9	3518.3	2775.5	1991.7	921.89	3105.5	2171.9	3136.2	3299.1	3797.7	5853.5
Picrocrocin	Monoterpenoids	1133.3	1023.5	2250.5	2302.1	1583.3	1287.5	4450.9	2264	3559.9	2865.6	3229.8	2652.1
Nicotinic acid	Nicotinic acid derivative	76963	153007	225906	107857	78190	95831	262344	225711	151365	247664	294826	241458
6-hydroxynicotinic acid	Nicotinic acid derivative	4484.1	3387.8	3433.8	3381.7	5640.9	7145.6	5493.6	9746.5	5276.1	7213.6	4266.5	9180.4
Uridine 5'-diphospho-D-glucose	Nucleotide and its derivative	472164	2E+06	742710	2E+06	1E+06	1E+06	528478	225014	514831	934884	719781	746402
Adenosine 5'-monophosphate	Nucleotide and its derivative	367017	421955	499092	504970	587756	648774	230027	431826	280589	365442	423836	571630
beta-Nicotinamide mononucleotide	Nucleotide and its derivative	81248	97196	160289	156846	107868	96660	146384	159049	121058	153810	346303	125530
Guanosine	Nucleotide and its derivative	4747	3241.9	399768	6734.1	3111.9	3621.3	5357	6836.7	376093	3607.8	4782.2	521688
Cytosine	Nucleotide and its derivative	12793	33397	26847	31304	16536	43990	39554	60403	40059	33341	54173	48735
Cytidine	Nucleotide and its derivative	12136	13207	25911	24938	13235	9498.7	55726	74748	29770	60623	61396	37488
Purine	Nucleotide and its derivative	3176.2	33208	3579.4	11348	7408.5	22752	19990	132852	153026	176611	8705.2	41505
3-Methylxanthine	Nucleotide and its derivative	5171.7	26935	16844	20211	4132.5	3491.7	1861.9	1396.5	2059.4	694.99	3108.1	342.43
5'-Deoxyadenosine	Nucleotide and its derivative	8267.6	6410.8	13117	6244.1	5465.4	12251	95071	536454	127501	126527	278243	299450
Cordycepin	Nucleotide and its derivative	8267.6	6410.8	13117	6244.1	5465.4	12251	95071	536454	127501	126527	278243	299450
1-Methylxanthine	Nucleotide and its derivative	2834.3	10690	9419.7	2538.7	2329.8	21673	1884.8	2600.9	1905.4	1479.8	1323	2403.6
Uridine 5'-monophosphate	Nucleotide and its derivative	4344	22485	1430	14615	1015.4	696.11	0	324.48	682.59	0	1014.9	18261

Uracil	Nucleotide and its de	5154.7	3190.5	4755.7	16103	8081.2	3617	7126.5	9997.3	43019	53446	73743	5461.1
2'-Deoxyuridine	Nucleotide and its de	6472.2	4270.8	3418.6	4911.4	4762.3	11064	8444.2	10364	9386.7	5513.2	8941.9	3599.3
Uridine	Nucleotide and its de	5582.1	4717.6	2941	4978.5	10949	4736.2	3393.6	3019	4934.1	4443.3	5935.4	6432.3
Thymidine	Nucleotide and its de	4537.2	4652	2261.5	5267.7	5979.4	7186	3558.9	2923.6	3693.6	4014.3	4452.1	4046.5
Deoxycytidine	Nucleotide and its de	4765.2	7935.5	4317.2	3375.9	2344.7	4752.9	3036.3	2297.4	4330.4	4076.8	5512.9	5924.3
Adenosine	Nucleotide and its de	4336.8	2385.6	6262.7	2925.9	1824.4	4263.1	8364.9	5046.5	8E+06	8023.1	12644	3E+06
Deoxyadenosine	Nucleotide and its de	4055.5	2442.1	2485.9	1096.9	1859.9	4186.2	1188.5	3747.1	2500.2	3020.3	2501.1	3079.9
7-Methylxanthine	Nucleotide and its de	1027.7	1700.5	2078.4	1663.5	2586.8	3366.3	4639.9	3831.2	7109.1	4454	1352.3	2663.8
2'-Deoxyinosine-5'-monop	Nucleotide and its de	1162.7	661.42	979.55	1382.9	1749	1440.4	164.68	1613	949.81	1452.1	877	781.19
Guanosine 3',5'-cyclic mor	Nucleotide and its de	1148.6	694.85	0	2140.7	0	477.58	5309.3	5463.5	2765	731.41	0	4880.9
Phosphoric acid	Organic acids	3E+06	2E+06	3E+06	3E+06	2E+06	2E+06	1E+06	1E+06	1E+06	1E+06	962578	620567
Argininosuccinate	Organic acids	581105	637262	559881	450524	516658	630254	6637.3	13191	3341.1	8741.7	6118.7	7304
2-Hydroxybutanoic acid	Organic acids	114464	164028	205623	209432	263149	194900	280268	327057	230051	368129	294017	436555
2-Picolinic acid	Organic acids	50274	45840	64169	36180	38369	20291	22724	112015	85417	122781	110123	18940
2-Hydroxyethanesulfonate	Organic acids	40426	29880	22426	49817	31252	20209	26387	26434	31813	33117	20197	25969
Aminomalonic acid	Organic acids	24560	24962	21122	14883	14485	5886	5236	9174.2	10755	6518.5	13559	8347.1
5-Aminolevulinate	Organic acids	18005	15330	6744.6	16606	5461.2	756.57	2055.6	10601	4155.2	1207.5	952.1	3098.3
Creatine Phosphate	Organic acids	19924	9761.9	11944	6618.9	8165.6	4450.5	14000	9774.9	5715.5	3144.9	5714.6	3551.9
Phosphonoacetate	Organic acids	7598.6	5688.9	4259.6	6552	7111.6	5676.4	36106	51900	3701.2	4822	47093	5197
Citric acid	Organic acids	5474.2	2583.4	5301.1	2851.6	5945.3	3434.2	4860.9	9718.9	4134.3	4330	3383.2	4088.9
Creatinine	Organic acids	1611.3	980.53	3290.7	1458.3	484.43	5030.1	661.94	3508.9	4920.8	3246.3	6639.7	5392.6
cis-Aconitic acid	Organic acids and de	150015	99460	160257	117394	149122	503624	140441	583115	363316	489404	746138	885573
Glutaric acid	Organic acids and de	97950	95355	94070	99955	98293	87442	84696	85854	104779	88884	72253	95274
Shikimic acid	Organic acids and de	40146	50015	77658	48326	59693	93235	123531	94907	75228	131865	135424	108824
Fumaric acid	Organic acids and de	11391	12471	11074	14305	11064	15141	24592	36199	24705	28388	27527	29224
Betaine aldehyde	Organonitrogen com	14085	16439	19491	20371	21163	19452	17268	24736	25943	22192	31371	28039
L-Carnitine	Organonitrogen com	18508	13535	28877	23388	11890	6597	33496	14180	11931	33814	19513	37188
Sphingosine	Organonitrogen com	5834.8	5649.5	4613.2	2342	5122.3	13837	11627	14224	10330	9197.9	9129.9	6344.5
Lactulose	Organooxygen comp	1E+07	1E+07	6E+06	1E+07	1E+07	9E+06	7E+06	7E+06	1E+07	1E+07	6E+06	6E+06
Galactose 1-phosphate	Organooxygen comp	1E+06	2E+06	2E+06	2E+06	1E+06	1E+06	642918	575586	565233	822759	400133	631223
Beta-D-Fructose 2-phosph	Organooxygen comp	382917	627008	419824	351012	616974	273653	246919	115952	229184	292747	285778	132807
Glucose 1-phosphate	Organooxygen comp	313332	145114	235266	549900	353943	317772	228767	354700	220633	232413	299974	263067

Maltotriose	Organooxygen comp	23712	112935	178001	37244	47329	23222	189255	158801	24461	90671	95327	98272
1-Kestose	Organooxygen comp	72231	41719	83826	0	0	66598	28404	3405	20804	13359	33724	7786
myo-Inositol	Organooxygen comp	0	57011	49877	0	65152	87045	72022	55629	90164	137178	82068	80002
Glyceric acid	Organooxygen comp	42389	25217	68834	25906	53466	24884	50241	30256	34216	62386	18712	17404
Stachyose	Organooxygen comp	29162	23943	16330	54121	31290	28769	12099	10032	0	13089	6393.9	4248.3
6-Phosphogluconic acid	Organooxygen comp	17511	44757	24390	23217	31552	9019	7066.2	16942	22576	12498	15476	19660
Mannose 6-phosphate	Organooxygen comp	26067	11721	7012.9	30735	21370	11992	13476	13606	7125.8	9411.9	30153	10616
Pseudouridine 5'-phosphat	Organooxygen comp	47076	3876.5	1791	46222	2108.8	1507.3	5124.7	17804	1581	38297	2729.5	3643.1
Streptozotocin	Organooxygen comp	5594	21828	3967.7	14255	0	19733	53969	56742	49113	9565.7	2269.4	6117.4
1-(alpha-Methyl-4-(2-meth	Organooxygen comp	10954	7628.9	8627.5	1537.1	13230	3027.2	12014	6509.9	7104	30558	4300.9	13224
Fructose 1,6-bisphosphate	Organooxygen comp	3219.6	5805.4	7764.3	3488.1	10608	11587	2194.8	1141.2	1587.9	2226.1	3258.5	2406.3
4-O-alpha-D-Galactopyran	Organooxygen comp	4520.3	2764.7	6214.2	8037.7	9411.1	5959.7	6638.6	36252	4294.5	40697	16210	5591.4
Quinic acid	Organooxygen comp	4039.7	4917.2	5396.7	6440.4	6089.7	7652.1	6465.9	7430.6	9010.1	4267.6	5921.1	9291.3
Beta-D-Glucose	Organooxygen comp	5301.7	2165.6	2145.6	1319.3	2092	1468.2	1840.3	1228	493.78	3879.7	2417.9	1516
Benzoyl glucuronide (Ben	Organooxygen comp	4864	2584.3	0	0	3081.9	0	14372	0	3915.8	0	0	0
Streptomycin	Organooxygen comp	492.18	0	0	2027.6	2372.6	5424.5	3022.9	3700.6	0	1421.8	5095.5	0
Galactinol	Organooxygen comp	1006.1	1031.7	323.45	1359.1	2950.7	673.13	1784.7	5993.3	2711.9	3945.9	2454.3	681.5
Raffinose	Organooxygen comp	0	0	0	0	6060.8	0	0	0	0	0	0	0
Phendimetrazine	Oxazinanes	13923	11516	9741.1	11508	25886	18444	10530	11478	14518	19561	15010	20317
Oxymorphone	Phenanthrenes and d	74773	92377	140399	121452	97080	120096	110463	246122	64002	128623	128320	142453
Trimethoprim	Phenol ethers	8E+06	6E+06	7E+06	5E+06	6E+06	2E+07	59433	223378	79776	78606	68113	86194
Venlafaxine	Phenol ethers	4896.6	1379.9	1415.9	1784.4	2614.9	1695.3	3631.5	2938.2	1262.1	1331	2323.4	662.04
N-p-Coumaroyl putrescine	Phenolamides	7091	8407.6	3637.5	4115.8	6657	4761.5	2273.7	2631.1	3947	5737.4	3554.3	5995.6
N-Feruloyl putrescine	Phenolamides	1047	753.03	2840.8	1519.3	1847.5	2760.5	19072	73790	15873	61125	75892	39593
3,4-Dihydroxybenzaldehy	Phenols	1E+07	9E+06	1E+07	1E+07	1E+07	1E+07	32377	124735	46963	13394	21937	28455
p-Octopamine	Phenols	8E+06	8E+06	7E+06	8E+06	8E+06	7E+06	7E+06	6E+06	8E+06	6E+06	7E+06	7E+06
Phloretic acid	Phenols	3E+06	8E+06	4E+06	9E+06	931399	115705	84571	119184	62339	118233	108906	74893
4-Hydroxybenzaldehyde	Phenols	3E+06	3E+06	87624	2E+06	1E+06	593311	600393	896445	522993	926211	619214	514871
2,5-Dihydroxybenzaldehy	Phenols	1E+06	1E+06	2E+06	998579	991490	2E+06	17799	53133	22822	26719	34111	26711
Benzaldehyde	Phenols	688391	2E+06	902033	2E+06	232038	137886	127857	91917	185859	79000	75261	79577
3-Ethyl-1,2-benzenediol	Phenols	1E+06	783369	1E+06	1E+06	383092	448782	846303	989931	1E+06	1E+06	716843	665853
Protocatechuic acid	Phenols	104292	151468	242709	114912	68968	265409	17115	24399	20755	17085	17773	15012

alpha-Tocopherol	Phenols	619142	36873	42508	138673	41805	33784	28642	166208	7712.6	8121.4	55858	72901
Syringic acid	Phenols	172073	155906	42464	160008	61456	12336	16621	38690	18109	80374	18905	46261
1,2-Dimethoxybenzene	Phenols	89781	59657	125569	114687	46083	117916	98421	97419	76722	143816	80922	81306
Moracin C	Phenols	94246	96610	118478	88056	63644	52265	239412	141181	121034	98879	127090	82155
Altholactone	Phenols	51558	41749	81597	53212	6381	65550	9997	7277.9	7693.4	7205.9	9812.5	7143.6
Ethyl orsellinate	Phenols	44347	57558	47549	44660	61274	38759	54095	52035	57072	42157	37072	64617
3-Hydroxyphenylacetic ac	Phenols	88395	28985	60587	24194	26956	46823	43541	32180	12026	40166	20735	22683
Dihydromethysticin	Phenols	68043	28858	12009	51100	5363.9	33684	304182	483058	367712	88235	752369	212225
4-Hydroxybenzoic acid	Phenols	26688	21940	35570	13948	23689	53102	55203	23381	48010	52365	28059	40772
3,4-Dihydroxymandelic ac	Phenols	28092	28772	27852	33634	24802	27241	33166	36966	25747	28923	25409	33173
Dihydrokavain	Phenols	17748	23181	32694	26108	20417	38008	2089.8	7292.1	6388.5	3301.1	10110	8420.6
Demethoxyencecalin	Phenols	21138	13605	51672	40193	12660	16117	26200	22217	28439	22634	22413	21884
Octyl Gallate	Phenols	20100	15191	29080	33452	31619	18569	35110	34859	21906	6086.3	38181	24679
4-Hydroxy-3-methoxyman	Phenols	4433.2	43238	13809	13423	18181	35472	131250	128308	80336	112943	143418	118854
Chavicol	Phenols	27858	17794	13266	24166	24220	20108	22950	30024	28444	27907	20221	24453
7-(4-Hydroxyphenyl)-1-ph	Phenols	19196	11878	10977	34438	9964.5	19634	18869	59553	16273	9172.7	25540	15869
3-Ethoxy-4-hydroxybenzal	Phenols	15594	19391	14891	14265	19518	11818	7990.2	21046	9610.9	12681	20819	27759
4-Methylcatechol	Phenols	25081	11466	7696.7	13371	14418	21478	0	588.91	586.75	563.77	0	1207.9
2-(4-Hydroxyphenyl)ethan	Phenols	14744	12437	17559	16873	10077	14342	21674	101266	12923	9759.4	56964	55515
Benzyl acetate	Phenols	25208	16942	18809	15104	0	9177.5	15349	5926.2	16260	10514	21002	14782
2,4-Dimethylphenol	Phenols	19449	15747	12730	13915	10609	12163	12160	12443	18879	9390.1	6953.4	12590
Broussonin C	Phenols	23987	12304	7663	4642.4	20063	15354	23838	22407	11101	10743	21641	2689.1
Methyl gallate	Phenols	4939.7	14802	5887.8	33814	6832.6	8387.4	95187	88129	114302	108968	47696	97198
1-Dehydro-6-gingerdione	Phenols	13645	8706.3	10689	5094.6	5215.9	30276	388.33	0	392.99	0	0	0
Yangonin	Phenols	16932	13483	17766	7803	11356	5951.7	10050	7948.7	6915.6	9007.8	28482	3501
Propyl paraben	Phenols	21337	8048.8	8154.1	11264	14016	8178.4	8394.5	6862	10021	12234	8289.1	7103.6
Precocene II	Phenols	9595.1	6815.5	10012	22945	13431	8017.1	13846	12839	4254.2	4446.9	17609	7694.4
Mulberrofuran Q	Phenols	8668.9	2968.5	20558	5107.2	26609	4603.8	13665	13295	2289.9	13161	13714	8061.2
6-Gingerol	Phenols	17299	6987.1	8945.7	9190.2	13702	8664.1	275406	984842	279800	346232	1E+06	226271
Guaiacol	Phenols	6085.1	7828.2	5457.3	2997.9	4194	31434	8352	7112.6	4425.3	6508.2	7136.2	7628.1
Beta-Tocopherol	Phenols	6454.2	9165	6567	7009.2	15663	11676	9585.5	9401	12254	5960.7	15004	4325.7
Sesamol	Phenols	8680.6	8468	6100.9	11867	7376.7	12517	5566.6	5460	7699.8	2488	6391.6	3392.5

4-Isopropylbenzaldehyde	Phenols	8697.7	6623	3482	15438	11182	9145.4	9082.5	16905	12367	18330	10558	18935
Acetovanillone	Phenols	7954.5	5357.5	7268.8	15381	5474.2	11274	8573.3	9225.4	4871.3	5395.7	8300	6512.5
3-Hydroxybenzoic acid	Phenols	3937.9	6738.6	7766.3	14450	6106.6	13049	11686	10029	8444.4	7212.2	6717.2	9518.5
1'-Acetoxychavicol acetate	Phenols	18215	5953.7	4662.6	9733.9	5795.2	7001.3	8191.8	5473.7	8072.6	8159.6	2478	5446.5
Kakuol	Phenols	5631.5	9415.3	10822	12520	3183.4	6204.7	8428.7	6433.7	3816.6	5274.4	11435	10459
Orsellinic acid	Phenols	26784	619.88	605.73	1215.1	16753	1202.3	655.18	0	2682.7	0	594.4	0
Ginkgolic acid C17:1	Phenols	0	0	9786.5	12560	24731	0	0	0	0	0	0	0
Vanillic acid	Phenols	3142.2	6039.7	5608.6	8758.9	14500	8830.9	149880	202061	159240	235105	179121	208273
Cinnamyl acetat	Phenols	6403.1	11769	8485.7	6498.3	9859.2	3851.5	7902.1	6365.6	6472.2	7696.8	10575	10501
Zingerone	Phenols	4726.7	2445.2	5509.1	10747	6780	10911	5441.2	4483.9	21743	7692.9	3858.6	3459.5
Encecalin	Phenols	10419	8123.7	5095.7	7333.8	4562.9	4677.7	7336.8	10360	3266.3	4982.1	11893	7682.6
4'-Prenyloxyresveratrol	Phenols	3358.1	4920	5397.5	7995.3	5516.6	11978	12156	8609.6	5368.9	7242.2	31841	6953.9
1-Phenylethanol	Phenols	5951.1	9988.4	8355.8	3298.5	5818.3	5581.7	5460.3	6979.5	7099.3	6751.6	3258	6597
Resorcinol	Phenols	589.24	601.4	18582	15357	905.09	586.91	4135.9	1194.3	1815.2	1192.6	1226.1	2447.9
10-Gingerol	Phenols	11173	4875.3	0	9647.5	2646.8	7846	11658	5095.5	2984.7	4985	4502	3381.2
Oleocanthal	Phenols	6508	4875.3	3197.9	10902	3947	6384.9	7942	10059	10144	3008.2	7119.9	13582
Cannabinol	Phenols	6268.3	0	5765.6	7392.4	4581	11415	0	48725	17295	19302	0	34314
Cardanol (C15:1)	Phenols	5285	3931.1	5723.6	8163	3691.6	6714.4	3966.1	5147.3	2293.6	1913.9	11350	6440.6
p-Hydroxymandelic acid	Phenols	9386.9	4070.8	3688.7	4685.1	3967.6	6404.1	19054	23000	12942	29359	31841	6233.4
N-(p-Hydroxyphenethyl)ac	Phenols	4045.4	4992	2692.8	7510.2	3966.2	6292.4	2974.2	4269.2	2896.8	3019.4	3125.9	3354.3
Piceatannol	Phenols	2981.5	9750.3	1202.3	3029	8135.6	2883	1816.5	4082.3	5299.8	3308.8	4958	5044.6
Oxyresveratrol	Phenols	4052.4	4895	5640.3	3756	3987.6	5132.2	4633.3	2757.4	5151	4701.3	5347.9	2195.5
Altechromone A	Phenols	4074.6	5519.8	3818.1	3641.4	3191.6	4125.4	5931.7	3918.1	6319.3	8873	6479.7	2676
beta-Glucogallin	Phenols	2811.5	2371.6	4019.6	1326.6	6359.3	5675.5	0	5092.3	1441.6	1898.4	1754.4	1900.9
4,4'-Methylenediphenol	Phenols	2748.4	8508.4	5364.8	1076.8	1726	2830.6	3143.3	7056.4	2218.4	2842.2	2814.7	2731.5
Batatasin III	Phenols	2867.2	1755.4	3217	4057.7	6916.2	3323	5250	1842.5	4410.9	4701.3	3147.9	2560.5
Ethyl 3,4,5-trimethoxyben	Phenols	4490.6	1583.5	4329.5	3864.5	3153.7	1458.2	2224.7	3426.9	2954.2	3853.6	6820.1	2315.7
5-Tricosyl-1,3-benzenedio	Phenols	4099.1	881.04	1315.1	6800.8	3369.7	1604.6	6072.6	4277.6	3162.3	2280.4	7048.4	2467.6
DL-alpha-Tocopherylacetate	Phenols	2845.3	781.06	202.18	5974.1	8103.4	0	2447	1885	1392.2	2169.3	1801.6	1173.1
Taxiphyllin	Phenols	3874.1	1668.7	1671.9	3066.2	2406.6	1341.3	1758.8	4808	1349.1	1352.8	5522.6	2199
Metanephrene	Phenols	2310.2	3833.6	1367.6	1891.4	1360.8	1177.6	4032.1	4003	958.19	1256.6	1163.7	1338.4
Methyl orsellinate	Phenols	1356.1	1513.2	2426.9	1444.5	2391.8	2037	1346.9	1521.5	1070.4	1371.7	2560.5	2325.2

Tetrahydrocurcumin	Phenols	931.09	624.83	216.63	1236.8	214.55	1033.3	1418.2	1860.3	1304.8	3263.3	1668.9	3089.9
Moracin O	Phenols	0	822.9	770.26	407.58	1119	665.34	1555.4	1767.5	2490.9	1214.6	1824.9	1601.4
Hamamelitannin	Phenols	0	0	0	0	0	0	725.61	0	0	3475.6	8633.5	0
4-Hydroxyphenyl-2-propic	Phenylpropanoic aci	7479.7	4696.2	6541.2	8678.6	23716	13713	6628.1	7813.5	10490	12992	9816.5	6940.9
Ethyl cinnamate	Phenylpropanoids	36659	39306	62934	16788	14099	31888	2947.9	13031	16555	8842.6	10743	7900.1
Caffeic acid	Phenylpropanoids	33136	29494	39117	25992	27461	33587	3797.9	3417.7	2826.7	4999.5	2954.4	1614
3-Methoxy-4,5-methylene	Phenylpropanoids	14180	40797	39985	23105	36996	30263	25801	25461	31353	47308	50755	24029
Methyl cinnamate	Phenylpropanoids	9431.8	16880	21430	25773	35727	30098	27021	56531	21089	49831	35444	24447
3,4,5-Trimethoxycinnamyl	Phenylpropanoids	28594	20197	28832	19240	17409	14625	9996	14472	19226	26169	30828	15929
Coniferylaldehyde	Phenylpropanoids	22390	9466.8	12033	15010	12042	27239	32778	58034	25698	32934	31605	25311
Ferulic acid	Phenylpropanoids	13804	9832.7	10637	17676	11534	20515	46776	63711	38469	6979.8	4387.8	6204.6
3-(4-Hydroxyphenyl)-1-pr	Phenylpropanoids	12223	10531	5817.3	16163	11441	20154	9578.7	8054.4	7102.6	5320.1	4222.8	7598.3
1-(4-Hydroxyphenyl)prop	Phenylpropanoids	11360	7788.3	8027	11120	20678	9937	14909	13189	5800.5	7724.2	13340	7142.8
Trans-caffeic acid	Phenylpropanoids	8248.2	16468	15836	7416.5	6996.4	9371.1	7090.7	25760	4169.2	10403	24088	6986.4
Cinnamic acid	Phenylpropanoids	2349.9	15784	17016	15617	3782.8	4997.1	6103	1618.9	2894.9	2183.1	2675.7	2628.8
Hydrocinnamic acid	Phenylpropanoids	7516.6	9298.2	8093.5	5815.5	11928	11313	10306	4330.2	7583.8	17737	7318.5	7379
Osthol	Phenylpropanoids	14330	7957.5	3845.8	5108.9	7794.6	10149	7951.3	9295.7	8683.5	12341	13071	6407.4
Angelicin	Phenylpropanoids	10202	4165.6	5906.1	6024.5	11133	9540.3	10902	9909.2	9935.8	5160	6481.5	5593.7
trans-3,5-Dimethoxy-4-hy	Phenylpropanoids	4429.3	10355	10276	4977.4	8406	6859.5	9526.6	12994	16975	6628.5	12245	6952.7
Cinnamyl alcohol	Phenylpropanoids	6843.8	6417.5	10851	3312.3	5722.3	2350.1	10258	14406	10361	10761	4277.6	7548.8
Dihydroconiferyl alcohol	Phenylpropanoids	6216.5	6265.6	2217.4	4910.5	8753.3	2023.7	9357	3977.9	5551.2	5724.7	2060.5	5317.9
Cinnamyl cinnamate	Phenylpropanoids	3086.6	3011.4	2224.7	2374	5293.1	13118	85084	435723	82314	346796	424562	189201
2-Hydroxycinnamic acid	Phenylpropanoids	7177.1	2775.2	2566.6	4638.1	9221.8	2542.7	4972.7	5518.2	9686.1	10853	5972.9	6134.6
3-Hydroxy-4-methoxycinn	Phenylpropanoids	5929.1	3960.3	4840.9	2296.6	3420.5	7355.9	26259	7889.1	15094	3944.4	2823.4	7259.2
Benzyl cinnamate	Phenylpropanoids	3919.9	1742.2	3007.4	4592.3	6349.4	7596.6	6442.2	3517.8	2268.9	3503	4388.5	6245.6
Coniferyl alcohol	Phenylpropanoids	2996.9	12099	1935	1593.5	4132.9	2213.7	4466.4	3479.1	23896	1077.6	710.22	1948.3
Isofraxidin	Phenylpropanoids	3028	2247.2	4840.8	3786.3	3049.9	5182.3	4159.1	4686.6	4862.9	5481.1	3725.2	2272.6
Imperatorin	Phenylpropanoids	5832	3446.2	1523.3	4335.5	4094.9	2567.7	2517	2689.2	2048.2	0	1476.7	1063.9
Echinacoside	Phenylpropanoids	2641.9	6193.2	3474.4	2632.2	2722.9	3398.3	209.63	215.59	0	0	0	417.48
4-Methoxycinnamaldehyd	Phenylpropanoids	4919.6	2572.9	1617.5	3865	3458.4	4626.4	2589.9	1199.9	776	2616.4	2396.6	3198.7
C-Veratroylglycol	Phenylpropanoids	2376.3	3021.4	5661.5	2140.2	3548.7	3191.7	3378.3	14403	3482.4	4448.8	6710.5	8250.5
Xanthotoxol	Phenylpropanoids	1627.5	2200.1	4515.2	3977.1	4086	2954.3	5220	2743.1	6974.9	1120.9	5320.9	2062.9

3,4-Dimethoxycinnamic acid	Phenylpropanoids	3628.3	4007.9	2709.3	2623.2	3217.4	2265.6	2087	3745.7	2619.2	3043.6	3203.7	3383.1
Magnolol	Phenylpropanoids	3372.8	1964.6	2195.3	3155.4	1319.8	1129	2448.9	3004.4	2908.4	2597.2	1649.3	3143.5
Syringin	Phenylpropanoids	1048.4	1047.8	1059.1	0	6456.5	2737.8	1092.6	1054.9	3020.4	1944.9	0	1055.9
5-O-Caffeoylshikimic acid	Phenylpropanoids	1207.6	1609.9	655.67	1085	1379.1	4219.3	1855.2	1548.2	2413.8	906.16	1139.9	1836.4
Phillyrin	Phenylpropanoids	931	238.11	483.97	741.53	1086.5	3457.5	966.42	1742.3	5491.5	4266.5	1000.2	1702.1
1-Aminocyclopropanecarboxaldehyde	phytohormone	66482	54508	580612	77559	68853	1E+06	12166	25870	7237.1	408986	13469	325317
trans-Zeatin-riboside	phytohormone	1753.5	63099	197351	70520	10094	2226.9	4706.6	2156.6	15118	7952.6	6726.1	3455
Indole-3-carboxaldehyde	phytohormone	19938	15358	28138	38599	32503	20638	47692	38970	34608	54021	31914	54872
N6-(delta 2-Isopentenyl)-adenosine	phytohormone	7986.2	8852.6	60004	17906	49807	4873.7	7359.9	6044.5	6836.8	2915.8	3622.9	10174
3-Indolebutyric acid	phytohormone	18088	26612	21319	30876	14175	18778	19560	13460	10256	17243	6335.9	19854
Indole-3-acetic acid	phytohormone	17005	19056	11638	16931	27191	0	17702	20653	19080	21613	16990	15744
trans-Zeatin	phytohormone	4388	4949.7	59589	5963	2083.1	5051.9	3187.8	2393.2	4348.3	6138.8	4366.3	4223.8
(±)-Jasmonic acid	phytohormone	27083	3607.1	12838	24816	4912.3	7755.8	2566.4	2891.8	334.72	7909.8	1896.7	1170.5
cis-Zeatin	phytohormone	4058.7	5795.6	22345	5963	7713.2	4643	3187.8	6647.9	2769.3	11281	4916.4	6495.1
N-((-)-jasmonoyl)-S-isoleucine	phytohormone	12452	584.15	5309.8	10955	6061.4	5385.9	1105.3	541.06	580.51	578.26	640.96	309.6
Gibberellin A7	phytohormone	2264.5	5351	2496.8	2677	2683.3	1206	3380.3	1349.2	1796.1	1697	2358	3724.3
Gibberellin A4	phytohormone	1678	1307.5	1682.1	2757.7	3431.5	3091.5	1207.5	1642.1	2338.4	793.37	1845.3	2297
(+)-Absciscic acid	phytohormone	796.66	0	1151.6	0	234.9	10132	1166.5	0	1171.7	4233.5	2407.8	0
1-Naphthylacetic acid	Phytohormones	8647.5	4260.1	6009.5	8859.1	15120	4701.9	9028.9	4656.3	7401.5	17891	9635.1	13942
alpha-Irone	Prenol lipids	68524	76826	59003	39412	72509	186232	17830	10001	19313	9906.3	19260	9352.9
(R)-Menthofuran	Prenol lipids	70675	79489	73078	72111	77819	83962	13959	10039	11923	24186	26769	7522.5
beta-Ionone	Prenol lipids	14544	13209	9824.4	6587.1	13811	5743.3	11642	8532	9234.4	11358	15176	26433
Capsidiol	Prenol lipids	6763.9	9980.3	10642	12902	5024.6	9708.6	11535	3849.9	3769.1	13397	6189.6	10162
4-Isopropylbenzoic acid	Prenol lipids	9933.2	5277.1	8636.3	9053.3	10095	2827.5	10100	13029	6201.2	6019.3	16782	5766.3
Lactaroviolin	Prenol lipids	2386.7	2353.4	1138.4	1221.3	5081.5	8754.7	1821.5	2342.7	3530	2950	8549.9	1196.9
Piperitenone	Prenol lipids	4794	3617.4	1980.4	1426	3445.4	4418.4	2592.4	3723.4	2978.6	9284	3229.5	2515.3
alpha-Cyperol	Prenol lipids	649.35	4686.4	1173.6	1279.3	0	3747	2863.7	1249.6	3935.9	2865	1745	0
Isoxanthopterin	Pteridines and derivatives	6688	5667.7	7280.9	4487.5	7532.8	3396.6	5064.8	5063.5	14309	11484	6686.1	6305.1
Vidarabine	Purine nucleosides	1E+06	675071	541878	2E+06	1E+06	243099	3E+06	5E+06	8E+06	2E+06	1E+07	3E+06
2'-O-Methyladenosine	Purine nucleosides	12373	0	20455	16134	32665	11238	9937.1	26527	6815.1	8904.2	16268	2428.4
Adenosine 2',3'-cyclic phosphate	Purine nucleotides	451.09	2359.5	461.48	3349.1	3186.6	1667.5	3098.3	3541.3	3974.3	489.6	3331.9	1101
3-Hydroxypicolinic acid	Pyridines and derivatives	14038	183435	11959	12092	7092.8	14108	5882.1	9513.1	5330.7	3947.4	3086.4	12282

5-(3-Pyridyl)-2-hydroxytetrahydro-2H-pyridine	Pyridines and derivatives	23623	57662	35963	84539	7379.2	3463.7	3248.4	2014	1035.2	3441.6	350.89	2134.2
3-Carbamyl-1-methylpyridine	Pyridines and derivatives	20287	9490.9	21170	17907	30670	23836	26583	92950	50169	49726	57762	47735
N1-Methyl-4-pyridone-3-carboxamide	Pyridines and derivatives	7040.2	4846.5	10186	14471	3805.2	6204	3253.4	19208	3603.1	0	951.18	9236.1
4-Pyridoxolactone	Pyridines and derivatives	9849.5	7363.1	4779.3	4815.1	6806.9	6340.7	10298	6093.3	5424.4	6022.5	8804.3	8286.3
Isonicotinic acid	Pyridines and derivatives	5603.4	2624.9	5060.3	4867.5	6911.4	13887	13141	2830.6	3613.9	4893.6	10665	6993.7
(S)-Actinidine	Pyridines and derivatives	5371.8	6112.1	5908.5	4841.8	4218.4	5777.6	5370.2	5883.7	5628.9	13474	8123.4	2982.2
gamma-Hydroxy-3-pyridinecarboxaldehyde	Pyridines and derivatives	3763.6	4324	5780.3	1875.6	2478.4	5610.8	764.46	1838.5	1310.1	2087.2	1055.9	2408.2
N1-Methyl-2-pyridone-5-carboxamide	Pyridines and derivatives	5740.1	2993.4	4365.4	2763.8	3259.5	2917.4	3113.3	4196.9	687.64	1373.8	1582.1	1190.8
Pyridoxal 5'-phosphate	Pyridines and derivatives	2041.2	871.28	1957.6	1229.7	1155.1	887.61	662.33	877.4	1301.3	1775.6	1243.5	727.1
Gemcitabine	Pyrimidine nucleosides	327891	262292	349350	215102	351606	847322	393933	382914	243820	222965	358768	621679
5-Methyldeoxycytidine	Pyrimidine nucleosides	4899.4	2930.5	3488.9	4626.9	2279.5	2817.8	3256.6	667.08	2293	2516.7	3148.1	259.51
dUMP	Pyrimidine nucleotides	38406	25558	20103	7509.8	15221	32985	26625	41690	39362	23621	35575	21039
Queuine	Pyrrolopyrimidines	13878	7829.1	7514.8	6743	1385.6	3424.9	17975	8238.5	6856	14847	2863.8	2753.8
D-(-)-Quinic acid	Quinolines and derivatives	6329.2	3605.1	6420.2	7116.5	2311.5	8337.1	5776.3	4273.6	4066.5	8098.1	4048.8	5063.4
Xanthurenic acid	Quinolines and derivatives	2276.7	5874.8	4482.7	9464.1	2123.1	5002.4	6220.5	11269	3645.2	15979	4450.8	3547.6
1,2,5,6-Tetrahydro-4H-pyrido[4,3-b]pyrimidin-4-one	Quinolines and derivatives	3027.3	5784	4471.8	6430.1	6368.4	2311.4	14591	7546.4	9864.2	4457.8	7255.5	5672.5
Shikonin	Quinones	100466	92077	69103	143266	142247	110712	5220	5037.4	7549.5	1191.6	15012	1844.5
9-Methoxy-alpha-lapachone	Quinones	40255	6694	26351	27726	63070	32695	1315.2	4096.9	2099.7	2465.5	2737.9	2210.2
Aristolindiquinone	Quinones	29154	27668	32832	55528	13270	17445	30985	15014	39533	15857	8971.4	12624
Juglone	Quinones	11446	9777.2	3791.6	5423.1	7032.6	16371	9816.4	10880	6985.2	11818	11317	6540.5
Vitamin K1	Quinones	5299.9	2663.4	12459	24326	2167	2514.5	6260.3	15424	2153.3	3065.7	2383.4	1321.4
Primin	Quinones	6308.4	6479.7	10736	7968.3	3501	2736.9	6645	7766.4	7773.8	9339.8	5997.4	9725.4
Embelin	Quinones	218.05	973.43	222.59	5284.9	1035.6	638.83	429.19	294.85	282.02	91.476	364.85	370.38
Artemisinin	Sesquiterpenoids	121998	37839	74769	136842	138177	74690	75790	167286	61134	40552	65942	86329
Picrotoxinin	Sesquiterpenoids	36424	43083	26643	19554	32887	89790	0	2549.4	649.13	988.65	0	0
trans-Caryophyllene	Sesquiterpenoids	32353	15824	53657	64269	41474	26794	57223	56315	37934	19963	52940	33055
Caryophyllene oxide	Sesquiterpenoids	37107	37573	37813	19111	32231	24701	25649	33570	13489	17875	41802	23216
Alpha-caryophyllene	Sesquiterpenoids	37698	18817	8943	22783	29039	24814	30962	17670	19969	10821	11141	16512
alpha-Cyperone	Sesquiterpenoids	35240	18650	9645.6	17449	18888	19921	14098	22700	13559	18126	21521	20449
Curzerene	Sesquiterpenoids	15707	18576	12618	13641	15036	22476	40937	57390	41491	52859	36037	33995
Alantolactone	Sesquiterpenoids	12077	15938	14665	16523	14139	7469.8	15841	23411	12128	17381	24532	12080
1beta-Hydroxyalantolactone	Sesquiterpenoids	9413.9	16001	11435	16979	6965.5	12594	1751.5	8527	0	2325.5	4658.7	3013.9



Valerenic acid	Sesquiterpenoids	2962.3	9366.3	15307	21028	4885.3	10678	2586.5	6381.3	9270.3	5160	11281	12918
Isoalantolactone	Sesquiterpenoids	9686.7	5594.7	5652.1	16523	12108	13747	13702	11618	16480	9858.8	14388	5090.5
Curcumol	Sesquiterpenoids	11245	7320.8	13386	7243.3	11448	10227	6940.8	4823	9428.5	5502	4949.3	4846.1
Alpha-Santonin	Sesquiterpenoids	3873	8423.3	10056	5566.1	5090.9	12336	4323.4	2022.8	2728.8	2136.8	6265.8	4697.6
Xanthatin	Sesquiterpenoids	8547.1	4393.9	6441	7959.9	4923.3	11093	3128.4	1735.7	3982.1	1928.3	2170.1	1695.5
Curcolone	Sesquiterpenoids	8547.1	4393.9	6441	7959.9	4923.3	11093	3128.4	1735.7	3982.1	1051.6	2170.1	1695.5
Bisabolol oxide A	Sesquiterpenoids	5550	4544.3	5904.8	4518.5	10066	8391.9	9422.6	8070.6	12242	12111	9391.8	7929
Macrocarpal B	Sesquiterpenoids	4760.3	4139.3	7192	3631	3047.1	6764.3	1223.6	3456	0	1775.2	3053.9	8426.3
Catalpalactone	Sesquiterpenoids	5349	2823.3	4298.5	3042.4	9675.8	1922.5	13959	8983.9	2063.3	7304.7	7147.9	2396.4
Anisatin	Sesquiterpenoids	4177.8	0	6185.8	2207.6	2208.1	6256.3	5291.4	1660.9	0	5532.3	8480.8	12991
Pyrocurzerenone	Sesquiterpenoids	3961.6	3369.4	4351.3	3149.2	2415.5	2896.1	2868.9	2741.2	1814.5	2220.1	2718.8	3164
Tenulin	Sesquiterpenoids	2762.9	3442.4	1130	3417.9	2633.9	1464.9	1036.7	2649.2	479.03	927.75	2176.8	1402
Pterosin D	Sesquiterpenoids	2843.4	2716.4	2452.9	3067.9	2133.1	478.85	993.36	2831.3	1763.8	3872	1469.8	1231.9
Eupatolide	Sesquiterpenoids	3329.1	1593.6	2029.5	2096.7	803.84	3408	512.17	499.71	498.07	1315.6	271.09	1142.1
Lactupicrin	Sesquiterpenoids	4439.6	1932.6	1080.5	3147.4	1055.9	1137.6	4503.9	1841.1	1315.4	726.4	2601.6	993.34
Cryptomeridiol	Sesquiterpenoids	488.43	1725.7	1013.8	2244.2	1785.7	1027.2	2020.7	3056.1	961.39	4533.1	2382.3	252.32
Testosterone	Steroids	57179	107202	92634	110042	76821	85945	6485.1	3541.3	2850.6	4873.7	1804.2	4400.9
Estriol	Steroids	25195	13448	26244	12757	15250	19440	0	321.51	961.45	0	0	0
Ursodeoxycholic acid	Steroids	6577.1	8393	1747.2	9723.2	6310.5	10478	8478.2	5594	6375	8856	6566.8	4921.6
Citrostadienol	Steroids	4654.3	4204	7486.1	6598.1	3735.7	4954.7	11169	11103	11679	4152	12741	10901
Lithocholic acid	Steroids	3546.7	3174.3	4350.9	2278.4	4213.2	3164.3	4913.5	3132.7	5256.5	3328.7	5484.9	4554.9
Bufotaline	Steroids	1548.4	3404.9	0	5412.6	2365	4397	12764	0	788.54	11946	5123.4	1522.1
Guggulsterone E&Z	Steroids	1796.2	2304.1	1787	4593.9	2905.3	2933.9	2299.8	15730	4923	1795	4625.9	2333.4
6-Hydroxystigmasta-4,22-	Steroids	1816	3544.5	1800.2	1803	465.69	1156.6	3791.9	1378	621.38	934.48	1890.2	462.85
Physalin C	Steroids	0	0	0	2206.2	3415.1	786.63	0	1063.7	0	0	541.21	0
Ergosterol peroxide	Steroids and steroid	8355.7	6129.1	57290	83154	5460.6	1437.4	7031.5	4745.5	23142	2532.1	8576	5700.8
Dehydroepiandrosterone	Steroids and steroid	26738	29439	27434	25520	14544	29606	0	631.87	961.45	0	0	0
Physalin D	Steroids and steroid	24134	6425.3	18067	18866	12167	29596	17464	33891	12783	31710	78954	15113
alpha-Spinasterol	Steroids and steroid	13766	23002	4739.4	26164	25028	9947.9	25417	8960.7	8530.5	2319.1	10708	12967
Exemestane	Steroids and steroid	8546.3	24885	24728	10821	10754	11534	16259	24159	18563	25728	37573	16100
Oleaside A	Steroids and steroid	7403.7	10914	18796	5937.3	23678	16767	25389	13672	9156.7	14022	9449.4	18760
Stigmasterol	Steroids and steroid	11379	24073	22110	3472.8	17837	2127.8	25417	8700.2	8530.5	3911.6	11954	7099

Campesterol	Steroids and steroid	17590	8950	17720	15286	13999	3757.3	27879	36887	8209.4	9465.7	28998	13090
7-Oxo-beta-sitosterol	Steroids and steroid	13493	10990	5717.7	7414.6	16962	15111	6334.5	8657.3	9610.5	5349.1	7911.7	7804.7
Physalin G	Steroids and steroid	9796.4	3634.1	3445.2	6496	22741	3885.8	3848.3	7908.2	4545.8	6585.5	8736.4	16303
Beta-Sitosterol	Steroids and steroid	11977	4360.1	3703.6	16851	8497.5	4268.9	19111	28863	3743.8	5671.5	10398	4743.3
Physalin A	Steroids and steroid	9796.4	3026.6	3445.2	2753.6	22741	3885.8	3908.3	7908.2	6114.1	6563	16916	16303
Lathosterol	Steroids and steroid	4930.4	7555.6	8310.9	9256.2	6185.6	6727.7	7885.4	24229	13411	25719	12875	35606
Dihydrotestosterone	Steroids and steroid	3860	5363.1	5121.1	8829.4	3167.9	16562	634.7	1858	618.88	0	0	1219.9
Physalin L	Steroids and steroid	8696.3	10173	3506.7	7066	4243.3	0	6748.2	9816.1	3649.9	5514	4771	8084
Sitostenone	Steroids and steroid	5732	3538.8	2393.2	4833.3	10256	2325.9	6673	5648.8	3654.5	2018.6	3829.5	2604.5
17-Hydroxyprogesterone	Steroids and steroid	5345.9	3879.2	0	5395.1	5492.2	8348.4	11014	11091	5019.4	9086.8	6680.9	6228.8
17alpha-Estradiol	Steroids and steroid	8145.7	1155.2	1236	4315	4048.9	5377.5	3437.7	5505	3200.6	2727.1	1778	5189.3
Vitamin D2 (Ergocalciferol)	Steroids and steroid	647.68	1285.6	5544.7	3412.9	8424	794.87	2105.5	0	5723.6	0	0	14374
11b-Hydroxyandrost-4-en-3-one	Steroids and steroid	2013	4892	3617.4	3069.1	1971.9	1733.9	3016.5	1113.4	753.25	1941	4380.4	1522.9
Adrenosterone	Steroids and steroid	1726.9	1640.8	2914.6	1457.8	2218.5	2374.7	2882.4	1631.1	3522.8	2813.5	4040.4	2675.1
Androstenediol	Steroids and steroid	0	1246	1251.2	4265.9	1219.9	3497.3	5596.7	18020	3064.8	22924	4195.2	4560.5
Ruscogenin	Steroids and steroid	4207	0	1799.5	0	1043.7	2534.1	2219.1	534.58	3145.4	1866.1	2623.5	3223.3
Deoxycorticosterone	Steroids and steroid	743.65	1096.4	2149.6	1695.6	1204.7	2363.5	1483.2	1874.9	1061.4	1325.5	2239.1	1581.8
Helveticoside	Steroids and steroid	1581	777.5	197.63	1052.3	409.91	863.26	1590.1	853.59	0	442.1	4286.2	2050.2
17a-Hydroxypregnenolone	Steroids and steroid	0	448.73	1950.6	919.02	0	898.75	348.36	1080.7	336.48	231.02	455.31	3279.6
Officinalisinin I	Steroids and steroid	293.46	1095.9	71.715	282.28	453.47	712.69	1573.6	341.53	69.72	429.94	984.7	773.51
Estradiol-17beta 3-sulfate	Sterol lipids	2723.2	0	2523.3	1897.6	2919.7	1808.9	1943.9	3081.5	3464.6	1501.3	1936.3	914.17
Loganin	Terpene	2334.7	0	0	609.06	0	0	591.57	0	594.74	4460.7	1207.3	0
Salsolinol	Tetrahydroisoquinol	8782.1	4424.6	7503.5	6181.1	3462.5	3581.3	996.7	2311.3	251.62	1103.6	3785.6	3740.6
(-)-Salsoline	Tetrahydroisoquinol	1961.8	737.79	3987.6	3585.8	1445.9	861.17	1296.6	2823.1	2338	3914.4	2137.1	961.93
Biliverdin	Tetrapyrroles and de	2622.8	975.18	2927.7	1733.8	0	1510.8	5523.9	9597.7	0	2164.7	5397.1	0
Deethylatrazine	Triazines	966139	180947	280904	368941	479845	168985	82161	128613	57442	241845	95167	63968
Epifriedelanol	Triterpenoids	6272.8	11333	279322	14910	11533	6201	54758	9232	32601	117396	94611	6306.2
Betulin	Triterpenoids	7822.7	7866.3	8521.1	7317.8	5297.7	8198.2	13439	17327	9322.1	13448	17667	10620
Shionone	Triterpenoids	9346	6474.4	11565	7471.6	2269.5	4954.7	7952.9	5453.4	6130.1	9338	4758.7	8623
Taraxerol	Triterpenoids	5691.1	3697	11369	5790.5	6886.7	4990.7	9905	9162.7	6979.5	5726.2	4269.7	3101.3
Dipterocarpol	Triterpenoids	5209.8	6654.2	8083.9	8089.7	1569.9	5980.3	11898	801.7	8570.4	4596.7	1563.8	2135
Lupeol	Triterpenoids	5494.2	3783.6	4643.5	7780.4	4659.7	5576.4	9564.1	3110.2	1435.1	7135.3	13285	4687.3

Germanicol	Triterpenoids	8181.2	1857	3013.9	6145.7	6886.7	3171.3	15025	5006.6	6979.5	6665.7	4269.7	5488.5
Ganoderic acid H	Triterpenoids	5942.5	2366.3	0	16208	0	3046.9	16641	12649	10757	14220	6277.5	0
Ginsenoside F2	Triterpenoids	0	1544.8	0	0	25994	0	17537	13025	0	0	4569	0
Simiarenol	Triterpenoids	5691.1	1857	3013.9	6145.7	6886.7	3171.3	15025	5006.6	6979.5	6665.7	4269.7	5206.5
Ganoderic acid F	Triterpenoids	4523.9	2340.3	4757.1	2998.4	6926	3340.8	18446	12954	5202.9	5064.7	16334	7540.8
Limonexic acid	Triterpenoids	3781.1	1857	4894.6	3980	5156.7	2460.7	4824.3	11038	15602	5156.6	8696.8	1249.6
Glycyrrhetic acid 3-O-mor	Triterpenoids	4788.4	3425.8	1598.1	3957.2	4148.3	3385.7	5466.4	2358.6	2231.3	3050.4	2143.2	2417.2
Taraxasterone	Triterpenoids	2235.6	1947.7	2377.8	5431.2	3287.6	3719.5	3138.9	3897.4	1609.5	3496.5	2892.4	2139
Jangomolide	Triterpenoids	2889.4	646.51	3289.1	2742.2	1747.2	1463.1	3269.3	2590.1	1512.6	739.09	4259.4	1082.5
11-Keto-beta-boswellic ac	Triterpenoids	2647.9	2569.6	2353.5	2585.1	524.34	1918.9	3163.5	2829.3	2812.3	813.4	2480.9	1895
N-Acetyl-5-hydroxytrypta	Tryptamine derivativ	3339	8180.1	10147	2473.4	10580	4556.3	5787.8	8948.9	5303.8	16271	7437.4	4747.3
N-Methyltryptamine	Tryptamine derivativ	3469.1	4027.9	5829.5	2970.6	1599.7	2531.6	2190.4	8002.1	4919.1	6359.8	3859	3968.2
Pyridoxine	Vitamins	258430	214777	216504	397032	273934	427050	51268	37639	55874	133536	31031	33620
Thiamine	Vitamins	78802	0	122605	116443	69508	113225	35376	21985	22093	40287	18758	63053
D-Pantothenic acid	Vitamins	1767.4	2673.5	1312.8	3596.2	992.91	1609.2	1929.2	640.37	2118.7	16759	998.01	1676.2
Garcinone D	Xanthones	13493	10990	5717.7	7729.7	16962	5980.2	6334.5	8657.3	9610.5	3832.7	7911.7	7804.7
Swertiaperennin	Xanthones	5335.5	7345.3	4412.7	10278	13352	5100.4	634.7	7073.3	1191.3	4584.2	1288	3226
Maclurin	Xanthones	1107.6	4428.9	13057	7871	6673.2	5495.3	1703.5	1206.6	6904.1	5339.6	4806.8	1729
Beta-mangostin	Xanthones	8270.4	3182.5	5743.5	8037.3	9167	3357.8	2912.9	8706.2	7660	2700.4	3907.8	8830
Mangiferin	Xanthones	13487	2418.7	4799.3	3106.5	7722	4214	0	3163.1	0	1863.5	0	2397.4
Isogentisin	Xanthones	3514.8	3570.9	6584.2	3038.6	5394.6	10429	1215.9	3355.7	935.09	1767.5	1250.1	3096
1,3,6-Trihydroxy-5-metho	Xanthones	3922.4	5958	1993.5	5455.5	4678.8	3558.2	3729.9	6789.1	2189.5	3843.3	5965.3	5879.8
Bellidifolin	Xanthones	3922.4	5958	1993.5	5455.5	4678.8	1578.1	3729.9	6789.1	3837.3	3843.3	5965.3	5879.8
2-Hydroxyxanthone	Xanthones	3639.2	3562.6	2055.2	1371.4	3851.4	3518.3	3027.5	2514.2	3235.2	2225.6	2194.1	2459.9
Lancerin	Xanthones	2423.8	2730	0	3540.7	1396.3	6306	2827.3	9103.3	2140	3546.9	19548	3512.4
4-Hydroxyphenylacetylglutamic acid		4E+06	2E+06	2E+06	7E+06	3E+06	4E+06	4E+06	6E+06	3E+06	3E+06	3E+06	3E+06
cis-9,10-Epoxystearic acid		3E+06	992079	1E+06	2E+06	3E+06	1E+06	3E+06	2E+06	1E+06	2E+06	2E+06	2E+06
5-Methyl-2-furaldehyde		526884	355500	499082	469644	274607	880243	510769	507606	369420	614187	358303	361305
6-Amino-2-oxohexanoate		280318	271347	206206	272689	215880	220448	35807	81354	154984	44069	270301	159870
Styrene-cis-2,3-dihydrodiol		139267	188461	186240	117585	100246	280328	5708.8	13708	16922	2976.3	6956.3	8981.8
2-Hydroxy-3-methylbenzalpyruvate		88436	50133	61875	46175	97985	89049	41647	53658	51287	25919	24892	48483
4-Sulfobenzoate		9578.5	50549	50679	53284	39440	76425	17276	19883	25816	14903	16281	15462

(2S,5S)-trans-Carboxymethylproline	18944	15039	10800	7926	17979	29847	7816.9	12705	5882.5	8006.7	11063	10185
3-Methylsalicylaldehyde	7099.6	17907	12637	19494	13098	10344	8753.2	9703.3	12687	10177	33273	10912
12-OPDA	42011	1246	695.47	5573.7	2804	3497.3	5596.7	18020	3591.6	22924	4195.2	4560.5
5-Hydroxyconiferaldehyde	7682.9	4496.1	12363	3579.1	10860	3813.5	6755.7	2641.3	3106.8	4136.2	3128.4	1526.8
Toluene-cis-dihydrodiol	5278.1	4053	9224	4665.6	3620.1	13024	4601.1	7270.6	3905.2	5721.2	4293.1	4091.7
2-Hydroxy-3-carboxybenzalpyruvate	6226.9	3451.5	13522	1882.5	4111.9	10345	2940.8	4550.1	4230.9	7988.8	6849.6	9110.1
S-(Phenylacetothiohydroximoyl)-L-cysteine	3887.3	5212.6	6365.3	4340.9	11144	3139	4663	15180	0	4364.8	5295.4	7551.2
N5-(L-1-Carboxyethyl)-L-ornithine	3522.5	8852.4	2641.3	6057.2	5121.6	7146.6	7891	4451	6794	3733.5	4166.8	6633.9
3-(2,3-Dihydroxyphenyl)propanoate	3269.3	3965.1	4712.8	5070	5574.3	5820.5	6578.3	6230.2	5441.5	3100.6	3441.6	5267.6
N,N-Dihydroxy-L-phenylalanine	3191.2	9827	2986.9	1848.5	2146	2779.9	2053.2	2923.3	981.03	4260.1	1595.2	785.56
9-Riburonosyladenine	2697.3	1224.9	663.84	2874.5	1931.8	10154	7160.3	4836	6944	4883	6536.5	3413.7
cis-3-(Carboxy-ethyl)-3,5-cyclo-hexadiene-1,2- $\alpha$	4314.4	543.35	1096.5	4143.7	4293.9	3823.1	2699.9	2223.5	3825.6	3822.1	1616.1	5843.1
O-Succinyl-L-homoserine	3324.9	1309.5	3974.9	2852.7	1859.4	1730.5	1679.2	2250.6	1540.9	4362	1676.3	2139.5