

Electronic Supplementary Information

Dissolved organic matter in urban stormwater runoff from three typical regions in Beijing: chemical composition, structural characterization and sources identification

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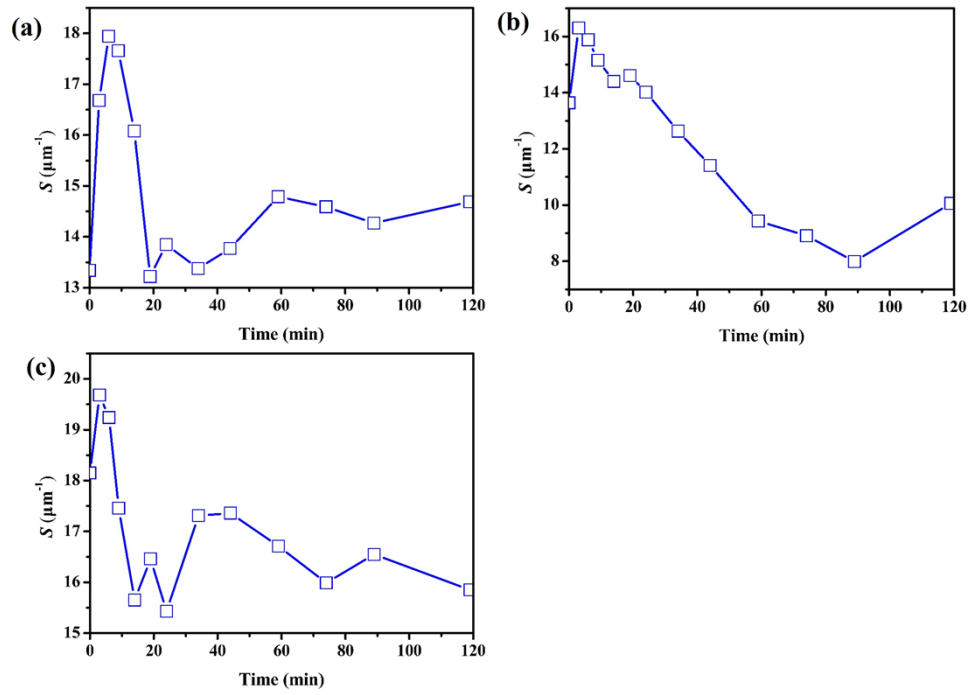


Fig. S1 Development of S values during storm event of three regions: (a) business; (b) campus; (c) residential.

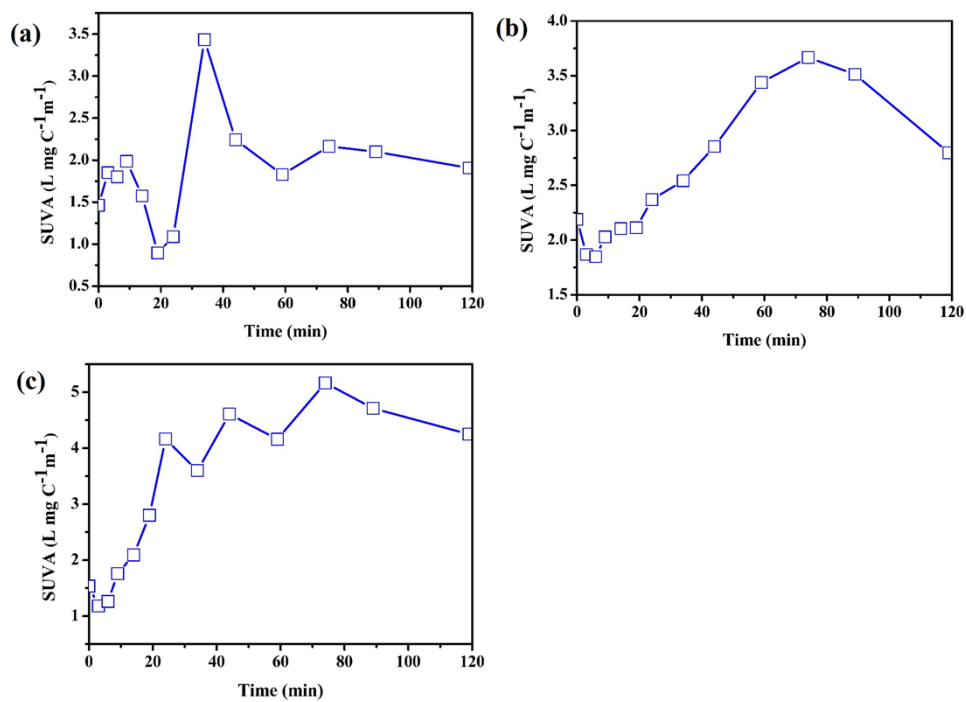


Fig. S2 Development of $SUVA_{280}$ values during storm event of three regions: (a) business; (b) campus;
(c) residential.

Table S1. Compounds information of B1 in negative ionization modes.

Retention Time (min)	Area	Intensity	S/N	Max. <i>m/z</i>	Max. MW	Formula	Possible Name	CAS
1.3	62974.68	10022	111.4	450.7944	451.8017	-	-	-
							2-Phenylpropanal	93-53-8
							(4-Methylphenyl)acetaldehyde	104-09-6
12.2	108147.91	10029	10	133.0659	134.0732	C ₉ H ₁₀ O	(Z)-4-(1-Propenyl)phenol	-
							Cinnamyl alcohol	104-54-1
14.8	133588.83	10089	15.2	514.2834	515.2907	C ₂₆ H ₄₅ NO ₇ S	Taurocholic acid	81-24-3
1.5	171627.8	10090	11.1	222.9915	222.0226	-	-	-
1.7	181020.58	10202	13.5	127.0037	128.0109	-	-	-
16	94263.15	10209	8.8	765.4422	766.4494	C ₄₁ H ₆₆ O ₁₃	Tautomycin	109946-35-2
2.9	70541.09	10241	26.2	541.1236	542.1309	-	-	-

7.9	85449.99	10249	23.6	365.0545	366.0618	C ₁₆ H ₁₄ N ₂ O ₆	6-Methoxy-2(3H)-benzoxazolone	532-91-2
8	30271.54	10264	228.1	265.092	266.0993	-	-	-
0.9	64831.35	10317	21.9	332.8605	1001.607	-	-	-
10.2	141268.45	10329	13.1	415.1604	416.1677	C ₁₉ H ₂₈ O ₁₀	Phenylethyl primeveroside	129932-48-5
13.8	64615.47	10330	12.4	152.0352	153.0425	C ₇ H ₇ NO ₃	3-Aminosalicylic acid	570-23-0
11.4	53949.68	10352	10.3	182.0092	183.0165	C ₇ H ₅ NO ₅	5-Nitrosalicylate	96-97-9
11.4	90158.51	10370	26.7	671.2176	672.2248	-	-	-
9.6	131636.91	10410	12.9	345.155	346.1623	C ₁₆ H ₂₆ O ₈	(1R,3S,4S,6R)-6,9-Dihydroxyfenchone 6-O-β-D-glucoside	217960-73-1
13.9	127740.62	10466	12.6	955.4875	956.4948	-	-	-
13	80859.13	10491	22.8	725.3741	726.3814	-	-	-
							D-Xylulose	551-84-8
1.1	141286.36	10508	17.3	149.0451	150.0524	C ₅ H ₁₀ O ₅	2-deoxy-ribonic acid	-
						C ₆ H ₁₄ S ₂	Methyl pentyl disulfide	72437-68-4

23.4	77612.29	10508	8.9	271.2272	272.2345	C ₁₆ H ₃₂ O ₃	2-hydroxyhexadecanoic acid	764-67-0
0.9	49721.27	10571	9.1	322.9041	323.9114	-	-	-
						C ₇ H ₁₆ N ₄ O	Acetylglutamine	3031-89-8
							Jasmine ketolactone	70981-24-7
11.9	55870.31	10576	15.3	207.1024	208.1097	C ₁₂ H ₁₆ O ₃	Isoamyl salicylate	87-20-7
							2-Phenoxyethyl isobutyrate	103-60-6
							Monoethyl phthalate	2306-33-4
12	86541.23	10608	8.3	193.0504	194.0577	C ₁₀ H ₁₀ O ₄	ferulic acid	1135-24-6
1	108219.63	10616	5.7	132.8676	133.8749	-	-	-
							Apigenin 7,4'-dimethyl ether	-
12.3	84536.75	10626	8.5	297.0764	298.0837	C ₁₇ H ₁₄ O ₅	3-HYDROXY-3',4'-DIMETHOXYFLAVONE	6889-80-1
						C ₁₄ H ₁₆ D ₄ N ₆ O ₅ S	S-Adenosylhomocysteine-d4	-
1.9	79319.04	10650	23.2	423.1145	424.1218	C ₂₁ H ₂₉ BrO ₄	bromovulone I	-

10.8	766997.31	10666	11.9	229.1077	230.1161	C ₁₂ H ₂₂ S ₂	Dicyclohexyl disulfide	2550-40-5
1	82938.53	10690	12.5	99.0088	100.0161	C ₄ H ₄ O ₃	Succinic anhydride	108-30-5
						C ₁₄ H ₂₆ O ₆	1-Octen-3-yl glucoside	209863-00-3
							5,5-Diisopropyl-2,2'-dimethylbiphenyl-3,3',4,4'-tetrone	122548-31-6
16.1	110615.03	10700	10.8	325.1448	326.1521	C ₂₀ H ₂₂ O ₄	1,2-Dihydrodehydroguaiaretic acid	135962-21-9
							Dehydrodieugeno	4433-8-3
10.3	107537.9	10714	7.6	463.2177	464.225	C ₂₂ H ₃₂ N ₄ O ₇	Tyr Val Ser Pro	-
9.2	84865.41	10720	13.3	119.0503	120.0575	C ₈ H ₈ O	3-Methylbenzaldehyde	620-23-5
9.9	121489.71	10753	32.7	600.1408	1202.296	C ₂₂ H ₂₈ N ₇ O ₉ P	N-Acetyl-N6,O-didemethylpuromycin-5'-phosphate	-
14.3	113075.98	10793	14.1	147.0272	148.0344	C ₂₀ H ₁₈ O ₆	Isolicoflavanol	-
						C ₁₅ H ₁₈ N ₄ O ₄	Gly Gly Trp	-
12.8	112980.94	10794	13.2	353.1024	354.1097	C ₂₀ H ₁₈ O ₆	Licoisoflavanone	-
0.9	114710.19	10848	34.5	294.8906	295.8979	-	-	-

0.9	87836.87	10866	120.7	602.6838	603.6911	-	-	-
9.5	148242.42	10867	23.2	619.13	1240.275	-	-	-
14.6	120659.5	10885	4.3	795.4512	796.4585	C ₄₂ H ₆₈ O ₁₄	Mabiogenin 3-[rhamnosyl-(1->6)-glucoside]	-
11.8	93098.84	10888	28	743.1459	744.1532	C ₃₀ H ₃₆ N ₄ O ₁₂ S ₂	Niazidin	198969-42-5
9.9	134749.67	10899	10.2	281.0694	282.0767	C ₁₃ H ₁₄ N ₂ O ₃	N-Acetyl-DL-tryptophan	87-32-1
							2,4,8-Trihydroxy-1-tetralone	88899-02-9
12.3	72812.59	10937	8.6	193.0504	194.0577	C ₁₀ H ₁₀ O ₄	Isoferulic acid	537-73-5
							Monoethyl phthalate	2306-33-4
1.3	290008.66	10954	15.6	167.0016	165.9934	C ₅ H ₁₂ S ₃	Methyl 1-(methylthio)propyl disulfide	53897-66-8
0.9	82901.08	10959	121.8	456.804	457.8113	-	-	-
0.8	79809.59	10983	58.7	759.7666	760.7739	-	-	-
						C ₉ H ₆ N ₂ O ₂	Quinoxaline-2-carboxylic acid	-
1.6	331821.41	10984	9	209.0121	210.0194	-	Methyl 1-(2-propenylsulfinyl)propyl disulfide	-

						C ₆ H ₇ FO ₇	Fluorocitric acid	357-89-1
12	102881.52	11011	5.2	293.103	294.1103	-	-	-
12.9	107247.79	11019	9.5	283.0613	284.0686	C ₁₆ H ₁₂ O ₅	Galangin 5-methyl ether	-
20.2	90788.98	11036	9.2	277.1446	278.1519	C ₁₆ H ₂₂ O ₄	Dibutyl phthalate	84-74-2
6.4	89610.09	11037	8	199.0069	200.0142	-	-	-
1.2	318575.28	11093	5	241.0018	242.0091	C ₇ H ₅ F ₃ N ₂ O ₂	4-Nitro-3-(trifluoromethyl)aniline	393-11-3
11.9	86502.97	11121	11.2	361.1652	362.1725	C ₁₃ H ₂₆ N ₆ O ₄ S	Met Arg Gly	-
0.8	109912.74	11157	18.4	372.9013	373.9086	-	-	-
9.2	151397.42	11195	124.4	116.0352	117.0425	C ₄ H ₇ NO ₃	Aceturic acid	543-24-8
1.5	249207.55	11245	7.4	213.0071	211.9991	C ₆ H ₆ N ₄ O ₃ S	Niridazole	61-57-4
9.4	81798.55	11246	9.8	387.1657	388.1729	C ₁₄ H ₂₄ N ₆ O ₇	Ala Asn Gln Gly	-
1.1	63489.82	11248	10.4	635.1789	636.1861	C ₂₇ H ₃₆ O ₁₅	Loganin pentaacetate	-
11.8	72361.95	11260	11.5	379.1663	380.1735	C ₂₁ H ₂₈ O ₄	4-[4-(3,4-Dimethoxyphenyl)-2,3-dimethylbutyl]-2-methoxyphenol	-

							11-Dehydrocorticosterone	-
							3-Dehydro-2-deoxy-D-gluconate	-
1.5	224938.16	11261	3.3	177.0401	176.0312	C ₆ H ₁₀ O ₆	2-Keto-3-deoxy-D-gluconic acid	-
							Gluconolactone	90-80-2
1.5	233856.69	11284	15.6	113.0244	114.0317	C ₅ H ₆ O ₃	3-oxo-4-pentenoic acid	-
						C ₂₂ H ₃₀ O ₅	Cicaprost	94079-80-8
11.9	85264.44	11343	11.9	409.1766	410.1838	C ₁₈ H ₂₆ N ₄ O ₇	Ala Ala Tyr Ser	-
						C ₈ H ₆ N ₂ O	1(2H)-Phthalazinone	119-39-1
1.5	223661.03	11346	8.5	181.0172	180.0085	C ₆ H ₁₄ S ₃	Ethyl 1-(methylthio)propyl disulfide	53897-67-9
1	121562.66	11512	7	134.8651	135.8723	-	-	-
11.3	100308.28	11512	9.8	251.059	252.0663	C ₁₂ H ₁₂ N ₂ O ₂	desethyletomidate	7036-56-8
						C ₂₁ H ₂₂ N ₂ O ₆	N-Feruloylglycyl-L-phenylalanine	40747-82-8
11.4	85016.73	11552	5.1	433.1129	434.1202	C ₂₁ H ₂₂ O ₁₀	5,7-Dihydroxy-3,6,8,3',4',5'-hexamethoxyflavone	-

							Naringenin-7-O-Glucoside	529-55-5
8.6	82840.61	11576	8.8	225.0404	226.0477	C ₁₀ H ₁₀ O ₆	Chorismic acid	617-12-9
13.6	100536.61	11636	5.5	271.0643	272.0716	C ₁₅ H ₁₂ N ₂ O	Glycosminine	4765-56-4
1.7	101824.11	11731	6.3	221.0662	222.0735	C ₈ H ₁₄ O ₇	Ethyl glucuronide	17685-04-0
							3-(m-Aminophenyl)-2-(p-methoxyphenyl)acrylonitrile	5462-59-9
15	162692.83	11777	9.7	285.0801	286.0873	C ₁₆ H ₁₄ N ₂ O		
							Methaqualone	72-44-6
1.2	65563.09	11830	131.4	237.0615	238.0687	-	-	-
						C ₁₂ H ₂₀ N ₂ O ₈	Isomugineic acid	74281-81-5
1.1	344556.09	11875	11.4	355.088	356.0944			
						C ₁₁ H ₂₀ N ₄ O ₅ S	Ala Ala Cys Gly	-
						C ₃₀ H ₆₂ O ₁₀	Polidocanol	3055-99-0
19.4	94255.47	11946	12.1	617.4053	618.4126			
						C ₃₆ H ₅₈ O ₈	19-Methoxypomolic acid 3-arabinoside	243470-00-0
16	94974.03	11981	37.8	662.3183	663.3255	-	-	-
6.1	106475.41	11985	8.3	153.0192	154.0265	C ₇ H ₆ O ₄	3,4-Dihydroxybenzoic acid	99-50-3

							Phloretin	60-82-2
13.1	83120.83	12062	7.7	273.0761	274.0834	C ₁₅ H ₁₄ O ₅	Corey Lactone Aldehyde Benzoate	39746-01-5
14.1	241528.91	12063	16.3	253.144	254.1512	C ₁₄ H ₂₂ O ₄	C ₇₅	191282-48-1
							Coronafacic acid	62251-98-3
15.8	88783.62	12066	17.4	207.1025	208.1097	C ₁₂ H ₁₆ O ₃	a-Asarone	2883-98-9
							Amyl salicylate	2050-08-0
							Digitoxic acid	-
1.5	301766.03	12116	7.9	163.0605	164.0677	C ₆ H ₁₂ O ₅	2-Deoxyglucose	154-17-6
							Butyl propyl disulfide	72437-64-0
							Gly Gly Arg Lys	-
8.5	86249.47	12119	8.2	451.2186	452.2259	C ₁₆ H ₃₂ N ₈ O ₅	Tyr Val Thr Ala	-
							5,6-dihydroxy stearic acid	-
19.3	123118.75	12137	17.4	315.2535	316.2608	C ₁₈ H ₃₆ O ₄	2-Hydroxy-2,4-pentadienoate	159694-16-3
1.7	109797.21	12144	16.8	113.0245	114.0318	C ₅ H ₆ O ₃		

19.3	84022.52	12152	10.1	269.2117	270.219	C ₁₆ H ₃₀ O ₃	2-methyl-4-oxo-pentadecanoic acid	-
4.1	78432.32	12175	4	379.1246	380.1319	C ₁₂ H ₂₄ N ₆ O ₄ S ₂	Cys Cys Arg	-
0.9	191602.19	12180	19.2	294.9535	295.9608	-	-	-
12.7	139933.22	12186	7	205.087	206.0942	C ₁₂ H ₁₄ O ₃	p-Methoxycinnamic acid ethyl ester	1929-30-2
11.7	78297.71	12192	135.5	599.2547	600.262	C ₂₂ H ₄₄ N ₈ O ₅ S ₂	Met Arg Met Lys	-
						C ₂₆ H ₃₆ N ₁₀ O ₅ S	Trp Arg His Cys	-
17.6	8316634.5	12242	3.5	129.9757	130.983	-	-	-
3.7	90156.72	12279	6.6	213.9764	214.9837	-	-	-
15.1	109107.84	12283	32.2	554.2445	555.2517	C ₂₂ H ₄₁ N ₅ O ₇ S	Glu Lys Leu Met	-
						C ₂₅ H ₄₁ N ₅ O ₅ S ₂	Met Met Phe Lys	-
12.2	236476.17	12331	4.5	257.0484	258.0557	-	-	-
8.7	29340.47	12463	277	309.1191	310.1264	-	-	-
0.9	113400.89	12523	24.6	270.8321	271.8394	-	-	-

						C ₈ H ₁₄ O ₅	Diethyl L-malate	7554-28-1
2.3	127897.35	12592	8.9	189.0766	190.0838			
						C ₈ H ₁₄ O ₅	3-Hydroxysuberic acid	73141-47-6
17.3	113705.88	12741	7.2	633.4	634.4072	C ₃₆ H ₅₈ O ₉	Maslinic acid 3-O-b-D-glucoside	163634-06-8
1.6	308660.59	12746	11.1	253.0019	254.0091	C ₈ H ₆ N ₄ O ₄ S	Nifurthiazole	3570-75-0
0.8	314766.94	12764	283.6	988.7235	1977.462	-	-	-
0.9	65324.05	12825	142.5	434.8187	435.826	-	-	-
1	169677.67	12841	142.7	835.0105	836.0178	-	-	-
9.2	115702.52	12874	36.4	703.1536	704.1609	-	-	-
						C ₂₄ H ₄₃ C ₁₅ O ₅ S	11,12,13,15,16-pentachloro-14-hydroxytetracos-1Z-enyl sulfate	-
1	69138.29	12928	287.3	617.1225	618.1298			
						C ₂₆ H ₃₀ O ₁₅	Okanin 4'-alpha-L-arabinofuranosyl-(1->4)-glucoside	-
10.7	84602.19	12941	15.2	154.0144	155.0216	C ₆ H ₅ NO ₄	4-Nitrocatechol	3316--09-4
0.8	450779	12971	144.1	1060.694	1059.703	-	-	-
0.9	110420.9	12993	144.4	494.7574	495.7647	-	-	-

1.1	214472.7	13096	51.2	179.0557	720.2414	C ₆ H ₁₂ O ₆	allo-Inositol	643-10-7
0.8	145568.08	13131	145.9	516.8969	517.9042	-	-	-
10.1	82348.44	13139	9.1	153.0195	154.0268	C ₇ H ₆ O ₄	2,3-Dihydroxybenzoic acid	303-38-8
9	67911.12	13169	12.7	199.0067	200.014	-	-	-
1.1	276286.84	13219	38.2	669.1136	670.1155	-	-	-
18.4	108781.44	13340	34.2	450.2624	451.2696	C ₁₈ H ₃₇ N ₇ O ₄	Lys Leu Arg	-
						C ₂₈ H ₃₇ NO ₄	Cytochalasin Opho	108050-26-6
4.8	198064.88	13393	7	187.0612	188.0685	-	-	-
0.8	290733.81	13423	5.5	874.2477	875.255	-	-	-
9.9	134516.63	13441	10	181.014	182.0213	C ₈ H ₆ O ₅	2-Hydroxyisophthalic acid	606-19-9
0.9	171621.28	13462	34.2	232.9222	233.9295	-	-	-
12.5	106820.94	13479	13.1	617.2606	618.2678	C ₂₈ H ₃₈ N ₈ O ₆	Trp Gln Leu His	-
						C ₃₂ H ₃₈ N ₆ O ₅ S	Met Pro Trp Trp	-

15.2	157603.08	13482	50	648.3024	649.3097	C ₃₃ H ₄₃ N ₇ O ₅ S	Lys Trp Met Trp	-
1.2	79699.43	13535	300.8	845.2756	846.2829	C ₃₀ H ₅₄ O ₂₇	3-O-alpha-L-Arabinopyranosyl-L-arabinose	79435-28-2
10.6	173709.5	13554	7.5	243.0326	244.0399	-	-	-
							Valerenolic acid	1619-16-5
22.2	100963.66	13573	20.5	249.149	250.1563	C ₁₅ H ₂₂ O ₃	Abscisic alcohol	-
							Octisalate	-
						C ₂₁ H ₂₆ N ₄ O ₁₁	Asp Asp Phe Asp	-
8.2	108632.3	13665	39.3	545.1287	546.1359	C ₂₆ H ₂₆ O ₁₃	Biochanin A 7-(6-methylmalonylglucoside)	34232-19-4
0.8	125233.66	13686	304.1	812.761	1624.546	-	-	-
15.5	111517.66	13709	31	268.9826	269.9899	-	-	-
0.9	162688.42	13731	152.6	608.6961	609.7033	-	-	-
						C ₃₅ H ₅₆ N ₄ O ₅ S	8-iso Prostaglandin A2-biotin	-
12.9	103466.4	13764	24.9	679.3685	680.3758	C ₃₇ H ₅₆ O ₉	O-Methylganoderic acid O	-

1	125645.59	13793	25.6	172.8811	173.8883	-	-	-
11	68833.09	13796	153.3	195.0409	196.0482	-	-	-
8.9	75211.47	13869	9.4	451.2186	452.2259	C ₁₆ H ₃₂ N ₈ O ₅	Gly Gly Lys Arg	-
						C ₂₁ H ₃₂ N ₄ O ₇	Ala Ile Ser Tyr	-
0.9	86481.3	14043	156	504.7172	505.7245	-	-	-
						C ₅ H ₈ N ₄ O ₂	1,2,4-Triazole-3-alanine	10109-05-4
11.4	88870.62	14089	11.6	191.0346	192.0419		2-Hydroxychromene-2-carboxylate	-
						C ₁₀ H ₈ O ₄	2,10-dihydroxy-4,6,8-decatriynoic acid	-
7.6	103589.95	14103	24.4	184.9912	185.9985	C ₇ H ₆ O ₄ S	4-Sulfobenzaldehyde	-
						C ₂₀ H ₂₈ N ₆ O ₉	Glu Pro His Asp	-
						C ₁₉ H ₃₂ N ₄ O ₉	Val Leu Asp Asp	-
9.6	97515.55	14153	17.2	495.1869	496.1941	C ₂₀ H ₂₈ N ₈ O ₅	His His Pro Ala	-
						C ₂₅ H ₂₈ N ₄ O ₇	Trp Tyr Glu	-

11.1	108692.98	14154	19.4	439.1242	440.1315	C ₁₅ H ₂₄ N ₄ O ₉	Glu Glu Gly Ala	-
1.3	106058.35	14180	157.6	108.9964	110.0037	C ₂ H ₆ O ₃ S	METHYLMETHANE SULFONATE	-
1	319354.56	14191	69.3	759.0295	760.0367	-	-	-
12	98583.64	14283	13.5	159.0814	160.0886	C ₁₁ H ₁₂ O	RETUSOQUINONE	-
							Propyl benzoate	2315-68-6
11.2	85893.05	14306	13.8	163.0761	164.0834	C ₁₀ H ₁₂ O ₂	4-Isopropylbenzoic acid	536-66-3
							THYMOQUINONE	490-91-5
							Nonanedioic acid	-
11.8	281101.88	14313	21.7	187.0971	188.1044	C ₉ H ₁₆ O ₄	Butyl ethyl malonate	17373-84-1
12.6	99222.2	14345	9.8	273.17	274.1773	C ₁₄ H ₂₆ O ₅	3-hydroxy-tetradecanedioic acid	-
4.1	160820.22	14384	11.5	197.0092	198.0164	C ₈ H ₆ O ₆	3,4-Dihydroxyphthalate	82784-82-5
							trans-Resveratrol 4'-O-glucuronide	-
1.2	332093.81	14430	22.9	439.0758	440.0831	C ₂₀ H ₂₀ O ₉	5,3'-Dihydroxy-3,6,7,4',5'-pentamethoxyflavone	-

10.5	104177.88	14473	18	119.0501	120.0574	C ₈ H ₈ O	4-Hydroxystyrene	2628-17-3
							Phenylacetaldehyde	122-78-1
							C ₆ H ₁₂ S ₂	1-Propenyl propyl disulfide
1.7	135128.42	14531	28.5	147.0297	148.0369	C ₅ H ₈ O ₅	Citramalic acid	2306-22-1
							D-Ribonolactone	5336—08-3
5	117116.55	14678	23.5	319.1034	320.1107	C ₁₇ H ₂₀ N ₂ S	Desmethyiltrimeprazine	22732-04-3
							Diethyl phthalate	84-66-2
15.3	95199	14843	7.9	221.0816	222.0889	C ₁₂ H ₁₄ O ₄	Diglycidyl resorcinol ether	101-90-6
							Valeroyl Salicylate	64206-54-8
14.5	146152.19	14852	17	184.984	185.9913	C ₄ H ₆ O ₆	Tartaric acid	87-69-4
						C ₃ H ₇ O ₇ P	D-Glycerate 2-phosphate	3443-58-1
0.8	172588.58	14996	16.2	118.9663	119.9736	-	-	-
15.4	106778.05	15006	7.9	221.0816	222.0888	-	-	-

7.8	94309.53	15109	25.2	315.0716	316.0788	C ₂₀ H ₁₃ ClN ₂	2-(4-Chlorophenyl)-3-phenyl-3-(2-pyridinyl)acrylonitrile	94546-56-2
0.8	157453.28	15113	335.8	946.7149	1895.444	-	-	-
11.8	125299.59	15126	25.7	634.2591	635.2664	C ₂₉ H ₄₁ N ₇ O ₅ S	Phe Phe Met Arg	-
1.2	124105.72	15182	12.4	152.0021	153.0094	C ₃ H ₇ NO ₄ S	3-Sulfinioalanine	1115-65-7
14.2	110942.75	15220	12.7	269.1754	270.1827	C ₁₅ H ₂₆ O ₄	Ethylene brassylate	105-95-3
10.7	159979.08	15262	18.9	323.0799	324.0872	C ₁₅ H ₁₆ N ₂ O ₄	3-Carboxy-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole-1-propanoic acid	-
24.9	143054.58	15346	20.1	387.1555	388.1628	C ₁₅ H ₂₄ N ₄ O ₈	Ala Asp Pro Ser	-
1.2	98160.78	15350	8.8	180.9809	181.9881	C ₅ H ₁₀ OS ₃	(Z)-Methyl 3-(methylsulfinyl)-1-propenyl disulfide	104228-50-4
9.6	93441.62	15372	5.3	199.0068	200.0141	-	-	-
14.1	132449.84	15409	6.1	275.0956	276.1028	C ₁₅ H ₁₆ N ₂ O	LY201116	787-93-9
1	133030	15487	104.2	856.9964	858.0036	-	-	-
1.8	88444.3	15537	33	222.0438	446.1016	C ₁₀ H ₉ N ₃ O	AMRINONE	60719-84-8
18.1	360077.38	15562	9.7	293.176	294.1833	C ₁₇ H ₂₆ O ₄	Tanacetol A	86778-06-5

						C ₁₇ H ₂₆ O ₄	Gingerol	58253-27-3
15.5	118287.6	15643	35.3	96.9907	97.9979	-	-	-
						C ₃₃ H ₄₀ N ₆ O ₅	Ile Pro Trp Trp	-
11.2	205418.42	15649	36.9	635.2708	636.2781	C ₃₈ H ₄₀ N ₂ O ₇	Calafatimine	77793-42-1
							Diethyl malonate	105-53-3
9	101897.27	15736	8.5	159.066	160.0733	C ₇ H ₁₂ O ₄	2-Methyladipic acid	626-70-0
10	204349.63	15742	44.5	703.1545	704.1618	-	-	-
0.8	143259.84	15768	24.5	486.8807	487.8879	-	-	-
							Adipic acid	124-04-9
8.6	113864.15	15911	20.2	145.0506	146.0579	C ₆ H ₁₀ O ₄	Dimethyl succinate	106-65-0
18.4	144382.75	15925	33.6	447.1343	448.1416	C ₁₆ H ₂₄ N ₄ O ₁₁	Ala Asp Asp Glu	-
11	107699.44	15973	32.8	609.1446	610.1519	C ₂₇ H ₃₀ O ₁₆	Isoorientin 7-glucoside	35450-86-3
3	7342735	16078	4.6	129.9757	130.983	-	-	-

0.8	258271.83	16166	107.9	923.7453	1848.511	-	-	-
						C ₂₄ H ₁₄	Dibenzo[a,e]fluoranthene	5385-75-1
1.5	280875.28	16183	27.5	337.077	338.0834	C ₁₂ H ₁₈ O ₁₁	L-Ascorbic acid-2-glucoside	129499-78-1
						C ₁₉ H ₁₅ ClN ₂ O ₂	Inabenfide	82211-24-3
							6,7,4'-Trihydroxy-3-methoxyflavone	-
14.4	132048.2	16186	7.8	299.0557	300.063	C ₁₆ H ₁₂ O ₆	8-Hydroxygalangin 3-methyl ether	-
							1,1-Dimethylethyl benzoate	774-65-2
12	121680.93	16253	16.8	177.0919	178.0992	C ₁₁ H ₁₄ O ₂	Phenylmethyl butanoate	103-37-7
							4-t-Butylbenzoic acid	98-73-7
							Butopyronoxyl	532-34-3
10.1	145984.03	16354	13.7	225.1128	226.1201	C ₁₂ H ₁₈ O ₄	Tuberonic acid	-
							cis-p-Coumaric acid	4501-31-9
8.9	132619.13	16404	26.2	163.0399	164.0472	C ₉ H ₈ O ₃	3-Oxo-3-phenylpropanoate	29285-17-4 614-

								20-0
							Salicylic acid beta-D-glucoside	10366-91-3
8.4	108288.84	16457	24.8	299.0768	300.0841	C ₁₃ H ₁₆ O ₈	Dimethyl fukiic acid	56158-55-5
							4-(β-D-Glucosyloxy)benzoate	-
						C ₇ H ₁₇ N ₄ O ₇ P	N1-Amidinostreptamine 6-phosphate	-
10.6	115297.05	16465	182.9	175.0973	176.1045	C ₈ H ₁₆ O ₄	6,8-dihydroxy-octanoic acid	-
4.3	165251.44	16535	8.7	207.03	208.0373	C ₁₀ H ₈ O ₅	FRAXETIN	574-84-5
0.8	991386.38	16553	367.8	1003.703	1004.711	-	-	-
22.4	208901.63	16564	13.8	269.2117	270.219	C ₁₆ H ₃₀ O ₃	Ambrettolic acid	-
						C ₅ H ₁₂ N ₄ O	4-Guanidinobutanamide	23256-39-5
10.6	129497.01	16649	6.8	179.0709	180.0781		1-(2,4-Dihydroxyphenyl)-1-butanone	4390-92-5
						C ₁₀ H ₁₂ O ₃	3-Methoxybenzenepropanoic acid	10516-71-9
							Coniferyl alcohol	458-35-5

0.8	376031.84	16686	370.8	930.7369	1863.488	-	-	-
9.2	196977.81	16724	76.8	835.1588	836.1661	-	-	-
						C ₁₉ H ₃₀ N ₈ O ₈	Thr Gln Asn His	-
11.2	136104.42	16738	26	533.1866	534.1921		Cys Ile Thr Tyr	-
						C ₂₂ H ₃₄ N ₄ O ₇ S	Cys Glu Phe His	-
0.9	245027.28	16931	15.7	310.9302	311.9359	C ₉ H ₁₄ Br ₂ O ₂	9,9-dibromo-8-nonenoic acid	-
0.8	185711.3	17024	17.4	384.8745	385.8818	-	-	-
13	120828.46	17085	27.4	133.0115	134.0188	-	-	-
							4-Coumaryl alcohol	3690—05-9
							hydrocinnamic acid	501-52-0
12.3	302987.66	17130	16.6	149.0605	300.1377	C ₉ H ₁₀ O ₂	2'-Methoxyacetophenone	579-74-8
							4-Vinylguaiaicol	7786-61-0
							Tolylacetate	140-39-6

13.9	148553.47	17218	15.2	294.0647	295.072	C ₁₃ H ₁₃ NO ₇	Caffeoyl aspartic acid	860295-20-1
							4-Hydroxyphenacyl alcohol	5706-85-4
							Methyl salicylate	119-36-8
9.6	119532.04	17225	16.5	151.0399	152.0472	C ₈ H ₈ O ₃	2',4'-Dihydroxyacetophenone	89-84-9
							2-Hydroxyphenylacetic acid	614-75-5
7.6	146316.61	17237	27.5	163.0421	164.0493	-	-	-
14.2	147655.8	17554	17.8	273.1158	274.123	C ₁₆ H ₁₈ O ₄	HETEROPEUCENIN, METHYL ETHER	26213-95-6
1.5	119009.74	17607	6.1	827.266	828.2733	C ₃₀ H ₅₂ O ₂₆	Maltopentaose	34620-76-3
10.7	232664.61	17700	13.9	193.053	194.0602	C ₁₀ H ₁₀ N ₂	1,5-Naphthalenediamine	2243-62-1
1.4	235800.33	17742	16.6	601.1281	602.1354	C ₂₆ H ₃₀ O ₁₄	Butein 4'-arabinosyl-(1->4)-galactoside	-
1.3	173557.27	17887	54.2	198.9916	199.9989	C ₇ H ₅ ClN ₂ O ₃	AKLOMIDE	3011-89-0
14.1	270990.25	18016	10.7	213.0148	214.0221	C ₇ H ₆ N ₂ O ₆	3,5-Dinitroguaiacol	63975-57-5
10.9	134683.39	18187	10.9	189.0553	190.0626	C ₁₁ H ₁₀ O ₃	Avenalunic acid	135754-92-6

							HYMECROMONE METHYL ETHER	2555-28-4
1.2	145577.2	18305	21.7	352.8298	353.8371	-	-	-
0.8	192734.78	18317	407	865.7593	1733.533	-	-	-
15.6	224252.59	18325	40.4	987.5136	988.5209	-	-	-
11.5	126891.48	18405	29.9	380.9919	381.9992	C ₁₅ H ₁₀ O ₁₀ S	6-Hydroxyluteolin 7-sulfate	-
18.9	171919.42	18461	26.5	315.2523	316.2596	C ₁₈ H ₃₆ O ₄	5,6-dihydroxy stearic acid	-
1.1	109856.54	18616	206.8	165.0403	166.0476	C ₆ H ₆ N ₄ O ₂	3-Methylxanthine	1076-22-8
						C ₅ H ₁₀ O ₆	L-Arabinonic acid	608-53-7
						C ₈ H ₁₀ N ₄ O ₃	1,3,7-Trimethyluric acid	5415-44-1
						C ₇ H ₁₄ O ₇	D-Glucoheptose	3146-50-7
15	101694.2	18628	20.4	245.0452	246.0525	C ₁₄ H ₁₄ S ₂	Dibenzyl disulfide	150-60-7
						C ₁₃ H ₁₀ O ₅	ISOPIMPINELLIN	482-27-9
						C ₆ H ₁₅ O ₈ P	Phosphatidyl glycerol	61468-73-3

0.9	112461.54	18717	39.4	412.7633	413.7705	-	-	-
1.9	130346.07	18730	4.8	377.1085	378.1158	C ₁₉ H ₂₃ ClN ₂ O ₂ S	Pyridate	55512-33-9
8.6	143448.23	18821	20.4	171.0662	172.0735	C ₈ H ₁₂ O ₄	3-Isopropenylpentanedioic acid	6839-75-4
							(-)-Corey Lactone Diol	32233-40-2
1	145828.09	18978	6.7	150.9702	151.9775	C ₄ H ₈ S ₃	3,5-Dimethyl-1,2,4-trithiolane	23654-92-4
4.3	211329.86	18982	23.7	269.0301	270.0374	-	-	-
11.5	149498.67	18991	20.5	457.1706	458.1778	C ₁₇ H ₂₆ N ₆ O ₉	Asp His Ser Thr	-
0.8	317083.84	19205	426.8	825.7484	826.7557	-	-	-
13	149528.06	19288	22.1	423.1289	424.1361	C ₁₅ H ₂₄ N ₄ O ₈	Ala Pro Ser Asp	-
						C ₂₀ H ₂₄ O ₁₀	Celereoside	74608-59-6
19	146998	19374	15.5	381.2252	382.2325	C ₁₇ H ₃₀ N ₆ O ₄	His Lys Val	-
1.1	156895.25	19423	30.8	633.1229	634.1302	C ₃₂ H ₂₆ O ₁₄	Actinorhodin	1397-77-9
24.5	296541.44	19448	17.4	327.1266	328.1339	C ₁₉ H ₂₀ N ₂ O	Vellosimine	6874-98-2

						C ₁₉ H ₂₀ O ₅	Libanorin	27303-26-0
							Decursin	5928-25-6
4.7	20495988	19512	5.7	174.9559	175.9632	C ₂ H ₅ O ₅ P	Acetyl phosphate	590-54-5
0.8	218289.64	19649	436.6	881.7364	1765.487	C ₅₄ H ₁₀₂ O ₆	TG(17:0-17:0-17:1(9Z))[iso3]	-
							cis-p-Coumaric acid	4501-31-9
9.2	188148.16	19788	31.6	163.0399	164.0471	C ₉ H ₈ O ₃	cis-2-Hydroxycinnamate	-
							3',4'-(Methylenedioxy)acetophenone	-
13.7	202875.58	19799	12.4	941.5097	942.517	C ₄₈ H ₇₈ O ₁₈	Lemmatoxin	53043-29-1
0.9	122017.39	19875	220.8	570.7398	571.747	-	-	-
20.2	156968.53	20131	27.2	267.1958	268.2031	C ₁₆ H ₂₈ O ₃	Methoprene acid	53092-52-7
						C ₇ H ₁₆ N ₄ O	Acetylarginine	3031-89-8
12.1	137988.09	20137	29.1	207.1024	208.1097		Isoamyl salicylate	87-20-7
						C ₁₂ H ₁₆ O ₃	Jasmine ketolactone	70981-24-7

							Isoelemicin	5273-85-8
							Coronafacic acid	62251-98-3
							2,5-Dimethoxy-4-(2-propenyl)phenol	90377-06-3
11.2	167765.7	20178	18.4	193.0865	194.0938	C ₁₁ H ₁₄ O ₃	Butyl salicylate	2052-14-4
							(R)-3-Hydroxy-5-phenylpentanoic acid	21080-41-1
0.9	40990.77	20197	448.8	446.8445	447.8518	-	-	-
1.1	203717.53	20296	30.3	607.1241	608.1314	C ₂₈ H ₂₈ O ₁₃	2'',4'',6''-Triacetylglycitin	-
1	97400.33	20622	87.5	292.895	293.9023	-	-	-
						C ₁₄ H ₂₆ O ₆	1-Octen-3-yl glucoside	209863-00-3
15.6	150998.5	20653	20.9	325.1444	326.1517		5,5-Diisopropyl-2,2'-dimethylbiphenyl-3,3',4,4'-tetrone	122548-31-6
						C ₂₀ H ₂₂ O ₄	1,2-Dihydrodehydroguaiaretic acid	135962-21-9
7.2	123349.58	20656	14.9	199.007	200.0143	-	-	-
0.8	814014.38	20701	460	1084.66	1085.667	C ₅₄ H ₉₉ NO ₁₈	Trihexosylceramide (d18:1-9Z-18:1)	-

12.1	222043.09	20866	37.8	679.3691	680.3764	C ₃₅ H ₅₆ N ₄ O ₅ S	Prostaglandin A2-biotin	-
15	303861.34	21098	12.4	793.4356	794.4429	C ₄₂ H ₆₆ O ₁₄	Calendulaglycoside E	38424-95-2
11.4	143547.75	21262	37.9	551.2123	552.2196	C ₁₈ H ₃₂ N ₁₀ O ₈	Asn Asn Asn Arg	-
						C ₂₇ H ₃₂ N ₆ O ₅ S	Cys Phe Phe His	-
13.5	168493.97	21275	22.6	811.4461	812.4534	C ₄₂ H ₆₈ O ₁₅	bayogenin 3-O-cellobioside	-
0.8	239561.72	21317	236.9	892.7323	893.7396	-	-	-
14.9	167627.31	21382	10.1	293.106	294.1133	-	-	-
0.8	138191.94	21473	477.2	876.7515	876.752	-	-	-
1	248217.53	21501	72.5	154.9175	155.9248	-	-	-
16.3	211298.13	21547	86.7	664.2975	665.3048	C ₃₃ H ₄₇ NO ₁₃	Natamycin	-
11.9	236141.72	21769	21.1	149.0606	150.0679	C ₉ H ₁₀ O ₂	Phenyl glycidyl ether	122-60-1
							p-Hydroxypropiophenone	70-70-2
							Tolylacetate	140-39-6

11.2	135778.44	21772	9.4	207.066	208.0733	C ₁₁ H ₁₂ O ₄	DIMETHYLCAFFEIC ACID	2316-26-9
12	140081.63	21825	26.5	447.093	448.1003	C ₂₁ H ₂₀ O ₁₁	KAEMPFEROL-7-O-GLUCOSIDE	16290-07-6
12.6	130231.43	22171	9.6	207.069	208.0762	C ₁₁ H ₁₂ N ₂	NORELEAGNINE	16502-01-5
						C ₁₁ H ₁₃ ClN ₂	Epibatidine	140111-52-0
9.4	150538.34	22298	23.9	431.192	432.1993	C ₁₆ H ₂₈ N ₆ O ₈	Ala Asn Gln Thr	-
16.9	140611.52	22578	14.1	293.1756	294.1829	C ₁₇ H ₂₆ O ₄	Gingerol	58253-27-3
1	325354.47	22592	251	224.9705	225.9778	-	-	-
1.1	548707.13	22599	21.1	659.0856	660.0929	-	-	-
9	247594.69	22668	15.7	229.0173	230.0245	C ₁₃ H ₁₀ S ₂	5-(1-Propynyl)-5'-vinyl-2,2'-bithiophene	17257-06-6
12	177612.61	22704	28.2	711.3955	712.4027	C ₃₆ H ₆₀ N ₄ O ₆ S	Prostaglandin D2-biotin	-
1.1	835002.31	22781	42.3	597.0957	598.103	-	-	-
16.1	275963.31	23038	92.7	664.2974	665.3047	C ₃₃ H ₄₇ NO ₁₃	Natamycin	-
1	265639.31	23046	42.4	79.9577	80.965	-	-	-

10.6	153728.06	23047	19.5	251.059	252.0663	C ₁₂ H ₁₂ N ₂ O ₂	L-1,2,3,4-Tetrahydro-beta-carboline-3-carboxylic acid	42438-90-4
0.8	284277.88	23154	257.3	816.7561	1635.527	-	-	-
1.1	299397.28	23353	62.1	639.0829	640.0902	-	-	-
1.2	214288.19	23413	260.1	197.8075	198.8148	-	-	-
1	319073.88	23425	13.4	377.0846	378.0919	C ₁₂ H ₂₂ O ₁₁	Gentiobiose	554-91-6
						C ₁₇ H ₁₈ N ₂ O ₆ S	carbenicillin	4697-36-3
						C ₄ H ₈ N ₄ O ₂	n,n'-dinitrosopiperazine	140-79-4
10.3	151832.69	23768	12.9	179.0347	180.042	C ₉ H ₈ O ₄	Caffeate	501-16-6
							Monomethyl phthalate	4376-18-5
13.8	162388.89	23913	9.5	275.0956	276.1029	C ₁₅ H ₁₆ N ₂ O	LY201116	787-93-9
1.2	270748.44	23937	44.1	79.9577	80.9649	-	-	-
15.5	186608.23	24075	41.2	262.9757	263.983	C ₁₃ H ₈ S ₂	Thiarubrine A	63543-09-9
1.1	474135.38	24092	267.7	701.1895	702.1968	C ₃₁ H ₃₈ O ₁₆	Tetramethylquercetin 3-rutinoside	58528-03-3

9.2	174178.47	24259	25	401.1447	402.152	C ₁₈ H ₂₆ N ₂ O ₆	Bufotenine O-glucoside	64656-15-1
						C ₁₈ H ₂₆ O ₁₀	Benzyl O-[arabinofuranosyl-(1->6)-glucoside]	88510-11-6
1.5	573729.75	24291	27.4	665.2136	664.2029	C ₃₁ H ₃₈ O ₁₆	Tetramethylquercetin 3-rutinoside	58528-03-3
1.5	228387.03	24358	22.6	182.9966	184.0039	C ₅ H ₁₂ OS ₃	Methyl 1-(methylsulfinyl)propyl disulfide	134018-95-4
8	152908.23	24377	13.8	215.0017	216.009	-	-	-
1.1	324993.72	24734	9.1	593.1569	594.1642	C ₂₃ H ₃₄ N ₄ O ₈ S ₂	Asp Met Met Tyr	-
						C ₂₇ H ₃₀ O ₁₅	Kaempferol 4'-glucoside 7-rhamnoside	205876-37-5
16	237965.97	24774	9.9	275.0957	276.103	C ₁₅ H ₁₆ N ₂ O	Prolyl-2-naphthylamide	-
14.9	220372.72	24924	27.1	953.4717	954.479	-	-	-
14	240671.25	25216	9.9	795.4507	796.4579	C ₄₂ H ₆₈ O ₁₄	Jujubasaponin VI	146445-94-5
22.2	181825.56	25303	20.5	311.201	312.2083	C ₂₁ H ₂₈ O ₂	Levonorgestrel	797-63-7
8.4	190414.41	25425	19	137.0243	138.0316	C ₇ H ₆ O ₃	Salicylic acid	69-72-7
							2-Methoxy-1,4-benzoquinone	2880-58-2

							Sesamol	533-31-3
							3,4-Dihydroxybenzaldehyde	139-85-5
0.8	525221.94	25550	567.8	695.7905	696.7978	-	-	-
1.1	357158.84	25626	113	617.1509	618.1582	-	-	-
0.4	304346.22	25740	7.4	129.9757	130.983	-	-	-
						C ₂₂ H ₃₀ N ₄ O ₁₀ S	Asp Asp Met Tyr	-
							4-O-8',5'-5"-Dehydrotriferulic acid	-
14	220305.06	25982	33.8	577.1338	578.141			
						C ₃₀ H ₂₆ O ₁₂	Procyanidin B2	-
							Pelargonidin 3-p-coumarylglucoside	-
							2-Nitrophenol	88-75-5
11.9	185160.7	26039	23.8	138.0196	139.0268	C ₆ H ₅ NO ₃		
							3-Hydroxypicolinic acid	874-24-8
0.8	311008.59	26277	7.7	114.9887	115.996	-	-	-
15.1	305708.38	26717	63.9	682.3644	683.3717	-	-	-

14.1	206299.47	26808	12.6	293.1059	294.1132	C ₁₅ H ₁₈ O ₆	Tutin	2571-22-4
						C ₂₂ H ₃₄ N ₄ O ₆ S ₂	Ala Met Met Tyr	-
1.5	333575	27123	44.1	549.1663	550.1736	C ₂₆ H ₃₀ O ₁₃	Neoliquiritin 2''-apioside	135432-48-3
1	147636.73	27226	58.4	166.9652	167.9725	C ₃ H ₄ O ₆ S	3-Sulfofpyruvic acid	98022-26-5
						C ₂₃ H ₂₈ N ₄ O ₇ S	Cys Gly Tyr Tyr	-
1.5	335475.66	27382	47.4	503.1609	502.1533	C ₂₅ H ₂₈ O ₁₁	6-Hydroxykaempferol 3,5,7,4'-tetramethyl ether 6-rhamnoside	-
							3-Aminopropanal	352-92-1
						C ₃ H ₇ NO	Aminoacetone	-
12.3	146914.75	27417	54.1	108.0218	109.029			
						C ₆ H ₅ O ₂	p-Benzosemiquinone	-
9.4	279067.56	27423	43.1	608.1392	1218.293	C ₂₆ H ₃₁ N ₅ O ₆ S ₂	Cys Cys Trp Tyr	-
0.9	200632.08	27441	17.7	164.9423	165.9496	-	-	-
0.9	177053.55	27586	306.5	586.7119	587.7191	-	-	-
1.1	445082.75	27712	307.9	162.8388	163.8461	-	-	-

						C ₂₈ H ₃₈ N ₈ O ₇	Glu His Lys Trp	-
11.3	922146.13	27827	29.8	633.2553	634.2626			
						C ₃₂ H ₄₂ O ₁₃	Myricanene B 5-[arabinosyl-(1->6)-glucoside]	-
0.9	26218.36	27830	618.4	174.9374	175.9447	-	-	-
0.8	507308.75	28015	25.9	568.8222	567.8382	-	-	-
18.5	196610.47	28039	44.9	266.1033	267.1106	C ₈ H ₁₇ N ₅ O ₃	Arginyl-Glycine	-
9.3	228353.48	28109	16.7	213.0224	214.0297	-	-	-
						C ₄₃ H ₆₆ O ₁₄	Gymnemic acid I	122168-40-5
11.9	224245.36	28297	74.1	841.4217	842.4289			
						C ₄₂ H ₆₆ O ₁₇	26-(2-Glucosyl-6-acetylglucosyl)-1,3,11,22-tetrahydroxyergosta-5,24-dien-26-oate	155510-76-2
1	387524.44	28862	8.2	643.1383	644.1455	C ₂₈ H ₃₂ O ₁₅	Physcion 8-gentiobioside	-
16.2	198923.52	28957	70.7	197.0202	198.0274	C ₇ H ₆ N ₂ O ₅	DNOC	534-52-1
15.6	364179.88	28959	18.2	941.5095	942.5168	C ₄₈ H ₇₈ O ₁₈	Jujubasaponin IV	146445-93-4
9.9	220018.94	28986	69.5	711.0843	712.0916	C ₂₀ H ₂₆ N ₁₀ O ₁₃ P ₂	Diadenosine diphosphate	14938-28-4
0.9	557731.75	29002	32.4	238.8897	719.6948	-	-	-

1.1	1115291.5	29017	135.7	675.0569	676.0641	-	-	-
0.9	238117.28	29042	36	278.8795	279.8863	C ₆ H ₃ Cl ₃ O ₄	2,3,5-Trichloro-cis,cis-muconate	-
						C ₂₁ H ₃₂ N ₄ O ₆ S	Ala Cys Ile Tyr	-
11.2	198141.78	29104	50.4	503.1762	504.1835	C ₂₂ H ₃₂ O ₁₃	(S)-Multifidol 2-[apiosyl-(1->6)-glucoside]	467437-62-3
						C ₁₈ H ₂₈ N ₆ O ₁₁	Asp Asp Gln Gln	-
0.8	322898.94	29390	326.6	746.7966	747.8038	-	-	-
9.3	208131.36	30144	22.5	181.0143	182.0216	C ₈ H ₆ O ₅	Stipititate	4440-39-5
1.2	404766.91	30270	49.2	94.9809	95.9882	CH ₄ O ₃ S	Methanesulfonic acid	75-75-2
						C ₄ H ₅ FN ₂ O ₂	Dihydro-5-fluorouracil	696-06-0
1.5	227215.81	30463	43.3	167.0016	168.0089	C ₅ H ₁₂ S ₃	Methyl 1-(methylthio)propyl disulfide	53897-66-8
1.1	369423.19	30568	30.7	613.0695	614.0767	-	-	-
						C ₁₂ H ₂₆ N ₄ O ₃	Lysyl-Lysine	-
17.3	266219.56	30852	19	309.1704	310.1777	C ₁₇ H ₂₆ O ₅	3-Hydroxy-6,8-dimethoxy-7(11)-eremophilen-12,8-olide	162613-65-2

						C ₈ H ₁₈ N ₄ O	Propanoylagmatine	-
15.7	240431.02	31055	40.2	221.1183	222.1256		Hydroxyibuprofen	51146-55-5
						C ₁₃ H ₁₈ O ₃	Isoamyl p-anisate	27739-29-3
							Dehydrovomifoliol	15764-81-5
1.5	254560.7	31322	5.2	151.0067	152.014	-	-	-
10.1	216130.7	31482	72.2	543.0445	544.0518	C ₂₁ H ₂₀ O ₁₅ S	8-Hydroxyluteolin 8-glucoside 3'-sulfate	63109-34-2
0.8	194416.17	31513	700.3	534.8729	535.8802	-	-	-
8	187663.92	31621	36	178.0541	179.0613	C ₆ H ₁₃ NO ₃ S	Cyclohexylsulfamate	100-88-9
15.1	293796.53	31664	36.8	575.1188	576.1261	C ₃₀ H ₂₄ O ₁₂	Proanthocyanidin A2	41743-41-3
0.8	322037.16	32048	356.1	616.8388	617.8493	-	-	-
0.9	230946.25	32190	41.9	198.9229	599.7913	-	-	-
0.9	440968.78	32398	60.3	310.8699	311.8785	-	-	-
9.1	340678.16	33023	32.7	435.1295	436.1367	C ₁₄ H ₂₄ N ₆ O ₈ S	Cys Asn Asn Ser	-

						C ₂₁ H ₂₄ O ₁₀	Epiafzelechin 3-O-beta-D-glucopyranoside	-
9.4	189763.36	33090	34.1	401.1447	402.1519	C ₁₈ H ₂₆ N ₂ O ₆	Bufotenine O-glucoside	64656-15-1
						C ₁₈ H ₂₆ O ₁₀	Benzyl O-[arabinofuranosyl-(1->6)-glucoside]	88510-11-6
4.1	423273.38	33321	23.2	153.0192	154.0265	C ₇ H ₆ O ₄	2,6-dihydroxybenzoic acid	303-07-1
						C ₇ H ₆ O ₄	Patulin	149-29-1
0.9	533647.5	33402	56.5	316.887	317.8929	-	-	-
0.8	225049.16	33520	24.4	502.859	503.8663	-	-	-
1.1	494784.66	33880	376.4	160.8418	161.8491	-	-	-
1.5	398189.25	33986	38	225.0072	226.0144	C ₉ H ₆ N ₂ O ₃	Nitroxoline	4008-48-4
							4-Nitroquinoline-1-oxide	56-57-5
9.9	302241.78	34078	113.1	757.0888	758.0961	-	-	-
0.9	232570.22	34216	380.2	472.7757	473.783	-	-	-
11.9	252335.06	35071	35.1	182.0094	183.0167	C ₂ H ₅ N ₅ O ₃	N-Methyl-N'-nitro-N-nitrosoguanidine	70-25-7

						C ₇ H ₅ NO ₅	5-Nitrosalicylate	96-97-9
						C ₁₉ H ₂₀ N ₂ O	Vellosimine	6874-98-2
						C ₁₉ H ₂₁ ClN ₂ O	Pencycuron	-
20.1	393493.5	35345	31.6	327.1267	328.134		SELINIDIN	-
						C ₁₉ H ₂₀ O ₅	2-Hydroxy-7,8-dehydrograndiflorone	-
							DEOXSAPPANONE B TRIMETHYL ETHER	-
							p-Anisaldehyde	123-11-5
10.3	263079.06	35760	46.8	135.0449	136.0522	C ₈ H ₈ O ₂	2-Hydroxyacetophenone	582-24-1
							Phenyl acetate	122-79-2
16.8	373517.88	35869	86.3	678.3138	679.3211	-	-	-
						C ₄₉ H ₇₆ O ₁₅	Avermectin A2a	-
14.7	409538.53	36143	18.7	939.4925	940.4998		Momordin IIa	95851-50-6
						C ₄₈ H ₇₆ O ₁₈	28-Glucosyloleanolic acid 3-[arabinosyl-(1->2)-6-methylglucuronide]	117804-22-5

							2-Hexyl-1,3-dioxolane-4-methanol	-
15.7	226909.89	36340	41.7	187.1337	188.141	C ₁₀ H ₂₀ O ₃	Hexyl (R)-3-hydroxybutyrate	-
							2-hydroxy capric acid	-
11.7	271060.53	36470	60.9	725.2073	726.2146	C ₃₆ H ₃₈ O ₁₆	Licorice glycoside C1	-
1.2	621195.69	36828	7.5	737.0502	738.0574	-	-	-
1	441682.09	37412	16.4	152.9861	153.9933	C ₄ H ₁₀ S ₃	Methyl propyl trisulfide	17619-36-2
0.8	531188.88	37802	30.5	130.9664	131.9737	-	-	-
1.1	465622.31	38543	428.3	804.2296	1610.474	-	-	-
1	219198.33	38975	52.4	314.8712	315.8785	-	-	-
1	373499.5	39884	84.8	170.884	171.8912	C ₂ H ₂ BrClO ₂	Bromochloroacetic acid	5589-96-8
1	490437.88	40231	8.5	721.0766	722.0839	-	-	-
0.9	364365.69	40236	447.1	488.7469	489.7542	-	-	-
8.7	244880.53	40270	36.5	258.9915	259.9988	C ₉ H ₈ O ₇ S	Caffeic acid 3-sulfate	-

0.9	347045.13	41342	26.4	368.7973	369.8046	-	-	-
13	335846.63	42232	76.5	679.3684	680.3757	C ₃₅ H ₅₆ N ₄ O ₅ S	Prostaglandin A2-biotin	-
						C ₃₇ H ₅₆ O ₉	O-Methylganoderic acid O	-
						C ₁₇ H ₂₈ N ₈ O ₄	His Pro Arg	-
8.4	232790.2	42445	52.8	443.192	444.1993	C ₂₂ H ₂₈ N ₄ O ₆	Mitoxantrone	65271-80-9
						C ₂₁ H ₃₂ O ₁₀	dihydrophaseic acid 4-O-beta-D-glucoside	-
						C ₁₇ H ₂₈ N ₆ O ₈	His Ser Thr Thr	-
0.8	507254.88	42936	299.8	662.8319	663.8392	-	-	-
							4-Nitroanisole	100-17-4
14.3	246441.39	43072	51.8	152.0352	153.0424	C ₇ H ₇ NO ₃	3-Hydroxy-2-methylpyridine-5-carboxylate	-
							3-Aminosalicylic acid	570-23-0
0.9	319748.34	43795	486.6	466.7626	467.7698	-	-	-
1.1	534437.75	43957	89.8	623.1052	624.1124	-	-	-

0.8	499304.13	44419	33.9	130.9832	131.9904	-	-	-
15.3	259230.97	45194	110.3	197.0201	198.0274	C ₇ H ₆ N ₂ O ₅	DNOC	534-52-1
2.2	61860232	45217	6.7	146.9646	147.9719	-	-	-
13.9	312507.81	45230	41.2	193.0899	194.0972	-	-	-
0.9	388559.91	45290	48	250.8844	251.8917	C ₅ H ₃ Cl ₃ O ₃	3-Chloro-4-(dichloromethyl)-5-hydroxy-2(5H)-furanone	77439-76-0
16	463501.81	45907	84.8	925.5139	926.5212	C ₄₈ H ₇₈ O ₁₇	Oleanolic acid 3-[rhamnosyl-(1->4)-glucosyl-(1->6)-glucoside]	160845-07-8
1.6	340231	46144	54.8	119.035	120.0422	C ₄ H ₈ O ₄	a,b-Dihydroxyisobutyric acid	21620-60-0
							L-Erythrulose	533-50-6
							Gravelliferone	21316-80-3
24.5	1653669.38	46199	41.8	297.1525	298.1597	C ₁₉ H ₂₂ O ₃	5-Hydroxy-7-(4-hydroxyphenyl)-1-phenyl-3-heptanone	83161-96-0
1.1	330355.19	46242	64.4	566.1568	567.164	C ₂₃ H ₂₉ N ₇ O ₆ S	Cys His Ser Trp	-
9.2	760692	47400	57.3	261.0878	262.095	C ₁₂ H ₁₈ O ₄	Tuberonic acid	-
						C ₁₃ H ₁₄ N ₂ O ₄	DMABA NHS ester	58068-85-2

							L-cis-Cyclo(aspartylphenylalanyl)	5262—10-2
							L-Tyrosine methyl ester	1080-06-4
18.3	288027.69	47533	41	194.0821	195.0894	C ₁₀ H ₁₃ NO ₃	O-BENZYL-L-SERINE	4726-96-9
16.7	584861.38	48180	67.5	779.4573	780.4646	C ₄₂ H ₆₈ O ₁₃	Carnosifloside I	109985-90-2
0.8	470703.34	48766	541.8	632.8163	633.8236	-	-	-
						C ₂₃ H ₃₄ N ₄ O ₈ S ₂	Asp Met Met Tyr	-
11.4	342961.78	48824	66.2	593.15	594.1572	C ₂₇ H ₃₀ O ₁₅	Kaempferol 4'-glucoside 7-rhamnoside	205876-37-5
						C ₂₇ H ₃₀ O ₁₅	Pelargonidin 3-galactoside-5-glucoside	-
						C ₃₄ H ₂₆ O ₁₀	Kuwanon Z	104931-21-7
						C ₄ H ₈ N ₄ O ₂	n,n'-dinitrosopiperazine	140-79-4
10.8	294786.59	49172	26.8	179.0346	180.0419		Aspirin	50-78-2
						C ₉ H ₈ O ₄	Monomethyl phthalate	4376-18-5
6.1	409958.59	49692	50.5	343.067	344.0743	C ₁₃ H ₁₆ N ₄ O ₃ S	Mecarbinzid	27386-64-7

						C ₁₄ H ₁₆ O ₁₀	Theogallin	17365-11-6
1.3	561977	50505	33.5	136.991	137.9983	-	-	-
1.5	388622.84	51780	22.6	152.9862	153.9934	C ₄ H ₁₀ S ₃	Methyl propyl trisulfide	17619-36-2
1.2	716561.75	53206	4.4	763.1803	764.1876	C ₃₂ H ₄₀ O ₁₉	Parishin B	-
1.2	438222.13	54064	23.6	152.9861	153.9933	C ₄ H ₁₀ S ₃	Diethyl trisulfide	3600-24-6
0.9	158987.83	54510	6.9	242.9433	243.9506	-	-	-
						C ₂₂ H ₂₉ BrO ₃	9-Bromo-16alpha-methyl-pregn-4-ene-3,11,20-trione	-
6.9	338569.66	55494	15.1	419.119	420.1263	C ₁₇ H ₂₄ O ₁₂	Secogalioside	61774-57-0
						C ₂₈ H ₃₈ N ₈ O ₇	Glu His Lys Trp	-
11.7	755918.13	57364	61.4	633.2558	634.2631	C ₃₂ H ₄₂ O ₁₃	Myricanene B 5-[arabinosyl-(1->6)-glucoside]	-
						C ₁₇ H ₂₄ N ₄ O ₆ S	Ala Cys Gly Tyr	-
7.9	474780	59684	70.3	447.1143	448.1215	C ₁₅ H ₂₄ N ₆ O ₆ S ₂	Cys Cys His Ser	-
0.8	1217572.38	60352	53.3	186.9293	939.7048	-	-	-

10.5	551166.94	61282	126	609.1455	610.1527	C ₂₇ H ₃₀ O ₁₆	6-Hydroxyluteolin 7-rutinoside	-
							Cyanidin 3-galactoside-5-glucoside	-
1.1	680481.81	71165	104.9	341.1083	342.1156	C ₁₁ H ₂₂ N ₄ O ₄ S ₁	Cys Gly Lys	-
						C ₁₂ H ₂₂ O ₁₁	Laminaribiose	34980-39-7
1.2	696425.88	74047	46.9	232.8824	233.8897	-	-	-
10.8	392171.66	74889	98	135.0449	136.0522	C ₈ H ₈ O ₂	p-Anisaldehyde	123-11-5
							m-Methylbenzoate	99-04-7
							Toluate	99-94-5
							Diglycidyl resorcinol ether	101-90-6
							Monoisobutyl phthalic acid	30833-53-5
16.1	879274.63	75277	29.5	795.4518	796.4591	C ₄₂ H ₆₈ O ₁₄	Valeroyl Salicylate	64206-54-8
							Saponin E	85191-73-7
1.5	1282590.75	78237	184.2	194.9966	196.0038	-	-	-

9.5	940937.38	78573	123.4	608.1388	1218.292	C ₂₆ H ₃₁ N ₅ O ₆ S ₂	Cys Cys Trp Tyr	-
1.2	804458.88	78906	229.1	216.9089	217.9162	-	-	-
						C ₉ H ₁₄ O ₉	Monoglyceride citrate	36291-32-4
13.2	514920	80080	69.2	301.0346	302.0419		5,7,8,2',4'-Pentahydroxyisoflavone	-
						C ₁₅ H ₁₀ O ₇	HIERACIN	1621-84-7
7.7	467333.53	82726	116.5	204.03	205.0373	C ₁₀ H ₇ NO ₄	6-Hydroxykynurenate	3778-29-8
							Diisobutyl phthalate	84-69-5
19.8	557210	89117	74.1	277.1442	278.1515	C ₁₆ H ₂₂ O ₄	Phthalic acid Mono-2-ethylhexyl Ester	4376-20-9
0.8	1685086.75	89441	94.1	158.9784	159.9857	C ₇ H ₆ Cl ₂	Benzal chloride	98-87-3
16.5	748531.38	89603	146.7	331.2487	332.256	C ₁₈ H ₃₆ O ₅	9,10,13-Trihydroxystearic acid	50439-74-2
15.1	843483.44	90493	167.9	728.3695	729.3768	-	-	-
1.1	1603897.63	102091	1134.3	1043.304	1044.309	-	-	-
7.7	623711.56	103824	89.5	160.0403	161.0475	C ₉ H ₇ NO ₂	Indole-3-carboxylic acid	771-50-6

							3-Formyl-6-hydroxyindole	192184-71-7
							4,6-Dihydroxyquinoline	3517-61-1
1	838775.88	116146	189	94.981	95.9883	CH ₄ O ₃ S	Methanesulfonic acid	75-75-2
						H ₄ O ₄ Si	Silicic acid	10193-36-9
0.8	1618671.13	117055	199.5	402.9165	403.9238	-	-	-
0.9	928242.5	122026	77.4	232.8805	233.8877	-	-	-
17	956901.25	125479	148.1	259.1008	260.1081	C ₉ H ₂₁ ClN ₂ O ₂	Propamocarb hydrochloride	25606-41-1
						C ₁₅ H ₁₇ ClN ₂	monodesmethyl chlorpheniramine	20619-12-9
0.9	816476.44	131739	186.6	180.9124	181.9197	-	-	-
2.2	2002539.5	142292	206.2	232.9758	233.9831	C ₉ H ₈ Cl ₂ O ₃	2,4-DICHLOROPHENOXYACETIC ACID, METHYL ESTER	1928-38-7
1	1509415.63	172322	508.6	138.9705	139.9777	C ₃ H ₈ S ₃	Methyl (methylthio)methyl disulfide	42474-44-2
10.1	1493113.38	187464	172	213.9635	214.9707	-	-	-
1	1196852	201975	327.5	330.842	331.8493	-	-	-

1.2	1632318.25	204963	383.1	194.9272	195.9345	-	-	-
0.9	2857131	223952	650.2	216.9089	217.9162	-	-	-
13.7	1533941.5	233054	244.6	183.0045	184.0118	C ₆ H ₄ N ₂ O ₅	2,4-DINITROPHENOL	51-28-5
0.8	1693704.63	238214	5293.6	548.8519	549.8592	-	-	-
0.8	3614480.75	244290	2714.3	272.9586	273.9659	C ₅ H ₁₁ AsO ₈	Ribose-1-arsenate	-
19	1963383.38	274462	230.7	313.2382	314.2454	C ₁₈ H ₃₄ O ₄	Dibutyl decanedioate	109-43-3
						C ₁₈ H ₃₄ O ₄	9,10-dihydroxy-12-octadecenoic acid	-
0.8	4227554	299172	44.1	146.9623	147.9695	CH ₅ O ₄ P	Hydroxymethylphosphonate	-
12.3	1785122.63	299711	274.5	138.0195	139.0268	C ₆ H ₅ NO ₃	2-Nitrophenol	88-75-5
						C ₆ H ₅ NO ₃	3-Hydroxypicolinic acid	874-24-8
0.8	3790413.25	322426	1240.5	418.8941	419.9013	C ₂ HF ₃ O ₂	trifluoroacetic acid	76-05-01
0.9	1521580.13	361776	80.7	112.9857	341.9782	-	-	-
1.1	2973463	374516	648.1	503.161	504.1683	C ₁₈ H ₃₂ O ₁₆	alpha-D-Glucopyranosyl-(1->6)-alpha-D-glucopyranosyl-(1->2)-D-glucose	40983-70-8

							MELEZITOSE	597-12-6
						C ₂₃ H ₂₈ N ₄ O ₇ S	Cys Gly Tyr Tyr	-
0.8	1829557.63	500608	11124.6	434.8716	435.8784	-	-	-
						C ₂₂ H ₃₄ N ₄ O ₆ S ₂	Ala Met Met Tyr	-
1.1	4293359	537070	872.4	549.1664	550.1736			
						C ₂₆ H ₃₀ O ₁₃	Liquiritin apioside	74639-14-8
0.8	8038385.5	618817	179.9	174.9559	175.9632	-	-	-
0.8	6274442	629338	275.5	288.9363	289.9435	-	-	-
1.1	12627112	758452	710.1	601.1284	602.1357	C ₂₆ H ₃₀ O ₁₄	5,7,4'-Trihydroxyflavanone 7-O-arabinosylglucoside	-
0.8	9155589	869922	537.9	304.9137	305.921	-	-	-
9.9	7399787.5	952958	2337	689.1019	690.1085	C ₂₇ H ₃₀ O ₁₉ S	Kaempferol 3-(6"-sulfogetiobioside)	-
						C ₁₈ H ₃₂ O ₁₆	beta-D-Galactopyranosyl-(1->4)-beta-D-galactopyranosyl-(1->4)-D-galactose	6118-87-2
1.1	20166640	1088750	5822.9	539.1377	540.145	C ₂₃ H ₂₈ N ₄ O ₇ S	Cys Tyr Gly Tyr	-
						C ₂₅ H ₂₈ O ₁₁	6-Hydroxy-7-methyl-3',4',5'-trimethoxyaurone 4-O-rhamnoside	-

1.2	27482636	2446520	448.9	96.9602	97.9675	H ₂ O ₄ S	Sulfuric acid	7664-93-9
0.9	26792800	3139490	576	96.9602	195.9343	H ₂ O ₄ S	Sulfuric acid	7664-93-9

Table S2. Compounds information of B1 in positive ionization modes.

Retention Time (min)	Area	Intensity	S/N	Max. <i>m/z</i>	Max. MW	Formula	Possible Name	CAS
8.3	281090.4	10010	8.3	167.1069	166.0996	C ₁₀ H ₁₄ O ₂	Karahana lactone	28449-87-8
							1,1-Dimethoxy-2-phenylethane	101-48-4
							2E,6Z,8E-decatrienoic acid	-
							Perillic acid	-
							Rotundifolone	3564-96-3
15.1	95093.03	10023	17.2	577.1337	576.1265	C ₃₀ H ₂₄ O ₁₂	4-n-Butylresorcinol	18979-61-8
							Proanthocyanidin A2	41743-41-3
							Polypropylene glycol (m w 1,200-3,000)	25322-69-4
9.9	96077.87	10038	7.2	580.3539	579.3466	-	-	-

						C ₈ H ₁₂ N ₄	1-(2-Pyrimidyl)piperazine	20980-22-7
7.3	71496.35	10049	8.8	187.0954	186.0881			
						C ₉ H ₁₄ O ₄	cis-2-Carboxycyclohexyl-acetic acid	14715-37-8
0.8	43242.08	10057	223.5	218.4564	217.4491	-	-	-
10.9	87368.41	10067	26	715.3722	716.3794	-	-	-
1.5	62543.61	10086	7.1	846.3075	845.3003	-	-	-
24.2	181549.9	10125	14.2	487.3599	486.3526	C ₂₃ H ₄₆ N ₆ O ₅	Ile Lys Lys Val	-
1.4	157375.2	10138	3.4	84.9597	83.9524	-	-	-
12	49056.62	10144	13.9	142.159	141.1517	C ₉ H ₁₉ N	Methylconiine	35305-13-6
						C ₁₇ H ₂₇ N ₇ O ₆	Ala Ala His Gln	-
8.3	47292.09	10173	19.1	448.1942	447.1869			
						C ₂₄ H ₂₅ N ₅ O ₄	Gly Trp Trp	-
16.3	84020.59	10195	23.8	242.2839	241.2767	C ₁₆ H ₃₅ N	1-Hexadecylamine	143-27-1
0.9	61006.57	10202	113.4	586.8724	585.8651	-	-	-
1.6	61316.15	10229	11.3	221.1194	219.1156	C ₁₃ H ₁₆ O ₃	2-ISOPROPYL-3-METHOXYCINNAMIC ACID	-

							Precocene II	644-06-4
							1-(5-Acetyl-2-hydroxyphenyl)-3-methyl-1-butanone	62458-64-4
1.7	149533.8	10242	4.7	163.0276	164.0349	-	-	-
0.9	63571.98	10246	7.5	179.9812	178.9739	C ₆ H ₄ ClNO ₂	2-Chloronitrobenzene	88-73-3
							Methyl acetyl ricinoleate	140-03-4
24.8	66059.33	10267	10.5	355.2809	354.2737	C ₂₁ H ₃₈ O ₄	1-Linoleoyl Glycerol	-
							PGF2 α Alcohol methyl ether	143656-18-2
15.5	85905.14	10272	18.6	230.2479	229.2406	C ₁₄ H ₃₁ NO	Xestoaminol C	-
							3 Hydroxycoumarin	939-19-5
14.2	66370.13	10305	14.7	163.0391	162.0318	C ₉ H ₆ O ₃	UMBELLIFERONE	93-35-6
						C ₁₉ H ₁₇ NO ₅	20-Hydroxyrutacridone epoxide	80565-10-2
1	201035	10319	5.3	362.0985	720.2273	C ₁₂ H ₁₉ N ₅ O ₄ S ₂	Cys Cys His	-
0.8	169033.9	10337	14.6	275.9879	274.9806	-	-	-

14.2	138121.3	10339	5.5	445.2764	444.2691	C ₁₉ H ₃₆ N ₆ O ₆	Ala Ile Lys Asn	-
						C ₂₇ H ₃₇ FO ₄	AL 8810 isopropyl ester	208114-93-6
							formyl 7-oxo-11E-tetradecenoate	-
							(3beta,9beta)-7-Drimene-3,11,12-triol	101470-79-5
17.4	73908.29	10347	5.3	277.1772	276.17	C ₁₅ H ₂₆ O ₃	cyclandelate	456-59-7
							[6]-Shogaol	555-66-8
							Onchidal	67656-42-2
							Propyl benzoate	2315-68-6
							2,4-Decadiynoic acid	-
8.7	58044.44	10352	9.1	165.0912	164.084	C ₁₀ H ₁₂ O ₂	Isoeugenol	97-54-1
							4-HYDROXYPHENYL-2-BUTANONE	5471-51-2
							4-Isopropylbenzoic acid	536-66-3
							THYMOQUINONE	490-91-5

							4-(3-Hydroxybutyl)-3,3,5-trimethylcyclohexanone	128660-70-8
10.4	51856.93	10352	14.1	213.1851	212.1779	C ₁₃ H ₂₄ O ₂	8E-Undecenyl acetate	-
							2-methylene dodecanoic acid	-
							1-(2-Methoxy-3,4-methylenedioxyphenyl)-1-propanone	-
9.6	83176.97	10381	5.5	209.0788	207.0536	C ₁₁ H ₁₂ O ₄	Benzylsuccinate	-
							Sinapyl aldehyde	4206-58-0
							DIMETHYLCAFFEIC ACID	2316-26-9
0.9	209087.6	10395	115.5	256.8746	767.6077	-	-	-
0.9	94833.36	10397	115.5	514.7538	513.7466	-	-	-
0.9	57539.57	10435	115.9	410.8006	409.7934	-	-	-
11.1	68417.64	10459	116.2	423.2753	844.5361	C ₂₄ H ₃₈ O ₆	3α,7β,12α-Trihydroxy-6-oxo-5α-cholan-24-oic Acid	-
0.8	123809	10461	4.3	334.9157	665.824	-	-	-
22.4	68532.2	10486	9.7	228.2322	227.2249	C ₁₄ H ₂₉ NO	Halaminol A	-

0.7	79027.14	10493	5.1	101.9499	100.9426	-	-	-
0.9	144276	10506	233.5	592.7581	593.7654	-	-	-
1.2	139671.5	10525	10.6	109.0287	540.1093	C ₆ H ₄ O ₂	1,2-Benzoquinone	583-63-1
							2,4-Dimethyl-1,3-dioxolane	3390—12-3
							(S)-2-Methylbutanoic acid	1730-91-2
7.1	49873.18	10528	17.6	103.0755	102.0682	C ₅ H ₁₀ O ₂	3-Hydroxy-2-pentanone	3142-66-3
							Tetrahydro-2-furanmethanol	97-99-4
							Ethyl propionate	105-37-3
10.5	84843.29	10551	13.3	334.0632	666.1118	C ₁₅ H ₁₃ C ₁₂ N ₅	Robenidine	25875-51-8
0.9	97991.41	10559	14.1	398.9874	397.9805	-	-	-
							5,7-Dihydroxy-8-C-(4-hydroxy-3-methyl-2-butenyl)flavanone	-
10.6	73758.81	10563	8.4	341.1389	340.1316	C ₂₀ H ₂₀ O ₅	Glyceollidin I	-
10.9	127426.8	10589	18.9	685.3251	686.3324	C ₂₆ H ₄₈ N ₆ O ₁₅	gamma-L-Glutamyl-butyrosin B	-

19	252403.4	10611	19.6	685.4171	686.4244	-	-	-
18.2	63151.5	10616	36.2	288.253	287.2457	C ₁₆ H ₃₃ NO ₃	Lauroyl diethanolamide	120-40-1
							2,2,6,7-Tetramethylbicyclo[4.3.0]nona-1(9),4-diene-7,8-diol	99901-24-3
13.7	84572.05	10618	5.5	209.1534	208.1461	C ₁₃ H ₂₀ O ₂	(S,E)-Lyratol propanoate	79507-85-0
							Eremopetasinorol	182127-77-1
							4-Heptyloxyphenol	13037-86-0
						C ₁₇ H ₁₈ N ₄ O	Alosetron	122852-42-0
10.8	57440.17	10630	6.9	317.1382	316.1309	C ₁₆ H ₂₂ O ₅	Tocopheronic acid	1948-76-1
							2'-Hydroxy-3',4',6'-trimethoxydihydrochalcone	-
						C ₁₈ H ₂₀ O ₅	EPIAFZELECHIN TRIMETHYL ETHER	-
7.3	42470.1	10669	118.5	179.0914	178.0841	C ₈ H ₁₈ S ₂	Dibutyl disulfide	629-45-8
						C ₇ H ₁₄ O ₅	Digitalose	4481-08-7
0.8	711977.6	10704	118.9	696.7946	2778.177	-	-	-

							Anthranilic acid	118-92-3
1.1	137988.6	10717	10.4	138.0551	137.0478	C ₇ H ₇ NO ₂	Salicylamide	-
15.8	93476.39	10752	16.2	272.2581	271.2508	C ₁₆ H ₃₃ NO ₂	2-aminohexadecanoic acid	7769-79-1
							4E,6E,10Z-Hexadecatrienyl acetate	-
22.1	79745.5	10755	7.6	279.232	278.2248	C ₁₈ H ₃₀ O ₂	estrane-3 α ,17 α -diol	-
							3E,9Z,12Z-octadecatrienoic acid	-
0.9	33919.55	10779	13.3	113.1074	112.1002	C ₆ H ₁₂ N ₂	2-Imino-4-methylpiperidine	165383-72-2
						C ₁₀ H ₁₈ O ₅	3-hydroxy-sebacic acid	-
7.9	107532.5	10779	9.2	241.1054	240.0982		Isopropyl 3-(3,4-dihydroxyphenyl)-2-hydroxypropanoate	-
						C ₁₂ H ₁₆ O ₅	2-Hydroxy-3-(4-methoxyethylphenoxy)-propanoic acid	56392-15-5
22.3	186585.2	10781	17	370.2009	369.1936	C ₂₀ H ₂₉ NO ₄	S-4-benzyl-3-((S)-3-hydroxy-2,2-dimethyloctanoyl)oxazolidin-2-one	-
						C ₂₂ H ₂₇ NO ₄	Corydaline	518-69-4
8.2	73420.05	10782	6.6	155.0706	308.1293	C ₈ H ₁₀ O ₃	Propyl 2-furoate	615-10-1

							Vanillyl alcohol	-
							3,4-Dihydroxyphenyl ethanol	10597-60-1
9.4	101741.4	10790	11.8	492.302	491.2947	C ₂₁ H ₄₁ N ₅ O ₈	N2'-Acetylgentamicin C1a	-
						C ₁₅ H ₁₉ N ₃ O ₂	N-Desmethylzolmitriptan	139264-35-0
7.9	51273.34	10803	19	296.1353	295.128	C ₁₂ H ₁₇ N ₅ O ₄	N6,N6-Dimethyladenosine	-
						C ₉ H ₂₀ S ₂	1,9-Nonanedithiol	3489-28-9
8.7	65742.99	10807	9.1	215.0893	214.0821	C ₈ H ₁₆ O ₅	5(S),6(R)-7-trihydroxymethyl Heptanoate	-
0.6	232824.1	10813	3.6	232.9797	231.9724	-	-	-
17.7	94978.11	10847	9.2	387.1933	386.1867	C ₂₄ H ₂₈ O ₃	3-(1,1-Dimethyl-2-propenyl)-8-(3-methyl-2-butenyl)xanthyletin	30310-55-5
9.2	98150.48	10867	7.6	235.1806	234.1733	C ₁₄ H ₂₂ N ₂ O	Angustifoline	550-43-6
24.1	98008.39	10877	10.7	399.3075	398.3003	C ₂₃ H ₄₂ O ₅	1-Oleoyl-2-acetyl-sn-glycerol	86390-77-4
16.2	120296.8	10931	32	867.4689	866.4616	C ₄₃ H ₇₂ O ₁₆	Cyclopassifloside III	292167-40-9
0.8	274029.1	10953	243.4	367.4204	364.3821	-	-	-

1.5	117348.5	10972	29.2	558.088	557.0807	C ₁₈ H ₂₆ N ₅ O ₈ PS ₂	Lipoyl-AMP	-
1.2	56882.49	11002	19.7	158.9124	157.9051	-	-	-
0.9	147037.4	11003	244.5	598.7173	596.7248	-	-	-
							(S)-2,3-Dihydro-5-hydroxy-2-methyl-1,4-naphthoquinone	76372-21-9
13.7	51604.81	11015	7.2	191.0701	190.0629	C ₁₁ H ₁₀ O ₃	1,2,3,4-Tetrahydro-4-oxo-1-naphthoic acid	-
							HYMECROMONE METHYL ETHER	2555-28-4
0.9	62600.56	11016	122.4	236.9853	235.9801	C ₆ H ₁₁ Cl ₃ O ₃	1,2,3-Tris(chloromethoxy)propane	38571-73-2
1.2	81526.59	11023	10.7	177.9483	176.941	-	-	-
							Salicylic acid beta-D-glucoside	10366-91-3
						C ₁₃ H ₁₆ O ₈	Dimethyl fukiic acid	56158-55-5
8.4	98901.13	11038	13.6	323.0744	322.0672	C ₇ H ₁₇ N ₄ O ₇ P	N1-Amidinostreptamine 6-phosphate	-
						C ₁₅ H ₁₄ O ₈	Elephantorrhizol	-
						C ₁₁ H ₁₈ N ₂ O ₅ S ₂	L-gamma-Glutamyl-S-allylthio-L-cysteine	-

0.9	81103.65	11045	245.4	774.7256	773.7183	-	-	-
0.8	119143.9	11051	11.5	270.9192	269.9119	-	-	-
0.9	83193.62	11053	15.7	452.7333	453.7406	-	-	-
							Ala Ile Asn Asn	-
9.4	88514.95	11087	13	453.2102	452.2183	C ₁₇ H ₃₀ N ₆ O ₇	Ala Glu His Pro	-
						C ₂₄ H ₃₀ F ₂ O ₆	Fluocinolone acetonide	67-73-2
0.8	501795.4	11113	34.9	848.7347	842.7564	-	-	-
0.8	123910.6	11120	16.8	132.9024	129.899	-	-	-
0.8	71757.23	11131	247.4	387.3935	385.3708	C ₂₆ H ₅₂	1-Hexacosene	18835-33-1
							(3-Methylcrotonyl)glycine methyl ester	-
1.5	124214	11145	13.4	172.0973	170.1058	C ₈ H ₁₃ NO ₃	Crotanecine	-
							N-butanoyl-lhomoserine lactone	67605-85-0
9.7	101197.5	11162	7.1	536.3275	535.3202	-	-	-

0.9	97763.93	11209	249.1	650.729	648.7308	-	-	-
0.9	67968.27	11225	4.7	115.9576	114.9503	-	-	-
							Prenylbenzoquinone	5594—02-5
11.2	63389.48	11226	10.5	177.0911	176.0838	C ₁₁ H ₁₂ O ₂	Ethyl cinnamate	103-36-6
							5,6,7,8-tetrahydro-2-Naphthoic Acid	1131-63-1
10.9	74291.96	11251	16.2	710.4166	709.4093	-	-	-
						C ₉ H ₁₆ O ₃	n-heptanoyl acetic acid	-
							Butylparaben	94-26-8
11.6	68583.66	11269	5.2	195.0997	194.0925		2,5-Dimethoxy-4-(2-propenyl)phenol	90377-06-3
						C ₁₁ H ₁₄ O ₃	Zingerone	122-48-5
							ORTHOTHYMOTINIC ACID	-
11.4	331313.6	11289	6.1	309.1674	308.1601	C ₁₂ H ₂₄ N ₂ O ₇	1-[(5-Amino-5-carboxypentyl)amino]-1-deoxyfructose	21291-40-7
22.1	120586.8	11315	12.3	415.209	416.2163	C ₁₈ H ₂₈ N ₆ O ₄	Phe Arg Ala	-

8.8	104408	11333	15.9	275.1464	274.1392	C ₁₇ H ₃₀ N ₆ O ₄ S ₁	Lys Met His	-
						C ₂₄ H ₃₀ O ₆	Eplerenone	107724-20-9
						C ₁₂ H ₂₀ N ₄ O ₂	Hexazinone	51235-04-2
						C ₁₁ H ₂₀ N ₃ O ₅	Lysyl-Glutamate	-
							Dimethyl succinate	106-65-0
0.8	186202.4	11341	11.7	169.0458	168.0386	C ₆ H ₁₀ O ₄	Mevaldate	541-07-1
							3-hydroxy-3-methyl-2-oxo-pentanoic acid	-
2.3	79492.16	11358	6.4	174.1238	173.1166	C ₁₀ H ₁₇ N	AMANTADINE	665-66-7
						C ₇ H ₁₅ N ₃ O ₂	Indospicine	16377-00-7
							Isoprocarb	2631-40-5
15	155090.2	11365	17.7	216.1013	215.094	C ₁₁ H ₁₅ NO ₂	Heliamine	1745-07-9
							SALSOLINE	89-31-6
						C ₁₃ H ₁₃ NO ₂	2-Naphthylalanine	58438-03-2

							Acetyl vitamin K5	523-68-2
						C ₈ H ₁₄ ClN ₅	Atrazine	1912-24-9
14	126412.4	11381	32.9	718.3072	717.2999	-	-	-
							1,3-Diacetoxy-4,6,12-tetradecatriene-8,10-diyne	29576-66-7
						C ₁₈ H ₂₀ O ₄	Toxyl angelate	-
23.9	68746.32	11389	32.8	323.124	322.1168		4'-Hydroxy-5,7-dimethoxy-8-methylflavan	-
						C ₁₅ H ₁₈ N ₂ O ₆	Binapacryl	485-31-4
							2,4,6-Trimethyl-4-phenyl-1,3-dioxane	5182-36-5
13.5	92089.98	11404	9.6	207.1378	206.1305	C ₁₃ H ₁₈ O ₂	xi-8,9-Dehydrotheaspirone	-
							Benzyl hexanoate	6938-45-0
						C ₃₃ H ₅₀ O ₁₀	(23S)-23,25-dihydroxy-24-oxovitamin D3 23-(beta-glucuronide)	-
10.1	133980.8	11405	24.2	629.3354	628.3281	C ₃₀ H ₄₄ N ₈ O ₇	Lys Arg Tyr Tyr	-
1.2	89995.36	11411	18	218.1023	217.0951	C ₁₀ H ₁₁ N ₅ O	Pymetrozine	123312-89-0

						C ₁₀ H ₁₉ NS ₂	1-Isothiocyanato-8-(methylthio)octane	4430-41-5
0.9	54496.37	11422	253.8	730.7439	728.7343	-	-	-
14.5	90613.2	11424	27	797.4679	796.4606	C ₄₂ H ₆₈ O ₁₄	Soyasaponin III	55304-02-4
0.9	51240.41	11469	31.5	258.8992	257.8919	-	-	-
13.8	164484.4	11469	11.6	442.3372	441.3299	C ₂₇ H ₄₁ D ₃ O ₃	(5E)-(24R)-24,25-dihydroxy-[6,19,19-trideutrio]vitamin D3 - (5E)-(24R)-24,25-dihydroxy-[6,19,19-trideutrio]cholecalciferol	-
16	98077.88	11485	23.6	503.7553	1005.496	-	-	-
0.8	84288.89	11507	9	464.875	926.6907	-	-	-
0.9	48884.41	11574	7.1	304.1504	303.1431	C ₁₂ H ₂₁ N ₃ O ₆	Asp Ala Val	-
							Nicotianamine	34441-14-0
0.9	54527.48	11585	15.8	134.9488	669.7029	-	-	-
1.5	97827.66	11648	3.3	125.9863	124.9791	-	-	-
1.9	72898.63	11663	39.6	396.1504	395.1431	C ₁₄ H ₂₃ N ₅ O ₇	Gly Asn Pro Ser	-

14.8	194701.2	11679	14.6	500.3793	499.372	-	-	-
14.2	141152	11712	14.3	619.2753	618.2681	C ₂₄ H ₄₀ N ₁₀ O ₆ S	Cys Arg Arg Tyr	-
						C ₃₂ H ₃₈ N ₆ O ₅ S	Met Pro Trp Trp	-
0.8	117840.9	11717	20	247.9027	246.8954	-	-	-
1.6	121129.7	11770	7.5	160.9894	159.9822	-	-	-
2.8	1926323	11792	3.4	125.9864	124.9791	-	-	-
9.9	49856.4	11809	131.2	143.1177	142.1104	-	-	-
						C ₁₃ H ₂₄ O ₂	Ethyl 10-undecenoate	692-86-4
							Polygodial	6754-20-7
17	84886.02	11809	8.3	235.1689	234.1617	C ₁₅ H ₂₂ O ₂	Alcyopterosins O	-
							Curmadione	-
							Macrophyllic acid A	-
18	79105.98	11820	8.7	337.2356	336.2283	C ₂₀ H ₃₂ O ₄	PGF2 α 1,9-lactone	55314-48-2

							12(S),20-DiHETE	89614-44-8
							15-epi-PGA1	20897-92-1
							3-(5-Methyl-2-furanyl)butanal	31704-80-0
9.3	123785.6	11876	10.9	153.0912	152.0839	C ₉ H ₁₂ O ₂	3-Isopropylcatechol	2138-48-9
							4-hydroxy Nonenal Alkyne	1011268-23-7
							Ethyl 2-furanpropionate	10031-90-0
9.5	69134.85	11892	9.5	169.0863	168.079	C ₉ H ₁₂ O ₃	2,6-Dimethoxy-4-methylphenol	621-23-8
							1,3,5-TRIMETHOXYBENZENE	621-23-8
0.8	90314.45	11895	264.3	229.8927	228.8854	-	-	-
0.8	104083.1	11904	264.5	186.9221	185.9154	-	-	-
0.9	91602.73	11915	132.4	628.7508	627.7435	-	-	-
1.2	76201.09	11941	11.7	188.0924	187.0852	C ₈ H ₁₃ NO ₄	6-Acetamido-3-oxohexanoate	-
0.8	63940.28	12026	133.6	256.42	255.4127	-	-	-

						C ₁₂ H ₂₀ O ₃	12-oxo-10E-dodecenoic acid	-
12.4	247844.2	12039	7.7	235.1311	234.1238	C ₁₄ H ₁₈ O ₃	Dehydrooreadone	124869-07-4
						C ₉ H ₁₈ N ₂ O ₅	2,6-Diamino-7-hydroxy-azelaic acid	-
						C ₁₅ H ₂₆ N ₆ O ₆	Asp Pro Arg	-
9.2	97555.67	12132	7.8	409.1832	408.1732	C ₂₂ H ₂₄ N ₄ O ₄	Gly Phe Trp	-
						C ₂₀ H ₂₈ N ₂ O ₅ S	Tamsulosin	106133-20-4
1.5	62921.05	12146	20.7	160.0609	159.0537	C ₆ H ₉ NO ₄	L-trans-alpha-Amino-2-carboxycyclopropaneacetic acid	117857-93-9
						Ala C _{ys} Gly Tyr	Ala Cys Gly Tyr	-
11.2	68278.24	12169	12.9	435.1283	868.2421	C ₂₁ H ₂₂ O ₁₀	3',5'-Dihydroxy-3,5,6,7,8,4'-hexamethoxyflavone	-
						C ₂₁ H ₂₂ O ₁₀	Naringenin-7-O-Glucoside	529-55-5
1.1	89105.76	12176	5.1	141.9587	140.9515	-	-	-
3.4	77843.02	12176	20.9	235.0493	234.042	C ₁₂ H ₈ N ₂ O ₂	Isophenoxazine	-
0.9	83241.98	12179	17.6	284.8895	283.8822	-	-	-

19.4	275683.9	12186	21.2	330.3365	329.3292	C ₂₀ H ₄₃ NO ₂	N,N-dimethyl-Safingol	-
							Yucalexin A19	119642-83-0
24.8	165143.6	12190	10.5	319.2263	316.2034	C ₂₀ H ₃₀ O ₃	Oxymesterone	145-12-0
							8(9)-EpETE	851378-93-3
						C ₁₃ H ₂₂ O	beta-Ionol	22029-76-1
							4-(3-Hydroxybutyl)-3,3,5-trimethylcyclohexanone	128660-70-8
9.4	56776.48	12199	13.9	213.1849	212.1776	C ₁₃ H ₂₄ O ₂	10-Undecenyl acetate	112-19-6
							2-methylene dodecanoic acid	-
10.4	57037.92	12214	16.4	195.1744	194.1672	-	-	-
10.7	181840.6	12218	22.8	359.7139	716.3559	-	-	-
8.3	71509.84	12224	20.5	774.3655	773.3582	-	-	-
						C ₉ H ₉ N ₅ O	(5-Phenyl-1,2,4-triazol-3-yl)urea	6642-32-6
1	117244.9	12231	15.1	204.0872	812.3212	C ₉ H ₁₇ NS ₂	1-Isothiocyanato-7-(methylthio)heptane	4430-38-0

							Methyl 3-phenylpropanoate	103-25-3
							Dihydrosafrole	94-58-6
8.6	66418.45	12262	10.8	165.0912	164.0839	C ₁₀ H ₁₂ O ₂	4-HYDROXYPHENYL-2-BUTANONE	5471-51-2
							4-Isopropylbenzoic acid	536-66-3
							THYMOQUINONE	490-91-5
0.8	564685.8	12268	30.5	466.8457	931.6768	-	-	-
0.4	356891.6	12274	7.8	97.9688	95.9539	-	-	-
1.8	77235.63	12288	16.1	224.0588	223.0515	-	-	-
							Rhein-9-anthrone	480-09-1
							Purpurin 1-methyl ether	94099-66-8
14.2	71595.26	12308	273.5	271.0602	270.0529	C ₁₅ H ₁₀ O ₅	Lucidin	478-08-0
							Emodin	518-82-1
0.7	162490.4	12328	9.5	194.9995	191.9946	-	-	-

0.7	146650.8	12328	9.5	194.9995	969.9675	-	-	-
1.3	156656.1	12328	2.1	90.526	447.5951	-	-	-
0.8	1365776	12339	6.3	688.7985	2759.223	-	-	-
							L-Cyclo(alanylglycyl)	4526-77-6
1.5	60657.81	12339	274.2	129.0649	127.0643	C ₅ H ₈ N ₂ O ₂	Squamolone	40451-67-0
							4-amino-4-cyano-butanoic acid	-
							2-(Methoxymethyl)furan	13679-46-4
6.2	84884.88	12340	10.6	113.0597	112.0525	C ₆ H ₈ O ₂	Cyclohexane-1,3-dione	504-02-9
							Sorbic acid	-
9.4	148064.2	12364	13	497.2576	496.2503	C ₁₉ H ₃₂ N ₁₀ O ₆	Ala Arg Asn His	-
						C ₂₂ H ₃₆ N ₆ O ₅ S	His Ile Met Pro	-
18.4	306142.2	12385	33.1	737.5009	736.4936	-	-	-
13	111047.8	12388	14.8	427.1609	425.1675	C ₁₉ H ₂₄ N ₄ O ₆	Ala Trp Glu	-

						C ₁₈ H ₂₆ N ₄ O ₆ S	Ala Ala Cys Tyr	-
						C ₂₀ H ₂₆ O ₁₀	6-(2-Carboxyethyl)-7-hydroxy-2,2-dimethyl-4-chromanone glucoside	-
						C ₁₆ H ₂₃ N ₃ O ₅	Ala Phe Thr	-
1.1	98968.36	12424	20.7	360.1496	359.1423	C ₁₆ H ₂₀ F ₃ N ₃ O ₃	TPPU	1222780-33-7
						C ₂₂ H ₄₂ N ₆ O ₆ S	Ile Lys Met Gln	-
9.7	127276.5	12432	15	541.2827	540.2754	C ₂₁ H ₃₆ N ₁₀ O ₇	Gln His Arg Thr	-
						C ₂₄ H ₄₀ N ₆ O ₆ S	Cys Lys Lys Tyr	-
1.9	278187.2	12446	35	417.0794	416.0654	C ₁₈ H ₁₈ O ₁₀	9-Hydroxy-4-methoxypsoralen 9-glucoside	115356-06-4
						C ₉ H ₁₂	Cumene	98-82-8
1	186189.7	12460	4.6	143.0817	141.0793		PIRACETAM	7491-74-9
						C ₆ H ₁₀ N ₂ O ₂	Ectoine	96702-03-3
							Tetrahydrofurfuryl propionate	637-65-0
8.3	121034	12500	5.2	181.0837	180.0765	C ₈ H ₁₄ O ₃	3-Oxovalproic acid	60113-81-7

1.1	164891.8	12534	31.8	573.1503	1144.286	C ₂₄ H ₃₀ N ₄ O ₇ S ₂	Cys Cys Tyr Tyr	-
							Citraconic acid dimethyl ester	-
1.1	178386.8	12535	3.8	159.0665	158.0592	C ₇ H ₁₀ O ₄	Succinylacetone	51568-18-4
							2-Isopropylmaleate	44976-69-4
							Laurencione monoacetate	-
							Isobutyric acid	79-31-2
11.2	113802.3	12567	21.2	89.0598	88.0525	C ₄ H ₈ O ₂	1,4-Dioxane	123-91-1
							Ethyl acetate	141-78-6
1.5	73303.71	12568	20.6	148.0969	147.0896	C ₆ H ₁₃ NO ₃	4-Hydroxyisoleucine	55399-93-4
							Fagomine	53185-12-9
							(E,E)-Boviquinone 3	34198-83-9
24.5	127235.6	12592	16	367.1885	366.1812	C ₂₁ H ₂₈ O ₄	Bisphenol A bis(2-hydroxypropyl) ether	116-37-0
							Formebolone	2454-11-7

						C ₁₈ H ₂₆ N ₂ O ₆	Bufotenine O-glucoside	64656-15-1
9	67209.01	12601	5.8	195.0938	194.0865	C ₁₀ H ₁₄ N ₂ S	Methiuron	21540-35-2
							Acamelin	74161-27-6
11.4	58583.91	12608	12.4	193.0497	192.0424	C ₁₀ H ₈ O ₄	4-METHYLDAPHNETIN	2107-77-9
						C ₂₆ H ₄₂ N ₈ O ₆	Phe Ile Gln Arg	-
9.9	145543.8	12628	13.8	585.3095	584.3022	C ₃₃ H ₄₄ O ₉	Euphornin	80454-47-3
						C ₁₇ H ₁₈ N ₄ O	Alosetron	122852-42-0
17.1	66244.63	12635	8.2	317.1355	316.1282	C ₁₆ H ₂₂ O ₅	Tocopheronic acid	1948-76-1
						C ₁₈ H ₂₀ O ₅	Combrestatin A4	117048-59-6
							Acetal R	7493-57-4
10.8	67369.23	12648	6.5	209.1537	208.1464	C ₁₃ H ₂₀ O ₂	(S,E)-Lyratol propanoate	79507-85-0
							4-Heptyloxyphenol	13037-86-0
8.4	111516.7	12664	9	321.1307	320.1201	C ₁₅ H ₂₂ O ₆	Sesamex	51-14-9

						C ₁₂ H ₂₀ N ₂ O ₈	D-Fructosazine	13185-73-4
							Isomugineic acid	74281-81-5
14.1	121600.4	12719	20.4	682.3447	679.3201	C ₃₄ H ₄₅ N ₉ O ₅	Ile Arg Trp Trp	-
0.9	94692.34	12752	141.7	414.7799	415.7872	-	-	-
						C ₄₃ H ₈₄ O ₁₆ P ₂	PIP(16:0-18:0)	-
14.7	176420.8	12794	24.8	941.5083	940.5015	C ₄₈ H ₇₆ O ₁₈	Colubrin	87834-09-1
						C ₂₁ H ₃₂ N ₄ O ₇	Ala Ile Tyr Ser	-
						C ₂₀ H ₃₂ N ₆ O ₄ S ₁	Phe Arg Met	-
9.1	163754.4	12799	15	453.2305	452.2233		Amoradinin	-
						C ₂₇ H ₃₂ O ₆	DEOXYANDIROBIN	-
11.2	65134.84	12803	21.2	511.1789	510.1716	C ₁₉ H ₃₂ N ₆ O ₅ S ₂	Ala His Met Met	-
10.5	74206.6	12810	11.8	592.3176	591.3104	C ₃₂ H ₄₁ N ₅ O ₆	Nummularine B	53947-96-9
1.7	58415.94	12811	12.5	138.0549	137.0477	C ₇ H ₇ NO ₂	2-Pyridylacetic acid	13115-43-0

							Anthranilic acid	118-92-3
							Methyl nicotinate	93-60-7
							3-Nitrotoluene	1999-08-1
							Eremopetasinorol	182127-77-1
12.8	81175.07	12822	6.6	209.1537	208.1465	C ₁₃ H ₂₀ O ₂	(S,E)-Lyratol propanoate	79507-85-0
							4-Heptyloxyphenol	13037-86-0
							2-(Ethoxymethyl)furan	6270-56-0
							3,4-Dimethyl-1,2-cyclopentanedione	13494-06-9
7.5	55338.92	12840	11.1	127.0756	126.0683	C ₇ H ₁₀ O ₂	Methyl sorbate	689-89-4
							1-Cyclohexenecarboxylic acid	636-82-8
0.7	160030.5	12851	8.1	179.0226	178.0153	C ₈ H ₉ ClO	chloroxylenol	88-04-0
							METHACHOLINE	62-51-1
1.5	46423.75	12880	4.6	160.1334	159.1261	C ₈ H ₁₇ NO ₂	3-amino-octanoic acid	-

							Isobutyl 2-furanpropionate	105-01-1
10.7	66103.97	12888	11.8	197.1173	196.11	C ₁₁ H ₁₆ O ₃	Hexyl 2-furoate	39251-86-0
							2,6-Dimethoxy-4-propylphenol	6766-82-1
12.1	257533	12944	12.5	441.2014	440.1946	C ₂₄ H ₃₁ FO ₅	Descinolone acetonide	2135-14-0
						C ₁₉ H ₂₈ N ₄ O ₈	Ala Ser Thr Tyr	-
11.3	611908.8	12962	11.7	450.2446	898.4746	C ₂₀ H ₃₁ N ₇ O ₅	Ala Phe Gly Arg	-
16.7	218822	12970	27.4	803.4536	804.4608	C ₄₂ H ₆₈ O ₁₃	Carnosifloside I	109985-90-2
8.4	123666.9	13076	13.6	365.1783	364.171	C ₁₇ H ₂₄ N ₄ O ₅	Ala Ala Phe Gly	-
						C ₂₃ H ₂₄ O ₄	Bisphenol A dimethacrylate	3253-39-2
24.5	1363272	13084	9.2	172.9813	171.974	-	-	-
							3-Propyl-1,2-cyclopentanedione	25684-04-2
1.5	89491.8	13096	31	303.1552	302.1479	C ₁₆ H ₂₄ O ₄	3,4-Epoxy-6-methylcyclohexylmethyl-3,4-epoxy-6-methylcyclo-hexanecarboxylate	141-37-7
						C ₁₁ H ₂₀ N ₅ O ₅	Arginyl-Glutamate	-

						C ₁₉ H ₂₈ N ₄ O ₆	Ala Ala Phe Thr	-
8.8	122437.1	13134	10.7	409.2042	408.1969		(E)-2'-Geranyl-3',4',7-trihydroxyflavanone	113866-90-3
						C ₂₅ H ₂₈ O ₅	2-Prenyl-6a-hydroxyphaseollidin	-
11.5	157707.8	13153	36	491.792	985.5986	-	-	-
						C ₁₂ H ₁₅ C ₁₂ NO ₂	Phenylacetic mustard	10477-72-2
21.7	187630	13179	26	276.0529	275.0457		L-Tyrosine methyl ester 4-sulfate	-
						C ₁₀ H ₁₃ NO ₆ S		
							Valyl-Histidine	-
						C ₁₁ H ₁₈ N ₄ O ₃		
7.2	153600.6	13184	18.8	277.1261	276.1245		Homoanserine	20314-38-9
						C ₁₂ H ₂₀ O ₇	Triethyl citrate	77-93-0
							Cycloionone	5552-30-7
							4-(4-Methyl-3-pentenyl)-3-cyclohexene-1-carboxaldehyde	37677-14-8
10.7	85488.59	13242	8.5	193.1589	192.1516	C ₁₃ H ₂₀ O		
							4-n-Heptylphenol	1987-50-4
							alpha-Ionone	127-41-3

1.1	165858.4	13265	23.6	259.0813	258.074	C ₁₀ H ₁₂ N ₄ O ₃	Didanosine	69655-05-6
5.6	83924.35	13266	7.6	157.0836	156.0763	C ₆ H ₁₄ O ₃	Polypropylene glycol (m w 1,200-3,000)	25322-69-4
15.1	81117.12	13280	35.6	370.6727	739.3308	-	-	-
1	384111	13301	21	160.0969	159.0905	C ₇ H ₁₃ NO ₃	Acetyl-DL-Valine	3067-19-4
23.1	6493397	13306	7.6	126.9667	123.957	-	-	-
0.9	42708.01	13335	296.3	514.813	513.8057	-	-	-
0.9	97089.51	13335	296.3	582.7417	583.749	-	-	-
23.5	3538205	13345	7	133.9739	132.9667	C ₃ H ₃ NOS ₂	Rhodanine	141-84-4
							5-Hydroxymethyl-2-furaldehyde	67-47-0
7.8	75134.34	13410	12.8	127.0391	126.0319	C ₆ H ₆ O ₃	1,2,3-Trihydroxybenzene	87-66-1
							4-HYDROXY-6-METHYLPYRAN-2-ONE	675-10-5
1.1	189864.1	13415	11.7	233.1242	231.114	C ₁₁ H ₁₈ N ₂ O ₂	L,L-Cyclo(leucylprolyl)	2873-36-1
						C ₈ H ₁₆ N ₄ O ₄	L-Acetopine	18416-86-9

15.4	107463.4	13453	11.4	283.1812	282.1739	C ₁₈ H ₂₂ N ₂ O	2-Hydroxydesmethylimipramine	1977-15-7
							Furfuryl isovalerate	13678-60-9
							3,4,5-Trimethoxytoluene	6443-69-2
7.9	94418.63	13508	10.2	183.1014	182.0941	C ₁₀ H ₁₄ O ₃	2-Oxo-delta3-4,5,5-trimethylcyclopentenyacetate	1130-49-0
							MEPHENESIN	59-47-2
11.5	79093.67	13671	151.9	241.0684	240.0611	C ₉ H ₁₄ O ₆	Triacetin	102-76-1
						C ₁₃ H ₁₃ P	Diphenylmethylphosphine	1486-28-8
19.1	95186.13	13674	20.8	223.0642	222.0569	C ₉ H ₁₈ S ₃	1-(1-Propenylthio)propyl propyl disulfide	143193-11-7
17.9	93950.63	13720	14.3	315.1205	314.1132	C ₁₄ H ₁₄ N ₆ O ₃	Dihydropteroic acid	-
10.7	111791.6	13746	26.3	641.2988	642.3061	-	-	-
						C ₁₇ H ₂₄ N ₄ O ₆ S	Ala Cys Gly Tyr	-
11.9	73593.35	13778	12.9	435.1285	434.1213		3',5'-Dihydroxy-3,5,6,7,8,4'-hexamethoxyflavone	-
						C ₂₁ H ₂₂ O ₁₀	Naringenin-7-O-Glucoside	529-55-5

0.8	191690.6	13790	12.3	200.9731	199.9665	-	-	-
3.5	155614.4	13793	13.8	187.0582	186.0509	C ₇ H ₁₆ S ₂	Butyl isopropyl disulfide	72437-53-7
						C ₆ H ₁₂ O ₅	2-Deoxy-D-galactose	1949-89-9
12.1	72448.22	13810	12.8	191.1066	190.0993	C ₁₂ H ₁₄ O ₂	1-(4-Methoxyphenyl)-1-penten-3-one	104-27-8
							Precocene I	17598-02-6
							Ascariadole epoxide	-
10.8	54935.93	13843	5.9	185.117	184.1097	C ₁₀ H ₁₆ O ₃	1-Acetylcyclohexyl acetate	52789-73-8
							(1'R)-Nepetalic acid	21651-54-7
1	136209.6	13861	35.4	683.101	682.0948	-	-	-
0.9	44521.92	13875	308.3	566.7803	565.773	-	-	-
1.1	211633.6	13878	8.3	200.0448	398.0755	-	-	-
21.7	158557.4	13894	19.6	297.0644	298.0717	C ₁₆ H ₁₅ C _l O ₂	PDM 11	-
11.5	194345.4	13913	20.1	472.2879	942.5621	C ₂₀ H ₃₇ N ₇ O ₆	Ile Pro Arg Ser	-

							Furfuryl pentanoate	36701-01-6
							3,4,5-Trimethoxytoluene	6443-69-2
10.1	148922.9	13915	10.5	183.1015	182.0942	C ₁₀ H ₁₄ O ₃	MEPHENESIN	59-47-2
							5-oxo-7-decynoic acid	-
23.4	2885956	13922	21	154.9667	152.9518	C ₂ C ₁ F ₅	Chloropentafluoroethane	76-15-3
12.4	106627.3	13943	36.3	172.0161	171.0088	-	-	-
0.7	250595.8	13948	28.2	133.0344	129.9944	-	-	-
							17beta-Hydroxy-17-methylandrosta-4,9(11)-dien-3-one	1039-17-4
23.6	87476.82	13990	15.5	301.2163	300.209	C ₂₀ H ₂₈ O ₂	8,11,14-Eicosatetraynoic acid	34262-64-1
0.8	73691.19	14012	311.4	478.8284	476.8066	-	-	-
10	176267	14055	27.8	787.2292	786.2222	C ₃₄ H ₄₂ O ₂₁	Peonidin 3-sophoroside-5-glucoside	-
15.6	171181.3	14086	26	500.2456	998.4767	C ₂₀ H ₃₃ N ₇ O ₈	Asp His Lys Thr	-
0.9	82318.99	14152	6.5	436.7611	435.7544	-	-	-

0.8	10163672	14188	10.8	752.7537	2261.283	-	-	-
1	240502.7	14206	7.5	167.0525	330.0845	C ₄ H ₈ N ₄ O ₂	n,n'-dinitrosopiperazine	140-79-4
1.5	56870.84	14212	13.5	114.0552	113.048	C ₅ H ₇ NO ₂	DL-Propargylglycine	-
18.1	100232.6	14220	10.5	337.2352	336.2279	C ₂₀ H ₃₂ O ₄	15-epi-PGA1	20897-92-1
16.7	123720.7	14225	22.1	425.3773	424.3701	C ₂₈ H ₅₀ O	Campestanol	474-60-2
						C ₃₀ H ₄₈ O	Glutinine	-
12.4	855783.1	14232	13.8	441.2018	440.1992	C ₁₉ H ₂₈ N ₄ O ₈	Ala Ser Thr Tyr	-
8.5	114276.2	14242	32.7	174.1854	173.1781	-	-	-
0.9	51028.29	14268	317.1	446.7667	447.7739	-	-	-
4.5	100103.5	14278	8.9	100.076	99.0687	C ₅ H ₉ NO	N-Methyl-2-pyrrolidinone	872-50-4
							1-Pyrrolidinecarboxaldehyde	3760-54-1
1	142097.1	14319	159.1	525.0794	524.0722	C ₂₇ H ₁₈ O ₁₀	Garcidul B	176257-86-6
15.5	73157.41	14331	318.5	207.0442	206.0369	C ₉ H ₁₂ O ₂ S	(+--)-3-[(2-methyl-3-furyl)thio]-2-butanone	-

11.2	215631.1	14354	24.2	481.1684	480.1611	C ₁₇ H ₂₆ N ₆ O ₉	Asp Asn Asn Pro	-
							D-(+)-3-Phenyllactic acid	-
3.4	100879	14366	21.5	189.0526	188.0453	C ₉ H ₁₀ O ₃	o-VERATRALDEHYDE	-
							MANDELIC ACID, METHYL ESTER	10606-72-1
							1-Ethyl-1H-pyrrole-2-carboxaldehyde	2167-14-8
							2-Propionylpyrrole	-
1.5	324152.9	14369	13	124.0759	123.0686	C ₇ H ₉ NO	ortho-Anisidine	90-04-0
							4-Amino-o-cresol	2835-96-3
0.9	86577.44	14402	160	312.8376	623.6704	-	-	-
0.8	148516.5	14404	6.3	277.9475	276.9403	-	-	-
0.8	139248.8	14416	160.2	350.8317	349.8244	C ₆ H ₄ C ₁₆ O ₄	TCA-ethadyl	2514-53-6
						C ₁₉ H ₂₆	18-Nor-4(19),8,11,13-abietatetraene	C19H26
11.3	255358.6	14427	7.3	277.1907	274.166	C ₁₆ H ₂₄ N ₂ O ₂	Noralfentanil, Norsufentanil	61086-18-8

13.9	208924.9	14454	22.4	684.3233	683.316	C ₂₈ H ₄₉ N ₃ O ₁₆	Chitin	-
0.5	497026.8	14461	5	113.9638	112.9566	-	-	-
0.8	140224.2	14467	31.7	190.0021	188.9948	-	-	-
1.6	94297.65	14469	20.1	132.0808	131.0735	C ₉ H ₉ N	Tolylacetonitrile	22364-68-7
1.6	151745.4	14477	21.9	100.9911	99.9838	-	-	-
1.1	55527.63	14479	5.4	247.0583	246.051	C ₁₁ H ₁₂ O ₅	Sinapic acid	530-59-6
							HAEMATOMMIC ACID, ETHYL ESTER	39503-14-5
							ISOPIMPINELLIN	482-27-9
							Phosphatidyl glycerol	61468-73-3
							8,8-Diethoxy-2,6-dimethyl-2-octanol	7779-94-4
20.2	523537	14510	13.1	269.2109	268.2039	C ₁₄ H ₃₀ O ₃		
21.7	132803.4	14543	30.6	381.1215	379.0942	C ₁₆ H ₂₈ O ₃	Methoprene acid	53092-52-7
						C ₁₉ H ₂₂ N ₂ O ₃ S	Deacetyl-N-monodemethyldiltiazem	86408-44-8
						C ₂₃ H ₂₁ ClO ₃	CHLOROTRIANISENE	569-57-3

0.8	363553.2	14552	161.7	310.4316	616.816	-	-	-
1.1	174631.1	14565	19.8	857.2605	1712.507	C ₄₀ H ₄₄ N ₂ O ₁₉	7-Hydroxylpradimicin A	-
21.9	474073.9	14620	10	297.2424	296.2353	C ₁₈ H ₃₂ O ₃	(±)9-HODE	98524-19-7
							N-(Acetyloxy)benzenamine	71825-04-2
3.5	140374.6	14691	10.9	152.0708	151.0635	C ₈ H ₉ NO ₂	Dopamine quinone	50673-96-6
							2-Phenylglycine	2835-06-5
1.6	78468.91	14738	163.8	365.138	364.1307	C ₂₀ H ₂₂ O ₅	Hydroxygaleon	61576-09-8
						C ₂₂ H ₂₀ O ₅	Carpachromene dimethyl ether	-
2	809908.6	14739	10.4	191.023	190.0157	-	-	-
0.8	303434.3	14755	44	432.8979	430.8762	-	-	-
							(R)-Bitalin A	35844-67-8
12.2	113781.3	14827	11.6	219.1012	218.0939	C ₁₃ H ₁₄ O ₃	EUPATORIOCHROMENE	19013-03-7
13.3	181159.2	14848	43.3	959.5187	958.512	C ₄₈ H ₇₈ O ₁₉	Asiaticoside	16830-15-2

9.4	111777.4	14867	20	629.1274	1256.24	-	-	-	
21.8	105425.5	14888	27.6	579.2928	578.2855	C ₂₅ H ₃₈ N ₈ O ₈	Glu Phe Gln Arg	-	
10.6	122461.1	14914	22.4	340.1782	678.3418	C ₂₀ H ₂₈ C _l N	terodiline hydrochloride	7082-21-5	
24.3	262576.9	14932	14	443.3339	442.3266	C ₃₂ H ₄₂ O	(all-E)-6'-Apo-γ-caroten-6'-al	22255-36-3	
1.1	157534.8	14962	7.5	687.2114	1372.408	-	-	-	
21.7	88702.91	14989	19.7	437.2089	872.4032	C ₁₇ H ₃₂ N ₄ O ₇ S	Cys Ile Thr Thr	-	
0.8	153781.9	15000	6.1	498.8656	497.8605	-	-	-	
1.7	142794.1	15012	22.6	277.0847	275.0832	C ₁₆ H ₁₄ O ₃	Ketoprofen	22071-15-4	
							3,6-Dimethoxy-4-phenanthrenol	481-81-2	
							6-Methoxyflavanone	3034-04-6	
							OBTUSAQUINONE	21105-15-7	
							C ₁₅ H ₁₃ FO ₄	3',4'-dihydroxyflurbiprofen	66067-41-2
							C ₁₂ H ₁₈ C ₁₂ N ₂ O	Clenbuterol	37148-27-9

0.8	96866.46	15030	334	404.8635	403.8652	-	-	-
0.8	366420.8	15112	21.3	403.9112	400.8592	-	-	-
23.2	3156298	15182	10.8	160.9492	159.9419	-	-	-
6.8	254618.6	15213	3.5	245.0635	244.0592	C ₈ H ₁₄ O ₇	Ethyl glucuronide	17685-04-0
						C ₁₀ H ₁₂ O ₇	1-O-Galloylglycerol	-
1.5	159774.6	15257	14.9	188.098	185.1059	-	-	-
0.7	86519.7	15274	6.3	176.9887	175.9814	-	-	-
11	98017.64	15307	170.1	789.4449	788.4376	C ₄₁ H ₆₆ O ₁₃	Tautomycin	109946-35-2
							4-tert-Octylphenol	140-66-9
1.1	74579.81	15316	15.8	229.1547	228.1475	C ₁₄ H ₂₂ O	(+)-trans-alpha-Irone	35124-14-2
						C ₁₁ H ₂₀ N ₂ O ₃	L-isoleucyl-L-proline	-
6.7	123558.3	15344	12.9	182.9876	181.9803	-	-	-
0.8	369573	15355	24.4	409.8548	817.695	-	-	-

19	765541.7	15368	16.6	371.2113	370.204	-	-	-
							8H-1,3-Dioxolo[4,5-h][1]benzopyran-8-one	4361-93-7
8.9	94780.57	15380	17.1	191.0341	190.0268	C ₁₀ H ₆ O ₄	Coumarin-4-carboxylic acid	27393-46-0
							3,5-Dihydroxy-1,4-naphthoquinone	-
0.9	96404.17	15386	171	146.9754	145.9682	C ₆ H ₄ Cl ₂	PARADICHLOROBENZENE	106-46-7
1	199228.8	15392	22.3	679.0504	678.0426	-	-	-
						C ₆ H ₁₀ O ₃ S	1,2-Dihydroxy-3-keto-5-methylthiopentene	746507-19-7
0.8	189761.7	15400	5	185.0232	184.016	C ₅ H ₁₀ C ₁₂ N ₂ O	N,N'-bis(2-chloroethyl)- Urea (Carmustine Metabolite)	2214-72-4
10.7	96848.41	15454	34.5	666.3905	665.3833	-	-	-
0.8	186211.1	15465	11.5	366.8772	364.8591	-	-	-
0.9	120583.6	15499	16.2	155.9806	309.9467	-	-	-
16.5	100814.9	15511	16.2	204.1193	406.224	-	-	-
1.1	195579.4	15523	19.2	97.0284	96.0211	C ₃ H ₄ O ₂	Protoanemonin	108-28-1

19	92636.88	15577	34.2	332.2793	331.2721	-	-	-
							Diisopropyl phthalate	605-45-8
18.4	118363.9	15586	13.4	251.1277	250.1205	C ₁₄ H ₁₈ O ₄	Ubiquinone-1	605-45-8
							δ-CEHC	1221504-67-1
0.8	51964.07	15587	3.9	274.4304	273.4231	-	-	-
13.1	178964.1	15640	13.7	387.2348	386.2275	C ₂₀ H ₃₄ O ₇	Oleandolide	-
0.8	183099.5	15691	4.2	252.9713	251.9641	CH ₃ C ₁ H _g	Methylmercury chloride	115-09-3
							Etrogol	119417-97-9
							2,4,6-Trimethyl-4-phenyl-1,3-dioxane	5182-36-5
10.2	126385.8	15776	9.1	207.1382	206.131	C ₁₃ H ₁₈ O ₂	Benzyl hexanoate	6938-45-0
							Eremopetasinorone A	182127-76-0
2.4	90246.83	15788	16.9	233.0998	232.0925	C ₁₀ H ₁₆ O ₆	Glycerol 1-propanoate diacetate	36600-62-1
17.4	119775.8	15790	15.3	258.5808	515.147	-	-	-

12	110416.1	15791	20.4	631.3826	630.3753	C ₃₄ H ₅₆ O ₉	Torvoside G	184777-22-8
						C ₃₆ H ₅₄ O ₉	2,3,23-Triacetylsericic acid	58096-15-4
11	146450.9	15792	24.2	605.2596	602.2371	C ₃₂ H ₃₆ N ₄ O ₈	Glu Phe Phe Tyr	-
						C ₃₁ H ₄₀ O ₁₂	6-Hydroxysandoricin	133585-56-5
24.8	98020.02	15797	11.1	351.216	350.2087	C ₂₀ H ₃₀ O ₅	15-keto-Prostaglandin E2	26441-05-4
							PGD3	71902-47-1
6.2	108000.2	15828	13.2	141.0547	140.0475	C ₇ H ₈ O ₃	Furfuryl acetate	623-17-6
							2-METHOXYRESORCINOL	29267-67-2
23.3	145151.5	15858	7.5	328.2846	327.2778	C ₁₉ H ₃₇ NO ₃	N-palmitoyl alanine	-
21	147167.7	15913	14.3	399.2507	398.244	C ₂₅ H ₃₄ O ₄	17-Propylestra-1,3,5(10)-triene-3,17beta-diol diacetate	-
						C ₁₈ H ₃₉ O ₇ P	Tris(butoxyethyl)phosphate	78-51-3
23.3	3191216	15916	10.3	138.9797	137.9724	-	-	-
21.8	107444.7	15964	43.9	658.2531	657.2458	C ₃₂ H ₃₇ N ₅ O ₉	Gln Tyr Tyr Tyr	-

23.1	4319217	15969	11.8	178.9595	177.9522	-	-	-
21.8	161731	15993	43.2	398.1121	397.1048	C ₁₅ H ₁₉ N ₅ O ₆ S	S-Adenosyl-4-methylthio-2-oxobutanoate	22365-11-3
10.7	140693.9	16027	16.5	671.346	672.3533	-	-	-
0.9	63799.84	16039	57.5	576.7842	575.7769	-	-	-
9.9	100830.4	16049	16.8	565.1551	564.1478	C ₂₂ H ₃₀ N ₄ O ₁₀ S	Cys Glu Glu Tyr	-
						C ₂₆ H ₂₈ O ₁₄	Kaempferol 3-rhamnoside 7-xyloside	132618-21-4
17.5	655447.2	16128	23.5	679.4595	680.4668	C ₃₅ H ₆₇ O ₁₀ P	PG(12:0-17:1(9Z))	-
6.9	115368	16133	15.4	127.0391	126.0318	C ₆ H ₆ O ₃	5-Hydroxymethyl-2-furaldehyde	67-47-0
							1,2,3-Trihydroxybenzene	87-66-1
0.9	190458.3	16146	42.8	324.8826	651.7798	-	-	-
2	623405	16310	12.4	107.0704	106.0632	C ₄ H ₁₀ O ₃	Diethylene glycol	111-46-6
0.9	112248.6	16354	21.5	274.8808	547.7424	-	-	-
11.1	118054	16417	182.4	428.2308	854.4471	C ₁₇ H ₃₅ N ₅ O ₄ S ₁	Met Lys Lys	-

14.6	193107.2	16428	36.5	698.3389	697.3316	-	-	-
22.1	171822.3	16524	8.2	149.0233	148.0161	-	-	-
12.3	134188.2	16546	29.1	571.2398	570.2325	C ₂₈ H ₃₄ N ₄ O ₉	Glu Glu Phe Phe	-
0.8	542694.6	16557	22	420.8906	838.7426	-	-	-
24	141689	16565	15.5	482.4043	481.397	-	-	-
1.2	94605.48	16573	26.8	174.8865	173.8792	-	-	-
						C ₁₇ H ₂₄ N ₄ O ₆ S	Ala Cys Tyr Gly	-
11.4	210593.8	16588	17.5	435.129	434.122		3',5'-Dihydroxy-3,5,6,7,8,4'-hexamethoxyflavone	-
						C ₂₁ H ₂₂ O ₁₀		
							Naringenin-7-O-Glucoside	529-55-5
						C ₁₅ H ₁₈ O ₅	Marasmone	122458-04-2
9.5	90600.46	16595	11.3	279.1208	278.1136	C ₁₃ H ₂₀ O ₅	1-Methoxy-1-(2,4,5-trimethoxyphenyl)-2-propanol	98205-47-1
						C ₁₅ H ₁₈ O ₅	Achimilic acid	110732-04-2
0.9	59948.84	16598	101.5	554.7942	553.787	-	-	-

1.5	71560.9	16605	13.6	168.0658	167.0586	C ₉ H ₉ N ₂	4-Aminomethylindole	3468-18-6
							Pyridoxal (Vitamin B6)	66-72-8
						C ₈ H ₉ NO ₃	p-Aminosalicylic acid methyl ester	4136-97-4
							4-Hydroxy-L-phenylglycine	32462-30-9
1.7	413134.6	16646	13.8	206.995	204.9804	C ₅ H ₄ N ₄ O ₂ S	6-Thiouric acid	2002-60-0
						C ₅ H ₁₂ OS ₃	Methyl 1-(methylsulfinyl)propyl disulfide	134018-95-4
							4-tert-Octylphenol	140-66-9
2.9	119944.3	16729	17.3	229.1549	228.1476	C ₁₄ H ₂₂ O		79-69-6
							alpha-Irone	35124-13-1
0.8	53652	16785	373	220.9576	219.9504	C ₁₁ H ₂₀ N ₂ O ₃	Ile Pro	-
						-	-	-
						C ₁₃ H ₁₈ O ₄	1,2,3,4-Tetramethoxy-5-(2-propenyl)benzene	15361-99-6
1.6	136805.4	16820	12.3	261.1119	259.1085	C ₁₅ H ₁₆ O ₄	3-(1,1-Dimethylallyl)scopoletin	19723-23-0

							Citrusal	5980-07-4
							Homobaldrinal	67910-07-0
							PEUCENIN	578-72-3
10.5	104861.2	16886	29.2	622.3645	621.3572	-	-	-
0.9	72234.09	16913	187.9	466.9238	465.9165	-	-	-
1.9	136054.7	16930	17.1	401.1053	400.098	C ₁₉ H ₂₃ C ₁ N ₂ O ₂ S	Pyridate	55512-33-9
						C ₂₀ H ₂₆ N ₂ O ₄	Quinidine-10,11-dihydrodiol	80227-26-5
11.8	165503.4	16936	15	381.1809	380.1742	C ₂₂ H ₂₄ N ₂ O ₄	Di-4-coumaroylputrescine	37946-59-1
0.9	91813.57	16984	27.5	174.8864	173.8791	-	-	-
0.8	79141.87	16994	188.8	265.4251	264.4178	-	-	-
12	119462	17022	18.1	449.1073	448.1	C ₂₁ H ₂₀ O ₁₁	Fisetin 7-glucoside	-
12.2	125238.2	17055	20.9	619.2757	618.2684	C ₃₂ H ₃₈ N ₆ O ₅ S	Met Pro Trp Trp	-
13	138663.2	17077	12.4	501.3208	500.3135	C ₂₈ H ₄₆ O ₆	Dolicholide	85228-11-1

						C ₂₀ H ₄₀ N ₁₀ O ₅	Ala Arg Arg Val	-
						C ₃₀ H ₄₄ O ₆	Ganoderic acid beta	217476-76-1
1.1	885314.6	17128	17.2	1083.268	2164.521	-	-	-
1.4	689723.4	17128	4.7	158.9616	157.9543	-	-	-
2.9	119295.3	17133	37.9	100.1123	99.105	C ₆ H ₁₃ N	2-Methylpiperidine	109-05-7
21.8	168870.7	17172	26	197.5809	393.1532	-	-	-
11.4	259175	17222	14.8	458.7885	915.5624	-	-	-
16.4	98077.05	17222	12.1	279.2315	278.2242	C ₁₈ H ₃₀ O ₂	α -calendic acid	-
							Dehydrozingerone	1080-12-2
8.7	222336.8	17226	18.3	193.084	194.0913	C ₁₁ H ₁₂ O ₃	Carpacin	23953-63-1
							ETHYL-p-COUMARATE	2979-06-8
10.3	95238.48	17276	24.3	548.2909	547.2836	C ₂₂ H ₄₁ N ₇ O ₇ S	Glu Ile Met Arg	-
16	202440.2	17292	59.1	927.5288	926.5217	C ₄₈ H ₇₈ O ₁₇	Oleanolic acid 3-[rhamnosyl-(1->4)-glucosyl-(1->6)-glucoside]	160845-07-8

						C ₁₂ H ₁₄ N ₄ O ₂ S	Thiamine acetic acid	-
							4-Hydroxymaackiain	-
14.4	103580.2	17294	3.2	301.0709	300.0636	C ₁₆ H ₁₂ O ₆	1,4,5,8-TETRAHYDROXY-2,6-DIMETHYLANTHROQUINONE	19079-10-8
							Diosmetin	520-34-3
19	10509316	17324	3	90.526	89.5187	-	-	-
1	130361	17351	50.6	633.1188	632.1116	C ₃₀ H ₂₆ O ₁₄	Delphinidin 3-(6"-p-coumarylglucoside)	-
1.2	142385.4	17416	14.5	195.959	194.9517	-	-	-
							4-Acetyl-2(3H)-benzoxazolone	70735-79-4
7.7	77319.63	17461	27.1	178.0502	177.0429	C ₉ H ₇ NO ₃	5-Hydroxyindol-2-carboxylic acid	21598-06-1
							Tetramethylquercetin 3-rutinoside	58528-03-3
						C ₃₇ H ₅₈ O ₆	Hericenone D	-
16.6	643591.4	17479	19.7	621.4177	622.425	C ₃₂ H ₆₀ O ₁₁	Butyl 4'-O-hexadecanoyl-neohesperidoside	-
1.6	74302.34	17480	61.5	349.1643	348.157	C ₁₉ H ₂₄ O ₆	Gibberellin A1	-

							L-Leucine n-butyl ester	2885-08-7
12	77651.13	17570	36.7	188.1645	187.1573	C ₁₀ H ₂₁ NO ₂	9-amino-decanoic acid	-
0.6	339653.8	17624	6.2	186.9565	185.9492	-	-	-
							His Glu	-
1	469921.4	17731	17.2	307.1022	306.0943	C ₁₁ H ₁₆ N ₄ O ₅	Coformycin	11033-22-0
0.8	383684.1	17740	58.5	679.7955	2712.201	-	-	-
0.8	130991.4	17741	394.2	395.3827	788.7508	-	-	-
0.8	276856.8	17793	25.2	414.8897	1238.543	-	-	-
0.6	263202	17796	4.4	98.5123	97.505	-	-	-
0.9	60887.13	17834	198.2	356.8497	355.8424	-	-	-
21.8	106875	17879	22.4	248.2007	247.1934	C ₁₆ H ₂₅ NO	alpha-Sanshool	504-97-2
1.5	137742.4	17899	11.3	149.1073	147.0897	C ₉ H ₁₂ N ₂	Nornicotine	494-97-3
0.9	106183.4	17931	54.5	516.8105	515.8032	-	-	-

13	624645.7	18015	25.7	585.2544	584.2471	C ₃₀ H ₃₂ N ₈ O ₅	Gly His Trp Trp	-
						C ₁₆ H ₂₂ O ₆	tetranor-PGDM lactone	-
							3',5'-Dihydroxy-2',4',6'-trimethoxydihydrochalcone	-
13	97965.76	18064	14.7	333.1311	332.1238	C ₁₈ H ₂₀ O ₆	DUARTIN (-)	52305-04-1
						C ₁₃ H ₂₀ N ₂ O ₈	Mytilin A	73112-73-9
1	185608.1	18072	27.5	118.0868	117.0802	C ₅ H ₁₁ NO ₂	4R-aminopentanoic acid	-
23.1	107381	18114	8.6	328.2847	327.2774	C ₁₉ H ₃₇ NO ₃	N-palmitoyl alanine	-
							2H-Indol-2-one, 1,3-dihydro-7-hydroxy-4-[2-(propylamino)ethyl]-	122570-33-6
7	98572.59	18156	14.8	235.1443	234.137	C ₁₃ H ₁₈ N ₂ O ₂	p-Coumaroylputrescine	34136-53-3
						C ₉ H ₁₄ O ₄	5-Butyltetrahydro-2-oxo-3-furancarboxylic acid	-
9.2	176167.2	18160	9.7	209.0789	416.1461		1-(2-Methoxy-3,4-methylenedioxyphenyl)-1-propanone	-
						C ₁₁ H ₁₂ O ₄	DL-Benzylsuccinic acid	884-33-3
0.9	102209.6	18238	6.8	367.0215	366.0142	-	-	-

						C ₁₂ H ₁₁ N	Diphenylamine	122-39-4
8.2	252141.8	18254	8.5	192.0769	380.123			
						C ₉ H ₉ N ₃ O ₂	Carbendazim	10605-21-7
0.8	209276.2	18259	10.1	140.9616	139.9544	-	-	-
0.9	132925.8	18427	8.2	154.9323	461.7836	-	-	-
16.7	141351.6	18428	31.7	700.2971	699.2899	C ₃₃ H ₄₃ N ₉ O ₅ S	Met Arg Trp Trp	-
11.7	122997.1	18438	15.3	650.3537	649.3464	-	-	-
0.9	141074.3	18446	51	445.9946	444.9873	C ₁₅ H ₁₂ F ₃ NO ₆ S ₂	O-Desmethyltolrestat sulfate	752952-17-3
1.1	305044.7	18452	16	695.2079	1386.391	C ₃₄ H ₃₄ N ₂ O ₁₄	Dexylosylpradimicin C	-
							Acetaldehyde di-cis-3-hexenyl acetal	63449-64-9
20.5	129136.1	18454	11.7	249.1848	248.1775	C ₁₄ H ₂₆ O ₂	10Z-Dodecenyl acetate	-
						C ₁₆ H ₂₄ O ₂	4,7,10,13-hexadecatetraenoic acid	-
10.8	288178.2	18485	15.9	239.0895	240.0967	C ₁₂ H ₁₄ O ₅	1-(2,4,5-Trimethoxyphenyl)-1,2-propanedione	-
							Trans-2, 3, 4-Trimethoxycinnamate	-

1.5	109284.2	18516	8	344.1336	343.1263	C ₁₅ H ₂₁ NO ₈	b-D-Glucopyranosiduronic acid	33150-82-2
0.9	128027	18540	206	278.8603	277.8533	-	-	-
							Unsaturated alcohol	-
11.2	167494.4	18543	29.6	101.0963	100.089	C ₆ H ₁₂ O	4-Methylpentanal	-
							Caproaldehyde	-
1	184759.7	18553	14.3	155.5445	307.0585	-	-	-
11.4	299545.8	18639	13.2	450.2752	898.536	C ₂₂ H ₃₅ N ₅ O ₅	Phe Gly Lys Val	-
						C ₂₁ H ₃₆ NO	Tridihexethyl	60-49-1
23.5	178875.3	18657	16	341.2662	342.2735		PGE1 Alcohol	21562-57-2
						C ₂₀ H ₃₆ O ₄	15(S)-HpEDE	145375-41-3
10.9	149462.4	18663	24.8	384.2048	766.395	-	-	-
0.6	471831.6	18707	9.6	159.9691	158.9618	-	-	-
0.8	595621.8	18725	416.1	513.3574	512.3583	C ₃₂ H ₄₈ O ₅	11a,12a-Epoxy-3b-hydroxy-28,13-oleananolid 3-acetate	35738-25-1

						C ₃₀ H ₅₀ O ₅	Barringtogenol C	17304-24-4
10.5	156405	18730	28.1	597.2731	598.2803	C ₃₂ H ₃₈ N ₄ O ₆	Phe Phe Val Tyr	-
11.7	619132.6	18768	8	185.1152	184.1079	C ₈ H ₁₈ O ₃	(3R,7R)-1,3,7-Octanetriol	217650-11-8
1.7	225273.9	18770	14.5	209.0333	208.0261	C ₉ H ₁₁ C _l O ₂	2-Chloro-1,3-dimethoxy-5-methylbenzene	27971-69-3
0.8	67304.42	18854	209.5	209.4516	208.4443	-	-	-
16.9	162577.2	18861	35	795.4507	794.4439	C ₄₂ H ₆₆ O ₁₄	Spinasaponin A	25406-56-8
1.2	154300.9	18885	27.4	679.0537	678.0465	-	-	-
							Vanillyl alcohol	498-00-0
11.6	106098.8	19080	11.7	155.0702	154.0629	C ₈ H ₁₀ O ₃	3,4-Dihydroxyphenyl ethanol	10597-60-1
						C ₁₇ H ₂₄ N ₄ O ₆ S	Ala Cys Gly Tyr	-
1.1	191743.8	19164	9.5	435.1273	868.24		5,7-Dihydroxy-3,6,8,3',4',5'-hexamethoxyflavone	-
						C ₂₁ H ₂₂ O ₁₀	Naringenin-7-O-Glucoside	529-55-5
1.5	115647.6	19168	16.4	262.1288	259.1511	C ₁₁ H ₁₉ NO ₆	Epidermin	126050-09-7

0.9	59016.91	19249	213.9	242.8649	241.8577	-	-	-
17.4	233301.6	19336	25.6	418.1858	417.1786	C ₂₂ H ₂₇ NO ₇	Tirandamycin	34429-70-4
8.1	100046.7	19346	27.9	146.0601	145.0529	C ₉ H ₇ NO	Quinolin-2-ol	70254-42-1
16.4	199820	19368	28.7	333.2629	332.2562	C ₁₈ H ₃₆ O ₅	9,10,13-Trihydroxystearic acid	50439-74-2
							10-Hydroxy-2,8-decadiene-4,6-dienoic acid	-
12	207795.5	19440	17.8	177.0546	176.0485	C ₁₀ H ₈ O ₃	1,3,8-Naphthalenertriol	-
							HERNIARIN	531-59-9
						C ₁₆ H ₃₁ ClO ₃	9-chloro-10-hydroxy-hexadecanoic acid	-
10.6	237818.8	19465	216.3	329.1873	660.3892	C ₂₄ H ₂₄ O	4-(3,5-Diphenylcyclohexyl)phenol	33330-65-3
						C ₁₉ H ₂₄ N ₂ O ₃	Labetalol	36894-69-6
22.9	4650342	19524	10.7	140.9515	139.9442	C ₃ H ₂ Cl ₂ O ₂	3,3-dichloroacrylic acid	-
0.9	137087.2	19531	217	394.8138	393.8065	C ₁₂ H ₂ C ₁₆ O	1,2,3,4,7,8-Hexachlorodibenzofuran	70648-26-9
16.5	183776.4	19554	33.6	700.2964	699.2891	C ₃₃ H ₄₃ N ₉ O ₅ S	Met Arg Trp Trp	-

0.9	96896.34	19596	87.6	434.8549	433.848	C ₉ H ₈ I ₂ O ₄	3-(3,5-Diiodo-4-hydroxyphenyl)lactate	-
1.5	112341.3	19611	19.1	138.0553	137.0481	C ₇ H ₇ NO ₂	Anthranilic acid	118-92-3
							4-Nitrotoluene	99-99-0
							6-Paradol	27113-22-0
14	89354.05	19624	12.6	279.1928	278.1856	C ₁₇ H ₂₆ O ₃	Panaxxytriol	-
							7-hydroxy-10E,16-heptadecadien-8-ynoic acid	-
21.7	154773.2	19639	41.1	320.0805	319.0732	C ₁₁ H ₁₅ N ₅ O ₃ S	5'-Deoxy-5'-(methylthio)adenosine	2457-80-9
							1,5-Dihydroxy-2-methoxy-6-methylanthraquinone	63965-45-7
12.9	112101	19657	20.9	285.0759	284.0686	C ₁₆ H ₁₂ O ₅	7,2'-Dihydroxy-5-methoxyflavone	-
							PHYSCION	521-61-9
							Furfuryl pentanoate	36701-01-6
7.6	137346	19694	14.9	183.1002	182.0929	C ₁₀ H ₁₄ O ₃	3,4,5-Trimethoxytoluene	6443-69-2
							MEPHENESIN	59-47-2

							Iridotrial	-
							5-oxo-7-decynoic acid	-
						C ₆ H ₁₀ N ₆ O	Dacarbazine	4342—03-4
9.1	149200.4	19727	18.3	437.1444	436.138	C ₁₄ H ₂₄ N ₆ O ₈ S	Asn Asn Ser Cys	-
						C ₂₁ H ₂₄ O ₁₀	Phenethyl 6-galloylglucoside	-
19.8	145397.6	19745	10.4	279.159	278.1522	C ₁₆ H ₂₂ O ₄	Phthalic acid Mono-2-ethylhexyl Ester	4376-20-9
1.4	316145.4	19748	5.6	125.9863	624.8958	-	-	-
13	149097	19835	10.4	519.3311	518.3238	C ₂₆ H ₄₂ N ₆ O ₅	Phe Lys Lys Pro	-
23.4	205064.7	19884	20.5	429.3183	430.3256	C ₂₄ H ₄₄ O ₆	Sorbitan oleate	1338-43-8
1	214979.9	19912	20.1	109.0286	108.0213	C ₆ H ₄ O ₂	Quinone	-
1.1	123553.4	19990	10	146.9965	145.9892	-	-	-
6.4	150574.3	20113	11.5	157.0837	156.0764	C ₆ H ₁₄ O ₃	Polypropylene glycol (m w 1,200-3,000)	25322-69-4
10.9	129297.4	20243	32.7	381.727	761.4394	-	-	-

0.9	53087.67	20321	26.4	320.8696	319.8623	-	-	-
10.3	131749.2	20345	44.7	578.3385	577.3312	C ₃₂ H ₄₃ N ₅ O ₅	Phe Ile Ile Trp	-
0.9	117168.6	20373	12	349.0115	348.0042	C ₁₀ H ₁₀ C ₁ F ₃ N ₄ OS	6-(2-CHLORO-5-(TRIFLUOROMETHYL)PHENYL)-1-PHENYL-2-THIOBIUREA	-
8.5	92084.76	20380	14.3	314.1813	313.1741	-	-	-
0.8	465453.6	20406	453.5	457.3837	916.7821	-	-	-
1.7	241219.8	20416	13.9	179	175.9998	C ₆ H ₁₀ S ₃	Diallyl Trisulfide	2050-87-5
10.5	196765.9	20526	13	627.3198	628.327	C ₂₄ H ₄₀ N ₁₄ O ₅	His His Arg Arg	-
						C ₂₈ H ₄₆ N ₆ O ₈ S	Benzylpenicilloyl Polylysine	2642-55-9
17.2	128419	20583	11.7	277.1432	276.1359	C ₁₆ H ₂₀ O ₄	Scorpioidin	76045-40-4
5.8	153531.1	20597	15.2	102.1278	101.1205	C ₆ H ₁₅ N	Hexylamine	111-26-2
8.4	101172.9	20626	18	245.0998	244.0925	C ₉ H ₁₈ O ₆	Isopropyl beta-D-glucoside	5391-17-3
						C ₁₁ H ₁₆ O ₆	threo-Syringoylglycerol	121748-11-6
10.5	137859.4	20686	22.9	177.1639	174.14	C ₁₃ H ₂₀	(6E,8E)-4,6,8-Megastigmatriene	51468-86-1

							Gentianadine	6790-32-5
1.5	109559.9	20736	22.1	150.0552	447.1426	C ₈ H ₇ NO ₂	N-Acetyl-p-benzoquinonimine	50700-49-7
2	107128.6	20738	45.9	100.1122	99.1049	C ₆ H ₁₃ N	2-Methylpiperidine	109-05-7
17.9	138725.1	20780	29.1	294.1005	293.0932	C ₁₄ H ₁₆ C ₁ N ₃ O ₂	TRIADIMEFON	43121-43-3
9.4	92551.34	20805	25.2	120.0557	119.0485	-	-	-
1.5	168697.6	20877	19.7	829.2808	828.2737	C ₃₀ H ₅₂ O ₂₆	Maltopentaose	34620-76-3
14.1	157290.6	20893	12.9	213.1098	212.1025	-	-	-
2.1	359952.7	20905	23.3	179.118	178.1107	C ₁₀ H ₁₄ N ₂ O	Glycine xylidide	18865-38-8
							Phenylpropionic acid	637-44-5
10.5	101661.9	20976	18.7	147.0443	146.037	C ₉ H ₆ O ₂	2-Benzofurancarboxaldehyde	4265-16-1
							Chromone	491-38-3
1.1	321429.9	21069	18.7	353.0919	352.0846	C ₁₁ H ₂₀ N ₄ O ₅ S ₂	Ala Cys Cys Gly	-
14.1	130971.8	21109	14	139.1118	138.1045	C ₉ H ₁₄ O	(Z,Z)-3,6-Nonadienal	21944-83-2

15.7	660601.6	21140	28.6	563.3761	564.3834	-	-	-
0.9	204482.1	21158	58.4	450.9499	449.943	-	-	-
8.8	198950.3	21264	13.1	213.1102	424.2038	-	-	-
19	132813.5	21333	38.9	334.2271	333.2198	-	-	-
0.9	60832.66	21369	237.4	440.8101	439.8029	-	-	-
11.3	174530.5	21410	21.7	436.7754	871.5364	-	-	-
10.3	159724.1	21452	36.4	553.2469	554.2542	C ₂₄ H ₃₆ N ₆ O ₇ S	Phe Met Gln Gln	-
0.8	330828.3	21506	17.4	226.9516	225.9454	C ₆ H ₄ C ₁₂ O ₅	2,5-Dichloro-4-oxohex-2-enedioate	-
						C ₁₃ H ₁₆	1,2-Dihydro-1,1,6-trimethylnaphthalene	30364-38-6
							3-Hydroxy-N-glycyl-2,6-xylidine (3-Hydroxyglycinexylidide)	112606-87-8
19	210221.8	21615	15.5	195.1143	194.107	C ₁₀ H ₁₄ N ₂ O ₂	Laccarin	175669-28-0
							Pilocarpidine	127-67-3
11.7	343031	21623	6.5	309.2266	308.2168	C ₁₄ H ₃₀ N ₄ O ₂	N1,N12-Diacetylspermine	-

						C ₁₅ H ₃₂ O ₆	1,2,3-Tris(1-ethoxyethoxy)propane	67715-82-6
15.6	204045.9	21639	20.6	271.1881	270.1808	C ₁₃ H ₂₈ O ₄	alpha-Butyl-omega-hydroxypoly(oxyethylene) poly(oxypropylene)	9038-95-3
						C ₁₅ H ₂₆ O ₄	Ethylene brassylate	105-95-3
20.2	120218.1	21725	18.5	251.2006	250.1934	C ₁₆ H ₂₆ O ₂	3-Methyl-alpha-ionyl acetate	68555-61-3
						C ₁₆ H ₂₆ O ₂	4,7,10-hexadecatrienoic acid	-
0.9	88107.95	21735	483	384.7957	362.4027	-	-	-
1.5	145753.6	21807	20.7	182.0812	183.0885	C ₉ H ₁₁ NO ₃	DL-o-Tyrosine	2370-61-8
10.1	143651.2	21808	33.2	504.265	503.2577	C ₂₈ H ₃₃ N ₅ O ₄	Trp Trp Leu	-
1.1	247893.7	21830	5.1	605.1768	1208.339	C ₃₄ H ₃₀ O ₉	Kuwanon Y	105016-28-2
23.5	454201.5	21857	23.3	385.2923	386.2995	C ₂₂ H ₄₀ O ₅	17,20-dimethyl Prostaglandin F1α	-
12.3	205304.3	21873	18.9	411.1913	410.1845	C ₁₈ H ₂₆ N ₄ O ₇	Ala Ala Ser Tyr	-
14.1	504962.1	21964	12.3	277.1383	278.1456	C ₁₄ H ₂₂ O ₄	C75	191282-48-1
						C ₁₁ H ₂₀ N ₂ O ₆	Saccharopine	997-68-2

7.9	183039.8	21974	43.2	321.1522	320.1449	C ₁₄ H ₂₄ O ₈	Valproic acid glucuronide	60113-83-9
11.2	218723.3	22032	50.2	447.7663	892.4611	-	-	-
0.9	132711.5	22127	34.2	164.9857	163.9784	C ₄ H ₈ C ₁₂ O	Bis(2-chloroethyl)ether	111-44-4
0.9	77770.94	22154	492.3	508.7969	507.7896	-	-	-
10.1	135549.7	22187	57.2	215.9785	214.9715	-	-	-
12.3	157603.2	22250	20.4	177.0546	176.0473	C ₁₀ H ₈ O ₃	3-(3,4-Methylenedioxyphenyl)propenal	14756-00-4
							4-Methylumbelliferone	90-33-5
							10-Hydroxy-2,8-decadiene-4,6-dienoic acid	-
							1,4,5-Naphthalenetriol	481-40-3
							Propyl 2-furoate	615-10-1
7.4	111319.3	22340	13.7	155.0705	154.0632	C ₈ H ₁₀ O ₃	3,4-Dihydroxyphenyl ethanol	10597-60-1
11.5	154759.8	22462	28.9	595.1658	594.1585	C ₂₇ H ₃₀ O ₁₅	Cyanidin 3-O-rutinoside	28338-59-2
4.3	170011.4	22483	17.6	99.0444	98.0371	C ₃ H ₆ O ₂	5-Methyl-2(3H)-furanone	591-12-8

							2-Furanmethanol	98-00-0
1.1	199178.2	22553	7.6	84.9597	83.9524	-	-	-
14.4	119950.3	22582	43.3	226.1804	225.1731	-	-	-
10.3	27805782	22704	5.6	98.5122	192.0148	-	-	-
0.9	58931.75	22762	252.9	310.8519	309.8446	-	-	-
0.8	277423.8	22823	5.7	218.9834	217.9761	-	-	-
0.8	288982.6	22827	41.6	171.9917	170.9844	C ₄ H ₅ C _a NO ₄	Calcium L-aspartate	21059-46-1
1.1	214046.8	22967	55	606.1188	607.1261	-	-	-
							N-Acetylanthranilate	89-52-1
6.6	157419.3	23063	25	180.0656	179.0583	C ₉ H ₉ NO ₃	Adrenochrome	54-06-8
1	258180.1	23143	6.6	125.9864	374.9378	-	-	-
0.9	102067.8	23153	13	152.9473	151.94	C ₂ H ₄ C ₁₂ O ₂	2,2-Dichloro-1,1-ethanediol	16086-14-9
10.8	213423.2	23251	19.4	167.1069	166.0996	C ₁₀ H ₁₄ O ₂	4-Butoxyphenol	122-94-1

							bornane-2,3-dione	-
							2E,6E,8E-decatrienoic acid	-
22.9	7255914	23396	15.6	201.9754	200.9681	-	-	-
1.2	174038.3	23410	38.3	663.0794	662.0721	-	-	-
1	189749.5	23423	31.2	297.0493	296.0421	C ₁₈ H ₁₀ O ₃	4-Phenyl-1H,3H-naphtho[1,8-cd]pyran-1,3-dione	56252-04-1
17.4	382643.3	23437	67.3	823.2924	822.2851	-	-	-
0.9	185732.2	23517	42.1	158.9123	315.8091	-	-	-
							Isoamyl 2-furonpropionate	7779-67-1
							1-Benzyloxy-1-(2-methoxyethoxy)ethane	7492-39-9
9.3	134409.5	23602	21	211.1329	210.1256	C ₁₂ H ₁₈ O ₃	(R)-8-Acetoxy-carvotanacetone	56691-69-1
							(±)7-epi Jasmonic Acid	62653-85-4
0.9	92641.11	23641	262.7	424.8354	423.8281	C ₃₂ H ₄₂ O	(all-E)-6'-Apo-γ-caroten-6'-al	22255-36-3
0.9	103641.3	23900	32.2	136.922	135.9147	-	-	-

24.1	197706.3	23977	22.5	443.3338	442.3265	-	-	-
1.6	108860	24159	18.4	170.0814	169.0741	C ₈ H ₁₁ NO ₃	Norepinephrine (noradrenaline)	51-41-2
0.8	384114.2	24173	44.4	480.8579	479.8525	-	6-Acetyl-2,3-dihydro-2-(hydroxymethyl)-4(1H)-pyridinone	214218-63-0
0.9	95094.56	24227	269.2	244.9025	487.7881	-	-	-
0.9	204162	24318	11.2	219.0266	218.0159	C ₉ H ₈ O ₅	HAEMATOMIC ACID	479-25-4
14.8	143479.4	24346	31.4	200.1282	199.1209	C ₁₀ H ₁₇ NO ₃	Ecgonine methyl ester	7143-09-1
1.7	219578.5	24366	31.5	102.5311	101.5238	-	N-hexanoyl-L-Homoserine lactone	147852-83-3
10.3	196606.2	24430	30.2	583.2932	584.3005	C ₂₉ H ₃₈ N ₆ O ₇	Lys Ser Trp Tyr	-
21.9	176623	24474	17.2	279.2318	278.2245	C ₁₈ H ₃₀ O ₂	3E,9Z,12Z-octadecatrienoic acid	-
0.8	325612	24708	21.4	223.9889	222.9817	-	-	-
1.6	147686.2	24745	50.4	349.0484	348.0411	-	-	-

11	250852.6	24746	12.8	403.7398	804.4042	-	-	-
							Norecasantalic acid	59300-52-6
							Dihydroactinidiolide	15356-74-8
15.5	162316.8	24833	24	181.1224	180.1151	C ₁₁ H ₁₆ O ₂	2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]nona-3,8-diene	15129-55-2
							3-tert-Butyl-5-methylcatechol	-
19	217984.5	24883	36.1	206.6223	411.23	-	-	-
11.3	299862.2	24901	24.6	428.2619	854.5097	C ₁₈ H ₃₃ N ₇ O ₅	Gly Pro Arg Val	-
15.6	202149.6	24973	24.3	225.0547	224.0477	C ₁₄ H ₈ O ₃	Hydroxyanthraquinone	129-43-1
9.8	160994.3	25038	41.4	460.2389	459.2316	C ₁₉ H ₃₃ N ₅ O ₈	Ala Glu Ile Gln	-
16.4	153336.8	25056	17.1	297.242	296.2347	C ₁₈ H ₃₂ O ₃	(±)13-HODE	73804-64-5
0.8	892154.6	25059	2.3	375.4103	752.8351	-	-	-
1.6	163472.3	25185	19.3	124.0969	246.1775	-	-	-
9.9	138072.9	25188	32.5	490.2858	489.2785	C ₂₁ H ₃₉ N ₅ O ₈	Glu Ile Lys Thr	-

10.1	138848.6	25212	37.8	534.3119	533.3046	C ₂₂ H ₄₃ N ₇ O ₆ S	Lys Lys Met Gln	-
0.9	89727.17	25300	12.8	226.891	225.8838	-	-	-
							Polygodial	-
							Alcyopterosins O	-
20.5	176960.2	25491	17.9	235.1691	234.1618	C ₁₅ H ₂₂ O ₂	Curmadione	-
							Macrophyllic acid A	-
							1,13-Dihydroxy-herbertene	-
						C ₂₂ H ₃₂ O ₆	Dihydrofukinolide	41059-95-4
18	334350.3	25553	27.9	415.211	414.2043	C ₁₇ H ₃₀ N ₆ O ₄ S ₁	His Met Lys	-
						C ₂₄ H ₃₀ O ₆	Magnoshinin	86702-02-5
							Fisetin 4'-methyl ether	-
14.3	170310.7	25568	4.8	301.0707	300.0634	C ₁₆ H ₁₂ O ₆	1,4,5,8-TETRAHYDROXY-2,6-DIMETHYLANTHROQUINONE	19079-10-8
							Diosmetin	520-34-3

11	282768.2	25845	61	392.7494	783.4841	-	-	-
								79-69-6
						C ₁₄ H ₂₂ O	alpha-Irone	
1.6	159356.5	25875	26.7	229.1548	228.1475			35124-13-1
						C ₁₁ H ₂₀ N ₂ O ₃	Leu Pro	-
11.1	356353.8	25887	81.3	425.7531	853.5207	-	-	-
10.9	169746.6	26000	39.5	745.4193	744.412	C ₃₉ H ₆₂ O ₁₂	Ophiopogonin C'	19057-67-1
24.3	718685.2	26088	35.3	345.2562	344.2495	C ₂₁ H ₃₂ N ₂ O ₂	3'-Hydroxystanozolol	125709-39-9
3.1	33051306	26136	7.2	158.9614	157.9542	-	-	-
0.8	1545067	26296	584.4	505.3684	506.3756	-	-	-
8.6	125116.9	26386	27.6	174.1489	173.1416	C ₉ H ₁₉ NO ₂	3R-aminononanoic acid	-
1.1	354478.7	26435	19.4	280.0547	279.0474	C ₁₄ H ₁₄ C ₁ NOS	2-Oxoticlopidine	-
23.2	6619368	26494	10.3	90.507	89.4998	-	-	-
10.9	322671.1	26705	73.8	740.464	739.458	C ₃₉ H ₆₅ NO ₁₂	Lycoperoside D	81037-16-3

11.8	151055.8	26738	18.7	199.0944	198.0871	C ₈ H ₁₆ O ₄	Metaldehyde	108-62-3
							2-hydroxyestradiol	362-05-0
1.5	169337.2	26841	10.9	311.1602	310.1529	C ₁₈ H ₂₄ O ₃	O-Geranylvainillin	151455-08-2
							Estriol	50-27-1
9.9	153361.2	26963	42	383.0069	381.9997	C ₁₅ H ₁₀ O ₁₀ S	6-Hydroxyluteolin 7-sulfate	-
7.8	124000.3	27050	17.4	265.1551	264.1478	C ₁₄ H ₂₀ N ₂ O ₃	Val Phe	-
1.4	136640.6	27061	12.8	281.0711	560.1276	C ₁₁ H ₁₂ N ₄ O ₃ S	SULFAMONOMETHOXINE	1220-83-3
9.1	125209.6	27180	53.7	372.1865	371.1792	C ₁₅ H ₂₅ N ₅ O ₆	Ala Ala Asn Pro	-
20.2	176855	27260	23	282.279	281.2717	C ₁₈ H ₃₅ NO	Oleamide	301-02-0
16	203765.6	27374	69.4	664.3329	663.326	C ₃₂ H ₅₁ NO ₁₂	(3a,5b,7a,12a)-24-[(carboxymethyl)amino]-1,12-dihydroxy-24-oxocholan-3-yl-b-D-Glucopyranosiduronic a	99794-78-2
8.7	127182.3	27421	47	328.1604	327.1531	C ₁₃ H ₂₁ N ₅ O ₅	Ala Thr His	-
10.7	197239.7	27495	18.5	273.1673	272.16	C ₁₃ H ₄ D ₁₀ N ₂ O ₄	DMABA-d10 NHS ester	1175002-05-7

						C ₁₈ H ₂₁ FO	(R*,S*)-4-[1-Ethyl-2-(4-fluorophenyl)butyl]phenol	-
10.1	214793.4	27503	32.8	509.2201	510.2274	C ₁₉ H ₃₆ N ₆ O ₆ S ₂	Cys Lys Met Gln	-
						C ₁₇ H ₂₄ O ₅	Inulicin	33627-41-7
12.3	519710.3	27633	22	331.154	330.1468		Gibberellin A105	114596-77-9
						C ₁₉ H ₂₂ O ₅	3-DESHYDROXYSAPPANOL TRIMETHYL ETHER	-
							6-Methylcoumarin	92-48-8
12.2	206288.1	27665	40	161.0598	160.0525	C ₁₀ H ₈ O ₂	2-Formyl-1-indanone	56794-24-2
							Naphthalene-1,2-diol	574-00-5
14.8	716516.2	27791	24.5	505.3344	506.3417	C ₂₇ H ₄₄ N ₄ O ₅	Phe Ile Ile Ile	-
1.5	118177.4	27824	20.5	280.1392	279.1319	-	-	-
12.2	136760.8	27921	32.7	243.1204	242.1131	-	-	-
						C ₁₂ H ₂₀ O ₄	2Z-Dodecenedioic acid	-
9.2	131106	27937	12.9	251.1256	250.1183	C ₁₄ H ₁₈ O ₄	Helinorbisabone	201288-95-1

							Diisopropyl phthalate	605-45-8
							Trolox	53188-07-1
							Ubiquinone-1	727-81-1
9.5	162737.3	27981	66	416.2134	415.2062	C ₁₇ H ₂₉ N ₅ O ₇	Ala Pro Gln Thr	-
0.7	425694	28105	140.6	460.8857	459.8784	-	-	-
21.7	170597.4	28414	35.3	307.138	612.2615	C ₁₄ H ₁₈ N ₄ O ₄	Trimethoprim 3-N-oxide	27653-67-4
1.5	271329.8	28442	53.5	487.1655	486.1582	C ₂₀ H ₃₀ N ₄ O ₆ S ₂	Ala Cys Met Tyr	-
9.6	140733.4	28514	27.1	135.0443	134.037	C ₈ H ₆ O ₂	6E-Octene-2,4-dienoic acid	-
15.3	128770.3	28516	14.2	149.0234	148.0161	-	-	-
7.5	150711.3	28521	44.6	384.1153	383.108	C ₁₂ H ₁₉ N ₅ O ₈	Asp Gly Gly Asn	-
10.6	612724.3	28554	20.6	229.1413	230.1486	C ₁₂ H ₂₀ O ₄	Traumatic Acid	6402-36-4
13.5	208181.3	28560	75.2	813.462	812.4548	C ₄₂ H ₆₈ O ₁₅	bayogenin 3-O-cellobioside	-
1.5	454478.7	28606	41.6	144.1021	143.0961	C ₇ H ₁₃ NO ₂	L-2-Amino-3-methylenehexanoic acid	29784-96-1

						C ₁₉ H ₃₀ N ₄ O ₇	Asp Pro Pro Val	-
16.1	248715.3	28734	30.7	427.2162	852.4179	C ₂₃ H ₂₇ FN ₄ O ₃	9-Hydroxyrisperidone	144598-75-4
						C ₁₂ H ₂₂ O ₁₁	3-b-Galactopyranosyl glucose	28447-38-3
1	414428.8	28743	5.1	365.1047	364.0974	C ₂₁ H ₁₆ O ₆	Gerberinol	84153-78-6
							Justicidin B	17951-19-8
10.1	226222.3	28793	17.7	539.2675	540.2748	C ₂₄ H ₃₈ N ₆ O ₆ S	Phe Lys Met Asn	-
1.1	343734.5	28952	56.6	443.1238	884.233	C ₁₅ H ₂₄ N ₄ O ₈ S	Cys Asp Pro Ser	-
8.9	182295	28954	40.4	215.1256	214.1183	-	-	-
13.9	155466.9	29035	27.5	359.2034	358.1961	C ₁₄ H ₂₆ N ₆ O ₅	Arg Pro Ser	-
1.6	235018.3	29057	53.9	314.0772	313.0699	C ₁₈ H ₁₃ NO ₃	Naptalam	132-66-1
						C ₉ H ₁₆ C ₁ N ₃ O ₇	Chlorozotocin	54749-90-5
9.6	537606	29060	39.2	629.1276	1256.241	-	-	-
1.5	133047	29087	34	158.154	157.1467	-	-	-

0.8	424426.2	29151	9.2	418.8658	417.8585	-	-	-
							1-(2-Methoxy-3,4-methylenedioxyphenyl)-1-propanon	-
							Furapiole	70874-90-7
9.5	222442.7	29348	15.6	209.0789	210.0862	C ₁₁ H ₁₂ O ₄	Sinapyl aldehyde	4206-58-0
							DIMETHYLCAFFEIC ACID	2316-26-9
0.9	84085.36	29365	326.3	294.8781	293.8708	-	-	-
							Creatine ethyl ester	15366-32-2
1.7	231394	29386	15.7	160.1082	159.1009	C ₆ H ₁₃ N ₃ O ₂	delta-Guanidinovaleic acid	462-93-1
1.2	288862.6	29707	22.3	127.0154	378.0314	C ₂ H ₇ O ₄ P	Dimethyl phosphate	813-78-5
11.1	419605.2	30039	24	406.2492	810.4841	C ₁₇ H ₃₅ N ₅ O ₄ S ₁	Met Lys Lys	-
						C ₂₄ H ₄₀ O ₇ S	Chenodeoxycholic acid 3-sulfate	128012-96-4
9.9	265867.8	30166	44	495.2412	496.2484	C ₂₃ H ₃₄ N ₄ O ₈	Ala Glu Ile Tyr	-
9.8	172547.7	30228	21.6	465.1943	464.1876	C ₂₁ H ₂₈ N ₄ O ₈	Ala Asp Pro Tyr	-

9.6	184764.7	30342	50.9	446.2595	445.2522	C ₁₉ H ₃₅ N ₅ O ₇	Ala Asp Ile Lys	-
1.4	644854.6	30364	12.8	141.9587	140.9515	-	-	-
11.9	369736.5	30433	26.3	411.1912	410.1843	C ₁₈ H ₂₆ N ₄ O ₇	Ala Ala Ser Tyr	-
15.1	619496.3	30463	71.1	650.3176	649.3109	C ₃₃ H ₄₃ N ₇ O ₅ S	Lys Met Trp Trp	-
19	202874.6	30523	59.2	667.4445	666.4372	C ₃₇ H ₆₂ O ₁₀	Notoginsenoside T2	343962-54-9
0.9	107533.4	30718	5.7	220.9348	219.9275	-	-	-
8.1	419145.3	30854	24.5	195.0632	196.0704	C ₈ H ₁₂ O ₄	Diethyl fumarate	623-91-6
							Ethyl 2,4-dioxohexanoate	13246-52-1
							3-Isopropenylpentanedioic acid	6839-75-4
							(-)-Corey Lactone Diol	32233-40-2
							Temozolomide	85622-93-1
							URB937	1357160-72-5
9.5	164315.9	30864	18.7	377.1463	376.1418	C ₂₀ H ₂₂ N ₂ O ₄		
						C ₁₇ H ₂₀ N ₄ O ₆	Gly Asp Trp	-

						C ₁₆ H ₂₄ O ₁₀	(1x,2x)-Guaiacylglycerol 3-glucoside	7094-73-7
14.7	202735.4	31052	25.7	227.1254	226.1182	C ₁₀ H ₂₀ O ₄	(2xi,3xi,6E)-3,7-Dimethyl-6-octene-1,2,3,8-tetrol	240495-79-8
						C ₁₁ H ₁₈ O	Limonene aldehyde	6784-13-0
1.5	128486.3	31141	40.8	189.1235	187.1211	C ₈ H ₁₆ N ₂ O ₃	Leucyl-Glycine	-
							Avenalumic acid	135754-92-6
12.3	170524.5	31184	20.4	191.0705	190.0633	C ₁₁ H ₁₀ O ₃	7-Hydroxy-2,5-dimethyl-4H-1-benzopyran-4-one	38412-47-4
							HYMECROMONE METHYL ETHER	2555-28-4
13.8	737370.6	31307	22.6	447.2928	448.3	C ₁₉ H ₃₈ N ₆ O ₆	Ala Lys Lys Thr	-
						C ₁₁ H ₁₂ N ₄ O ₂ S	SULFAMERAZINE	127-79-7
11.5	165182.4	31308	37.7	287.0553	286.048		Cyanidin	528-58-5
						C ₁₅ H ₁₀ O ₆	Fisetin	528-48-3
9	159777.6	31386	42.1	358.2073	357.2	C ₁₅ H ₂₇ N ₅ O ₅	Gly Gly Lys Pro	-
9	146718.8	31763	14.7	251.1257	250.1184	C ₁₂ H ₂₀ O ₄	Traumatic Acid	6402-36-4

							Helinorbisabone	201288-95-1
							Diisopropyl phthalate	605-45-8
						C ₁₄ H ₁₈ O ₄	Ubiquinone-1	727-81-1
							δ-CEHC	1221504-67-1
11.7	194959	31839	62.8	262.2376	261.2303	-	-	-
6.9	310439.3	32274	36.5	421.1346	420.1276	C ₁₅ H ₂₄ N ₄ O ₈ S	Cys Asp Pro Ser	-
1.6	186556.8	32614	32.3	118.0553	234.0978	-	-	-
8.4	164972.4	32663	21	265.1499	264.1426	-	-	-
0.9	258424.3	32665	24.4	266.1236	265.1163	C ₁₁ H ₁₅ N ₅ O ₃	N6-Methyl-2'-deoxyadenosine	2002-35-9
10.7	748606.2	32710	18.5	340.2097	678.4051	--	-	-
21.7	684011.9	32765	23.9	383.2038	384.2111	C ₁₆ H ₂₆ N ₆ O ₅	Ala Gly His Val	-
1.1	370708.2	32826	47.7	144.102	143.0947	C ₇ H ₁₃ NO ₂	L-2-Amino-3-methylenehexanoic acid	29784-96-1
13.8	253098.3	33062	88.6	290.2691	289.2618	-	-	-

1.5	196121.6	33146	20.9	684.2556	683.2483	-	-	-
11	522799.7	33213	20.7	384.236	766.4576	C ₂₇ H ₂₉ NO	JWH182	824960-02-3
15.7	530496.6	33214	78.1	362.3261	361.3188	-	-	-
						C ₁₀ H ₁₆ O ₃	(E)-10-Oxo-8-decenoic acid	69152-89-2
10.8	442463.5	33862	36.5	207.0995	206.0922		Cuelure	3572-06-3
						C ₁₂ H ₁₄ O ₃	p-Methoxycinnamic acid ethyl ester	1929-30-2
2.1	1314291	33877	17.3	163.1233	162.116	C ₁₀ H ₁₄ N ₂	Trimethyl-2-propenylpyrazine	55138-71-1
10.9	605130.9	33968	24.4	362.2231	722.4316	C ₂₁ H ₂₉ N ₃ O	Disopyramide	3737—09-5
17.3	486974.6	34161	38.4	302.305	301.2977	C ₁₈ H ₃₉ NO ₂	Sphinganine	764-22-7
0.8	381666.9	34182	56.9	398.9068	397.8995	-	-	-
0.9	161735.6	34234	58.3	266.16	265.1527	-	-	-
1.2	246689.1	34234	17.9	209.102	208.0947	C ₈ H ₁₆ O ₆	Ethyl beta-D-glucopyranoside	3198-49-0
1.6	297103.3	34403	37.2	134.0303	263.0424	-	-	-

11.7	197838.1	34445	56.4	547.1595	546.1522	C ₂₂ H ₂₈ N ₄ O ₁₁	Asp Asp Glu Phe	-
						C ₁₀ H ₁₃ C ₁ N ₂ O	Chlorotoluron	15545-48-9
10.9	164598.1	34808	39.7	235.0604	234.0531		7-Hydroxy-2-methyl-4-oxo-4H-1-benzopyran-5-acetic acid	94356-34-0
						C ₁₂ H ₁₀ O ₅	7-Acetoxy-6-methoxycoumarin	56795-51-8
0.8	14277713	34813	59.7	558.8401	1679.542	-	-	-
							2-Pyrimidine Acetic Acid	66621-73-6
1.8	161328.2	34860	7.2	139.0504	138.0431	C ₆ H ₆ N ₂ O ₂	methyl 2-Pyrimidine Carboxylate	34253-03-7
12.1	285740.8	34882	23.4	273.1672	274.1745	C ₁₃ H ₄ D ₁₀ N ₂ O ₄	DMABA-d10 NHS ester	1175002-05-7
						C ₁₄ H ₂₄ N ₆ O ₉	Asn Asn Ser Ser	-
9.5	218682.3	34914	49.5	421.1686	422.1759			
						C ₂₅ H ₂₄ O ₆	Pomiferin	572-03-2
						C ₁₃ H ₁₃ P	Diphenylmethylphosphine	1486-28-8
15.8	257012.1	35130	53.5	223.0636	222.0563			
						C ₉ H ₁₈ S ₃	1-(1-Propenylthio)propyl propyl disulfide	143193-11-7
15.9	205599.7	35161	8.1	219.1488	218.1419	C ₁₃ H ₁₈ N ₂ O	5-Methoxydimethyltryptamine	1019-45-0

0.8	315290.4	35262	783.6	327.4258	652.837	-	-	-
9.6	276999.4	35399	32.2	451.2153	429.7971	C ₂₁ H ₃₀ N ₄ O ₇	Ala Asp Phe Val	-
0.9	180470.4	35534	45.1	213.9693	212.962	C ₆ H ₆ ClNO ₂ S	p-Chlorobenzenesulfonylamide	98-64-6
9.3	174966.3	35703	47.4	402.2335	401.2262	C ₁₇ H ₃₁ N ₅ O ₆	Ala Ala Ile Gln	-
0.9	96629.38	35708	396.8	90.9767	89.9694	-	-	-
0.9	119197.4	35771	397.5	196.8685	195.8612	-	-	-
20.5	217657.1	35878	30.2	282.279	281.2718	C ₁₈ H ₃₅ NO	Elaidamide	4303-70-2
1.1	474114.8	36417	52.8	289.0919	288.0846	C ₁₆ H ₁₄ N ₂ O ₂	AG-1296	146535-11-7
						C ₁₂ H ₁₆ O ₈	Glucosylisomaltol	85559-61-1
19	371342.1	36574	406.4	651.4795	652.4868	-	-	-
10.7	420842.4	36848	96.1	701.3923	700.3876	-	-	-
3.6	14000109	37210	15.7	141.9587	140.9514	-	-	-
21.7	285400.3	37422	69.4	579.2921	578.2849	C ₂₅ H ₃₈ N ₈ O ₈	Glu Phe Gln Arg	-

						C ₁₆ H ₁₄ N ₂ O ₂	AG-1296	146535-11-7
6.9	184950	37491	35.4	289.0923	288.085			
						C ₁₂ H ₁₆ O ₈	Glucosylisomaltol	85559-61-1
18.2	246783.3	37634	49.7	182.1177	181.1104	C ₁₀ H ₁₅ NO ₂	beta-O-Methylynephine	60094-92-0
							1-Hydroxyepiacorone	185154-96-5
17	367822.4	37695	32.3	275.1614	276.1687	C ₁₅ H ₂₄ O ₃	Juvenile hormone III acid	-
							(+)-2-Sterpurene-6,12,15-triol	-
15.2	212704.8	38066	43.9	192.1382	191.131	C ₁₂ H ₁₇ NO	4 Methyl N-ethylcathinone	1225617-18-4
1.6	197160.6	38363	55.7	104.0309	206.0473	-	-	-
0.8	562337.3	38422	4.3	383.3995	382.3922	-	-	-
							Laurencione monoacetate	-
6.2	394122.9	38530	37.2	181.0473	182.0546	C ₇ H ₁₀ O ₄	2-Isopropylmaleate	44976-69-4
							Succinylacetone	51568-18-4
1.5	353817.5	39081	2.4	163.0602	162.0535	C ₆ H ₁₀ O ₅	Levoglucosan	498-07-7

							Dimethyl D-malate	70681-41-3
							3-hydroxy-adipic acid	-
							3,6-Anhydroglucose	7625-23-2
							Piperidione	77-03-2
14	238332.3	39376	54.7	170.1175	169.1102	C ₉ H ₁₅ NO ₂	Homoarecoline	28125-84-0
							Triethyl citrate	77-93-0
5.3	290801.3	39623	56.4	277.1261	278.1333	C ₁₂ H ₂₀ O ₇	Homoanserine	20314-38-9
							2-Ethylisonicotinic acid	3376-96-3
1.5	475264.8	39774	29.4	152.0705	153.0778	C ₈ H ₉ NO ₂	C-8 Ceramide	74713-59-0
0.8	538512.8	39878	886.2	448.3785	447.3713	C ₂₆ H ₅₁ NO ₃	Thr Pro Asp Gly	-
1	242799.3	39885	31.6	411.1475	410.1402	C ₁₅ H ₂₄ N ₄ O ₈	Gly Gly Lys Lys	-
12.8	876194.4	40129	18.2	389.2507	390.258	C ₁₆ H ₃₂ N ₆ O ₅	-	-
0.8	205617.5	40318	28.6	430.8743	429.867	-	-	-
1.6	455919.1	40466	26.6	145.0251	144.0179	C ₇ H ₆ O ₂	Benzoic acid	65-85-0

							4-Hydroxybenzaldehyde	123-08-0
1.9	393269.4	40479	35.5	94.0653	93.058	C ₆ H ₇ N	Aniline	62-53-3
						C ₁₁ H ₁₂ N ₄ O ₃ S	SULFAMONOMETHOXINE	1220-83-3
13.2	247133	40807	77.1	303.0498	302.0425	C ₁₅ H ₁₀ O ₇	HIERACIN	1621-84-7
1	499805.1	41010	24.2	195.0864	194.0791	C ₇ H ₁₄ O ₆	QUEBRACHITOL	642-38-6
						C ₁₉ H ₂₆ N ₄ O ₆	Ala Gly Pro Tyr	-
9.3	282462.4	41049	40.5	407.1885	408.1958		Minimiflorin	-
						C ₂₅ H ₂₆ O ₅	Lupalbigenin	-
1.2	352304.4	41235	55	641.09	640.0822	-	-	-
1.8	211644.4	41446	21.2	121.0399	120.0326	-	-	-
0.8	5527479	41636	5	606.8235	603.7854	-	-	-
0.8	374449.9	41836	32	268.9491	267.9418	-	-	-
0.9	240934.4	41921	465.8	164.9205	165.9278	-	-	-

0.9	168578.6	42429	37.5	350.8941	349.8872	-	-	-
							Amyl 2-furoate	4996-48-9
							3,4,5-Trimethoxytoluene	6443-69-2
8.7	265256.4	43064	32.6	183.1017	182.0944	C ₁₀ H ₁₄ O ₃	Dihydroconiferyl alcohol	2305-13-7
							MEPHENESIN	59-47-2
							5-oxo-7-decynoic acid	-
10.3	325397.9	43261	163.5	182.1906	181.1833	C ₁₂ H ₂₃ N	Dicyclohexylamine	101-83-7
						C ₁₀ H ₁₈ O ₄	Diethyl adipate	141-28-6
							Acoramone	2020-90-8
8.3	1173910	43369	31.7	225.1102	224.1029	C ₁₂ H ₁₆ O ₄	Dhelwangin	23800-56-8
							Diplosporin	69199-05-9
							Aspidinol	519-40-4
1.6	218916.8	43491	10.7	113.0362	224.0578	-	-	-

18.3	411714.5	43748	16.1	200.201	199.1937	C ₁₂ H ₂₅ NO	dodecanamide	-
21.7	273154.1	44011	120.9	658.253	657.2457	C ₃₂ H ₃₇ N ₅ O ₉	Gln Tyr Tyr Tyr	-
1.3	746677.9	44116	87	689.2104	688.2031	C ₂₄ H ₄₂ O ₂₁	3-beta-Glucosylcellotriose	58484-04-1
18.2	291815	44365	38.1	275.1752	274.1679	C ₁₄ H ₂₄ N ₂ O ₂	LUPANYL ACID	-
						C ₁₆ H ₂₂ N ₂ O ₂	Allyxycarb	6392-46-7
1.5	521149.9	44596	10.7	132.1021	131.0955	C ₆ H ₁₃ NO ₂	L-Norleucine	327-57-1
22.9	427896.1	44887	66.2	441.3721	440.3648	C ₃₀ H ₄₈ O ₂	Sebiferic acid	52809-09-3
							Karounidiol	118117-31-0
10.7	363255.1	44960	98.7	696.4375	695.4311	C ₃₇ H ₆₁ NO ₁₁	Mycinamicin IV	73684-71-6
11.2	429160.7	45121	40	107.0704	106.0631	C ₄ H ₁₀ O ₃	Diethylene glycol	111-46-6
1.5	576779.7	45378	89.5	689.2105	690.2178	C ₂₄ H ₄₂ O ₂₁	3-beta-Glucosylcellotriose	58484-04-1
						C ₃₁ H ₃₈ O ₁₆	Tetramethylquercetin 3-rutinoside	58528-03-3
3.7	336000.9	45469	67.2	160.1334	159.1262	C ₈ H ₁₇ NO ₂	DL-2-Aminooctanoic acid	664-90-6

16.3	459823.9	46108	108.3	666.3122	665.3055	C ₃₃ H ₄₁ N ₉ O ₅	Pro Arg Trp Trp	-
1.3	419168.8	46159	97.5	278.1233	277.116	C ₁₂ H ₁₅ N ₅ O ₃	Queuine	72496-59-4
						C ₁₀ H ₁₆ O ₄	Decenedioic acid	-
8.7	276770.1	46885	22.1	223.0943	222.087		Monoisobutyl phthalic acid	30833-53-5
						C ₁₂ H ₁₄ O ₄	APIOLE	523-80-8
							Valeroyl Salicylate	64206-54-8
9.1	301783.2	47379	28.7	377.1418	354.8403	C ₁₇ H ₂₀ N ₄ O ₆	Asp Gly Trp	-
						C ₁₆ H ₂₄ O ₁₀	(1x,2x)-Guaiacylglycerol 3-glucoside	7094-73-7
0.8	737335.5	48548	60.7	428.8816	426.8583	-	-	-
1.1	511520.8	48839	46.1	829.2805	828.2731	C ₃₀ H ₅₂ O ₂₆	Maltopentaose	34620-76-3
0.8	486004.2	48909	101.4	102.9702	101.9629	-	-	-
1.3	781880.7	49057	30.9	684.2552	683.2479	-	-	-
21.8	368189	49709	47	243.1354	244.1427	C ₁₄ H ₂₀ O ₂	13-Tetradecene-1,3-diyne-6,7-diol	122855-49-6

							Hexyl phenylacetate	5421-17-0
							13-Nor-6-eremophilene-8,11-dione	348119-85-7
						C ₁₁ H ₁₈ N ₂ O ₄	N-Hydroxypentobarbital	62298-51-5
0.9	264221.7	50026	48.6	177.9482	176.9409	-	-	-
0.9	298984.5	50660	56.2	300.914	299.9067	-	-	-
0.9	159836.2	50724	49.1	180.8945	179.8873	-	-	-
0.8	1189484	50747	80.1	501.8511	500.8438	-	-	-
							5-Hydroxymethyl-2-furaldehyde	67-47-0
1.1	803536.8	50909	48.6	127.0392	126.0319	C ₆ H ₆ O ₃	1,2,3-Trihydroxybenzene	87-66-1
9	333722.6	50942	75.8	363.1627	364.1699	C ₁₇ H ₂₂ N ₄ O ₅	Ser Trp Ala	-
						C ₁₃ H ₁₆ N ₄ O ₃	3'-Hydroxytrimethoprim	27653-69-6
14	349960.2	51088	4.6	299.1098	298.1026	C ₈ H ₁₉ N ₄ O ₆ P	Thalassemine	40524-74-1
17	450788.3	51315	87.2	680.3274	679.3202	-	-	-

3.5	488579.2	51482	49.3	184.0972	183.0899	C ₉ H ₁₃ NO ₃	Methylnoradrenaline	6539-57-7
9.2	320379.7	51505	71.9	215.1256	214.1183	-	-	-
7.7	315738.3	51766	32.4	114.0916	113.0843	C ₆ H ₁₁ NO	2-Acetylpyrrolidine	60026-20-2
16.1	545907.3	51849	121.8	666.3133	665.3064	C ₃₃ H ₄₁ N ₉ O ₅	Pro Arg Trp Trp	-
17.2	362463.5	52423	33.8	317.1355	318.1428	C ₁₆ H ₂₂ O ₅	Tocopheronic acid	1948-76-1
							Sorgolactone	141262-39-7
						C ₁₈ H ₂₀ O ₅	Flavokawin A	3791-75-1
							Combrestatin A4	117048-59-6
1.5	387197.6	52697	46.7	353.0924	352.0833	C ₁₁ H ₂₀ N ₄ O ₅ S ₂	Ala Cys Cys Gly	-
8.2	337304.6	52755	48.2	231.1205	232.1278	-	-	-
21.8	809393.2	52783	27.9	279.1592	278.1522	C ₁₆ H ₂₂ O ₄	Dibutyl phthalate	84-74-2
9.9	646483.1	53231	158	729.0641	728.0575	-	-	-
7.4	277577.8	53452	42.4	195.0629	194.0557	C ₈ H ₁₂ O ₄	Diethyl fumarate	623-91-6

							Ethyl 2,4-dioxohexanoate	13246-52-1
							3-Isopropenylpentanedioic acid	6839-75-4
							(-)-Corey Lactone Diol	32233-40-2
						C ₆ H ₆ N ₆ O ₂	Temozolomide	85622-93-1
0.9	129258.2	53656	33	304.8959	303.8886	-	-	-
1.2	524999.4	53735	78	272.0656	542.1166	C ₈ H ₁₅ N ₃ O ₄ S ₁	Gly Cys Ala	-
1.7	769954.7	54034	38.2	191.0229	190.0156	-	-	-
15.4	262088.4	54246	26.9	149.0234	148.0161	-	-	-
							L-Alanine n-butyl ester	2885-02-1
2	290094	54291	100.7	146.1177	145.1104	C ₇ H ₁₅ NO ₂	N,N-dimethyl-L-Valine	2812-32-0
11.8	937102.8	55130	17.2	331.2088	332.216	C ₁₃ H ₂₆ N ₆ O ₄	Gly Val Arg	-
						C ₁₉ H ₁₉ C ₁ N ₂	Descarboethoxyloratadine	100643-71-8
8.7	270223	55152	46.4	333.1159	332.1101	C ₁₄ H ₂₀ O ₉	Leonuriside A	121748-12-7

								1031799-40-2
0.9	331623.1	56031	25	212.1131	211.1058	C ₆ H ₁₅ N ₅ O ₂	NG-amino-L-Arginine	(HCl)
19	398585.2	56543	69.7	356.2796	355.2723	-	-	-
23.3	19896780	56876	17.5	108.5176	215.0206	-	-	-
14	712791.3	56902	77.5	216.1594	215.1524	C ₁₁ H ₂₁ NO ₃	Ethyl 3-(N-butylacetamido)propionate	52304-36-6
0.4	1449468	57076	24.1	141.9587	140.9515	-	-	-
8	253935.9	58544	55.2	289.0898	288.0825	C ₁₂ H ₁₆ O ₈	Glucosylisomaltol	85559-61-1
0.8	781763.3	58620	4.6	241.9996	240.9923	C ₈ H ₁₀ ClNO ₂ S	4-AMINO-3- (5-CHLOROTHIEEN-2-YL)BUTANOIC ACID	-
1	932866.6	58703	78.3	641.0904	640.0846	-	-	-
23.3	27481230	58835	19.1	115.964	114.9567	-	-	-
10.6	1096019	58910	39.6	273.1673	270.1447	C ₁₃ H ₄ D ₁₀ N ₂ O ₄	DMABA-d10 NHS ester	1175002-05-7
						C ₁₈ H ₂₁ FO	(R*,S*)-4-[1-Ethyl-2-(4-fluorophenyl)butyl]phenol	-
11.8	734404.4	59260	53.4	635.271	634.2641	C ₂₇ H ₃₆ N ₁₀ O ₇	Asp His Arg Trp	-

						C ₃₂ H ₄₂ O ₁₃	Myricanene A 5-[arabinosyl-(1->6)-glucoside]	-
10.6	486856.7	59334	61.4	657.3666	658.3738	C ₃₅ H ₅₄ O ₁₀	Digitoxigenin bisdigitoxoside	16479-50-8
0.8	687332.9	59491	38.8	130.9652	519.8329	C ₂ H ₄ C ₁₂ O ₂	2,2-Dichloro-1,1-ethanediol	16086-14-9
							3,4,5-Trimethoxytoluene	6443-69-2
8.6	451948.8	59909	45.3	183.1016	182.0943	C ₁₀ H ₁₄ O ₃	2-Oxo-delta3-4,5,5-trimethylcyclopentenylacetate	1130-49-0
							MEPHENESIN	59-47-2
1.5	385941.8	60118	154.2	522.2029	521.1956	C ₂₃ H ₃₁ N ₅ O ₇ S	Ala Asp Met Trp	-
11.7	420229.1	60871	43.8	229.141	230.1483	-	-	-
							L-erythro-5-(1-Hydroxyethyl)-2(5H)-furanone	54621-96-4
							Osmundalactone	69308-39-0
0.8	717113.9	61497	4.8	151.0354	150.0281	C ₆ H ₈ O ₃	Dihydro-4,4-dimethyl-2,3-furandione	13031-04-4
							6-hydroxy-2-hexynoic acid	-
1.5	294569.3	62226	154.1	465.2079	464.2008	C ₂₀ H ₂₈ N ₆ O ₇	Ala Asn Phe Asn	-

0.8	2356867	62657	101.9	436.8706	435.8633	-	-	
1.5	737383.6	62775	71.7	325.1132	326.1205	C ₁₃ H ₁₆ N ₄ O ₆	Levofuraltadone	3795-88-8
						C ₁₂ H ₂₀ O ₁₀	Bis-D-fructose 2',1:2,1'-dianhydride	3568-49-8
0.9	340399.3	63218	52.7	195.9588	194.9516	-	-	-
19.8	351740.4	64121	122.1	167.034	166.0267	C ₈ H ₆ O ₄	Terephthalic acid	100-21-0
6.6	411288.4	64455	80.6	231.084	230.0779	C ₈ H ₁₆ O ₆	Ethyl beta-D-glucopyranoside	3198-49-0
23.1	440259	64783	54.6	282.279	281.2718	C ₁₈ H ₃₅ NO	Elaidamide	4303-70-2
0.9	229785.5	65792	8.4	288.9219	287.9146	-	-	-
1	828196.4	66272	54.4	579.0997	1156.185	-	-	-
10.5	442159.8	66290	78.4	611.1607	610.1539	C ₂₇ H ₃₀ O ₁₆	Cyanidin 3-galactoside-5-glucoside	-
1.1	363338.9	66998	25.7	1028.821	1027.814	-	-	-
23.3	496855.3	67026	56.4	282.2792	281.272	C ₁₈ H ₃₅ NO	Elaidamide	4303-70-2
8.6	529337.5	67230	31.7	223.0944	222.0872	C ₁₀ H ₁₆ O ₄	Decenedioic acid	-

							Dillapiole	484-31-1
						C ₁₂ H ₁₄ O ₄	Monoisobutyl phthalic acid	30833-53-5
							Valeroyl Salicylate	64206-54-8
							2-amino-octadecanoic acid	-
23.9	503635.5	68196	55.3	300.2897	299.2825	C ₁₈ H ₃₇ NO ₂	Palmitoyl Ethanolamide	544-31-0
1.1	271772.6	70381	57.7	579.0994	578.0921	-	-	-
0.8	962928.7	70656	31.6	162.0074	160.0048	-	-	-
16.8	973175.3	70784	120.2	680.328	679.3212	-	-	-
12.5	518019.2	71378	87.3	619.276	618.2688	C ₂₄ H ₄₀ N ₁₀ O ₆ S	Cys Arg Arg Tyr	-
						C ₁₀ H ₁₀ O ₅	Vanilpyruvic acid	1081-71-6
0.9	626657.3	71390	31.3	233.0423	232.035	C ₁₂ H ₈ O ₅	4-Hydroxy-8-methoxy-2H-furo[2,3-h]-1-benzopyran-2-one	196503-96-5
1.3	1584331	71432	63.3	353.0923	704.172	C ₁₁ H ₂₀ N ₄ O ₅ S ₂	Ala Cys Cys Gly	-
1.1	836691.4	71771	50.5	516.1616	1030.309	C ₂₀ H ₂₉ N ₅ O ₇ S ₂	Cys Cys Gln Tyr	-

1.4	982871.5	72306	70.7	543.1322	542.1218	C ₃₀ H ₂₂ O ₁₀	Rugulosin	23537-16-8
16	393561.2	73565	58.8	225.196	224.1887	C ₁₃ H ₂₄ N ₂ O	Anapheline	19519-53-0
10.6	429716.9	73708	140.2	652.4111	651.4044	-	-	-
11.3	1509650	73770	66.5	635.2707	634.2641	C ₂₇ H ₃₆ N ₁₀ O ₇	Asp His Arg Trp	-
						C ₃₂ H ₄₂ O ₁₃	Myricanene B 5-[arabinosyl-(1->6)-glucoside]	-
6.7	885422.4	73885	26	236.0119	237.0192	C ₅ H ₁₂ NO ₄ PS	Omethoate	1113-02-6
11.2	675828.9	74273	64.7	637.2863	636.279	C ₃₈ H ₄₀ N ₂ O ₇	Calafatimine	77793-42-1
8	624458.4	74909	68.8	130.1592	129.152	C ₈ H ₁₉ N	Octylamine	111-86-4
8.5	454921.1	76311	44	319.1368	320.144	-	-	-
0.8	1044746	76400	17.7	99.5312	197.0478	-	-	-
							Isobutyric acid	79-31-2
1.6	351457.3	76473	129.2	89.0599	88.0526	C ₄ H ₈ O ₂	Propyl formate	110-74-7
							1-Hydroxy-2-butanone	5077-67-8

							1,4-Dioxane	123-91-1
							Ethyl acetate	141-78-6
							benzocaine	1994-09-7
1.2	448916.3	76600	81.4	166.0863	165.079	C ₉ H ₁₁ NO ₂	4-Hydroxy-1-(3-pyridinyl)-1-butanone	59578-62-0
							D-Phenylalanine	673-06-3
1.1	919849.8	76938	53	1047.299	2092.582	-	-	-
7.3	382653	76944	57.8	201.0735	200.0662	C ₈ H ₁₈ S ₂	Dibutyl disulfide	629-45-8
1.1	895076.3	77750	83.7	589.1284	588.1221	C ₃₁ H ₂₄ O ₁₂	Kolaflavanone	-
						C ₁₉ H ₁₄ O ₂	Bakers yeast extract	8013-01-2
1.6	714859.1	78266	104	297.0857	296.0784	C ₁₆ H ₁₂ N ₂ O ₄	5,5',6,6'-Tetrahydroxy-3,3'-biindolyl	-
							3,3'-Dimethoxybenzidine-4,4'-diisocyanate	91-93-0
10.4	439971.1	78397	112.9	608.3854	607.3782	-	-	-
19.8	422873.3	78436	39	149.0234	148.0161	-	-	-

							6-Hydroxypentadecanedioic acid	38076-52-7
						C ₁₅ H ₂₈ O ₅		
17.3	716473.4	78843	34.7	311.1849	310.178		1,2-Dihexanoyl-sn-glycerol	30403-47-5
						C ₁₇ H ₂₆ O ₅	3-Hydroxy-6,8-dimethoxy-7(11)-eremophilen-12,8-olide	162613-65-2
1.5	931301.6	79248	135.1	527.1582	528.1655	C ₂₁ H ₂₆ N ₄ O ₁₂	Asp Asp Asp Tyr	-
1	656954.5	80322	95.5	369.1054	736.1962	C ₁₇ H ₁₈ N ₂ O ₆	Nifedipine	21829-25-4
10.4	691533.3	80791	72	613.3408	614.3481	C ₃₀ H ₄₄ N ₈ O ₆	Phe Arg Lys Tyr	-
11.5	483412.1	81784	139.4	218.2115	217.2042	-	-	-
0.8	1081674	83205	25.9	81.5206	161.0266	-	-	-
11.4	831060	83718	230	230.0071	229.0001	C ₅ H ₁₂ NO ₃ PS ₂	DIMETHOATE	60-51-5
8.8	385662.1	84258	5.1	344.2279	343.2207	-	-	-
10.2	481211.4	85151	117.3	564.3588	563.3515	-	-	-
1.6	342516.5	85298	57.8	237.0915	236.0843	C ₈ H ₁₆ N ₂ O ₄ S	Methionyl-Serine	-
0.8	1041296	85977	53.6	146.0298	145.0226	-	-	-

1.6	278377.9	86212	118.3	213.1333	212.1261	-	-	-
1	634796.9	87342	121.3	132.0769	129.0794	C ₄ H ₉ N ₃ O ₂	3-Guanidinopropanoate	353-09-3
15.6	1219718	87709	250.5	943.5249	942.518	C ₄₈ H ₇₈ O ₁₈	Carnosifloside III	109985-92-4
11.4	447713.8	90027	110.1	198.9649	197.9576	-	-	-
1	542284.4	90844	78.9	127.0729	126.0656	C ₃ H ₆ N ₆	Melamine	108-78-1
10.2	794068.9	91832	96.4	569.3144	570.3216	C ₂₆ H ₄₄ N ₆ O ₆ S	Lys Lys Tyr Met	-
15.1	736128.8	91975	99.6	684.3797	683.3728	-	-	-
7.9	556268.2	93101	116.1	275.1107	276.1179	C ₁₀ H ₂₀ O ₇	2,3-Butanediol glucoside	146763-54-4
						C ₁₀ H ₁₆ N ₃ O ₆	Gamma-glutamyl-Glutamate	-
							5-Hydroxy-7-methoxy-8-C-methylflavanone	-
9.2	1163963	94906	56.3	307.0926	306.0858	C ₁₇ H ₁₆ O ₄	3,4-DIMETHOXYDALBERGIONE	41043-20-3
							LIQUIRITIGENIN DIMETHYL ETHER	95753-46-1
12.4	704573.2	94965	83.7	187.0396	186.0323	C ₁₁ H ₆ O ₃	Psoralen	66-97-7

1.1	2253280	95626	52.2	1031.325	1032.332	-	-	-
1.1	963316.8	96614	338.3	649.2179	648.2107	C ₂₄ H ₃₄ N ₈ O ₁₂	Tetrahydropteroyltri-L-glutamate	-
10	529106.4	97601	123.3	520.3328	519.3256	-	-	-
13.6	684659.3	97812	178.2	246.2426	245.2353	-	-	-
9.9	587552.6	99502	214.7	545.0594	544.0521	C ₂₁ H ₂₀ O ₁₅ S	8-Hydroxyluteolin 8-glucoside 3'-sulfate	63109-34-2
							7-Ethoxy-4-methyl-2H-1-benzopyran-2-one	87-05-8
21.8	822535.6	99631	72.7	205.086	204.0787	C ₁₂ H ₁₂ O ₃	Anofinic acid	34818-56-9
							3-Butylidene-7-hydroxyphthalide	93236-67-0
10	829628.5	99781	100.6	525.2884	526.2957	C ₂₄ H ₄₀ N ₆ O ₅ S	Cys Phe Lys Lys	-
19	727857	101015	69	297.2425	296.2352	C ₁₈ H ₃₂ O ₃	(±)13-HODE	73804-64-5
						C ₁₂ H ₂₀ O ₄	9,12-dioxo-dodecanoic acid	-
9.3	586982.6	101468	47	251.1255	250.1182		Diisopropyl phthalate	605-45-8
						C ₁₄ H ₁₈ O ₄	Ubiquinone-1	727-81-1

							δ -CEHC	1221504-67-1
1.6	508604.9	102311	113.9	179.1179	178.1107	C ₁₀ H ₁₄ N ₂ O	Glycine xylidide	18865-38-8
9.7	842916.3	103787	114.7	481.2621	482.2693	C ₂₃ H ₃₆ N ₄ O ₇	Phe Thr Ile Thr	-
							Methyl beta-D-glucopyranoside	709-50-2
1	787607.3	104583	98.8	217.0684	216.0612	C ₇ H ₁₄ O ₆	QUEBRACHITOL	642-38-6
2.1	8774786	104624	57	129.0525	128.0452	C ₄ H ₁₀ O ₃	Diethylene glycol	111-46-6
9.7	548629.3	104956	138.5	476.3067	475.2994	C ₂₂ H ₄₈ NO ₆ P	PC(O-12:0-O-2:0)	-
7.1	723223.9	105274	92	187.0944	188.1017	C ₅ H ₁₀ N ₆ O ₂	Dinitrosopentamethylenetetramine	101-25-7
15.8	694740.7	106746	124.8	158.1539	157.1466	-	-	-
9.2	518950	107437	112.8	388.2543	387.247	C ₁₇ H ₃₃ N ₅ O ₅	Ala Ala Lys Val	-
2.4	627480.2	107733	238.6	100.1123	99.105	C ₆ H ₁₃ N	2-Methylpiperidine	109-05-7
10.8	513664.8	109040	59.7	163.0392	162.0319	C ₉ H ₆ O ₃	UMBELLIFERONE	93-35-6
1.6	723502.7	112177	196.5	266.0451	265.0378	C ₁₀ H ₁₃ NO ₄ S	Mono-N-depropylprobenecid	10252-65-0

21.7	1365294	112903	59.6	279.1592	278.1522	C ₁₄ H ₂₄ O ₄	Monomenthyl succinate	188709-97-9
						C ₁₆ H ₂₂ O ₄	Diisobutyl phthalate	84-69-5
9.5	546749.2	113955	288.6	432.281	431.2738	C ₁₉ H ₃₇ N ₅ O ₆	Ala Lys Leu Thr	-
1.1	1145509	113969	78.5	1009.344	1008.336	-	-	-
21.7	713794.7	119328	87.1	205.0861	204.0788	C ₁₂ H ₁₂ O ₃	Anofinic acid	34818-56-9
							3-Butylidene-7-hydroxyphthalide	93236-67-0
9.5	879937.1	120040	64	437.2363	438.2436	C ₂₁ H ₃₂ N ₄ O ₆	Ala Ala Tyr Ile	-
9.2	938549.4	122481	125.3	393.2095	394.2168	C ₁₉ H ₂₈ N ₄ O ₅	Ala Phe Gly Val	-
						C ₂₅ H ₂₈ O ₄	Glabrol	-
							7,4'-Dihydroxy-6,8-di-C-prenylflavanone	-
19	891656	122701	86.4	279.2318	278.2246	C ₁₈ H ₃₀ O ₂	10E,12E,14E-Hexadecatrienyl acetate	-
							3E,9Z,12Z-octadecatrienoic acid	-
8.8	963253.1	131375	130	349.1835	350.1907	C ₁₆ H ₂₈ O ₈	(1S,2S,4R,5S,7S)-2,5,7-Fenchanetriol 2-O-b-D-glucoside	217960-85-5

							Foeniculoside VIII	219583-13-8
						C ₁₂ H ₂₄ N ₆ O ₆	Ser Ser Arg	-
0.9	440260.3	138522	63.1	150.1127	149.1054	C ₆ H ₁₅ NO ₃	Trolamine	102-71-6
0.8	2807301	139565	148.7	474.8332	473.8259	-	-	-
23.4	50420036	143497	23.6	99.5123	197.0101	-	-	-
1.1	1710231	146592	293.6	505.1762	504.1692	C ₁₈ H ₃₂ O ₁₆	alpha-D-Glucopyranosyl-(1->6)-alpha-D-glucopyranosyl-(1->2)-D-glucose	40983-70-8
						C ₂₃ H ₂₈ N ₄ O ₇ S	Cys Gly Tyr Tyr	-
3.4	1288340	148816	82.7	173.0787	174.086	-	-	-
0.8	1742794	149780	39.4	239.9665	238.9592	-	-	-
0.8	2238259	160238	210.9	344.8753	343.8688	C ₈ HC ₁₄ F ₃ N ₂	4,5,6,7-Tetrachloro-2-trifluoromethylbenzimidazole	2338-29-6
21.7	966462.5	160279	79.6	149.0235	148.0162	-	-	-
8.4	1210031	164208	178.3	305.1574	306.1647	-	-	-
-0.8	2134545	167521	29	90.5259	179.0373	-	-	-

6.4	1411354	168382	112.9	217.1049	218.1122	-	-	-
9.6	1129605	168828	33.5	212.1184	211.1112	C ₁₃ H ₁₃ N ₃	Varenicline	249296-44-4
7.8	1223030	171134	275.3	261.1311	262.1384	C ₁₂ H ₂₀ O ₆	Glycerol tripropanoate	139-45-7
17.4	1261417	171401	172.9	401.1592	400.1523	C ₁₅ H ₂₄ N ₆ O ₅ S	Ala Ala Cys His	-
0.8	2117061	175166	150.5	380.8966	379.8893	-	-	-
25	1699958	176342	232.1	256.2632	255.2559	C ₁₆ H ₃₃ NO	Palmitic amide	629-54-9
0.8	2649421	180288	4006. 4	492.8438	491.8366	-	-	-
0.8	2228431	189123	31.2	234.9611	233.9539	C ₇ H ₇ O	2-Iodophenol methyl ether	-
0.8	2284120	190048	2111. 6	198.94	197.9327	-	-	-
0.8	2801875	193581	32.4	362.8859	361.8793	C ₁₂ H ₈ C ₁₆	ALDRIN	309-00-2
1.1	2386787	199090	374.4	487.1656	486.1583	C ₂₀ H ₃₀ N ₄ O ₆ S ₂	Ala Cys Met Tyr	-

15.6	2462854	202587	167.8	318.3002	317.293	C ₁₈ H ₃₉ NO ₃	Phytosphingosine	-
19	1776963	212361	156.1	337.2349	314.4753	C ₁₈ H ₃₄ O ₄	9,10-dihydroxy-12-octadecenoic acid	-
0.8	2634564	213108	164.3	257.9771	256.9698	-	-	-
9.9	1755358	213952	467.7	691.1174	690.1105	C ₂₇ H ₃₀ O ₁₉ S	Kaempferol 3-(6''-sulfatogetiobioside)	-
1.1	2209205	223045	243.5	776.235	1550.456	-	-	-
16.1	2191768	232275	548.2	797.4666	796.4598	C ₄₂ H ₆₈ O ₁₄	Jujubasaponin VI	146445-94-5
0.8	2906972	254438	34.3	216.9505	215.9433	-	-	-
1.1	3299686	276960	316.4	325.113	324.1057	C ₁₃ H ₁₆ N ₄ O ₆	Levofuraltadone	3795-88-8
24.2	1848552	279527	196.5	398.2326	397.2253	C ₂₄ H ₃₁ NO ₄	Drotaverine	985-12-6
0.8	2743515	282097	21.3	255.9441	253.9247	-	-	-
0.8	3091203	333203	6.7	273.9547	272.9474	-	-	-
2.4	2067288	345497	640.9	146.1178	145.1105	C ₇ H ₁₅ NO ₂	2R-aminoheptanoic acid	-
1.6	2890217	356379	181.7	163.1231	162.1159	C ₁₀ H ₁₄ N ₂	L-Nicotine	54-11-5

11.2	6432258	468420	200.8	185.115	186.1223	C ₈ H ₁₈ O ₃	(3R,7R)-1,3,7-Octanetriol	217650-11-8
0.8	4664973	490043	144.1	250.9388	249.9315	-	-	-
1.1	8360441	498040	848.8	527.1582	526.1497	C ₂₁ H ₂₆ N ₄ O ₁₂	Asp Asp Asp Tyr	-
1.1	4917180	523253	49.1	524.1506	1046.287	C ₁₈ H ₂₇ N ₇ O ₈ S	Cys Glu Asn His	-
0.8	6769420	537126	211.1	143.9968	142.9896	-	-	-
1.1	6359267	556187	1426. 6	522.2029	521.1956	C ₂₃ H ₃₁ N ₅ O ₇ S	Ala Asp Met Trp	-
0.8	7319421	625464	545	128.0193	127.012	-	-	-
7.7	2948171	651869	708.6	206.0451	205.0378	C ₁₀ H ₇ NO ₄	6-Hydroxykynurenate	3778-29-8
15.4	6801574	655451	980.7	274.2741	273.2668	C ₁₆ H ₃₅ NO ₂	C16 Sphinganine	-
1.1	14047175	691576	1003. 4	272.0658	542.1208	C ₈ H ₁₅ N ₃ O ₄ S	Cysteinyl-Gamma-glutamate	-
1.6	3516920	713224	550.8	126.0441	250.0741	-	-	-

0.8	9018643	777100	666.7	110.0087	109.0014	-	-	-
0.8	7785947	789291	315.9	232.9282	231.9209	C ₇ H ₅ Cl ₃ O	2,4,6-Trichloroanisole	87-40-1
1.6	9645236	956032	724.9	107.0705	106.0635	C ₄ H ₁₀ O ₃	Diethylene glycol	111-46-6
0.8	9541449	975668	356.5	214.9176	213.9104	-	-	-
0.8	16288420	1541158	439.7	125.9863	124.979	-	-	-

Table S3. Compounds information of R1 in negative ionization modes.

Retention Time (min)	Area	Intensity	S/N	Max. <i>m/z</i>	Max. MW	Formula	Possible Name	CAS
9.1	47215.16	10039	18	199.0067	200.014	-	-	-
0.8	413671.03	10233	27.1	1052.7051	3161.1372	-	-	-
1.6	52835.08	10243	21.1	117.0192	118.0265	C ₄ H ₆ O ₄	4-Hydroxy-2-oxobutanoic acid	22136-38-5
							Methyl oxalate	553-90-2
10.1	62246.99	10292	9.6	485.2226	486.2299	C ₂₀ H ₃₄ N ₆ O ₆ S	His Ile Met Ser	-
6	69618.71	10316	15.4	287.0439	288.0512	C ₁₁ H ₁₂ N ₂ O ₅	N5-(3,4-Dioxo-1,5-cyclohexadien-1-yl)-L-glutamine	30382-25-3
0.9	26927.59	10395	30	514.8315	515.8388	-	-	-
0.8	353945.97	10455	64.5	1006.7086	2009.4252	-	-	-
7.5	45536.3	10455	116.2	271.049	272.0563	C ₁₁ H ₁₂ N ₂ O ₄	L-Formylkynurenine	1022-31-7

0.9	85272.01	10518	5.3	684.6773	685.6845	-	-	-
							1,1-Dimethylethyl benzoate	774-65-2
							4-t-Butylbenzoic acid	98-73-7
12	49684.85	10544	19.6	177.0917	178.099	C ₁₁ H ₁₄ O ₂	Methyleugenol	93-15-2
							PPHP	87864-20-8
0.8	274007.41	10579	40.6	1011.6951	2025.4047	-	-	-
						C ₁₄ H ₂₆ O ₆	1-Octen-3-yl glucoside	209863-00-3
							Licarin A	51020-86-1
16.1	59802.82	10690	15.1	325.1437	326.151	C ₂₀ H ₂₂ O ₄	Dehydrodieugenol	4433-08-3
							Uncinatone	99624-92-7
1.6	55871.98	10700	11.2	397.0653	398.0726	C ₁₂ H ₂₂ N ₄ O ₅ S ₃	Ala Cys Cys Cys	-
10	316183	10821	17.9	225.0793	226.0866	C ₁₁ H ₁₄ N ₂ O	5-Methoxytryptamine	608-07-1
0.8	35395.17	10899	121.1	774.7469	1551.5083	-	-	-

0.9	85341.04	11096	12.9	690.6887	691.6915	-	-	-
1.3	53751.16	11151	8.6	108.9964	110.0037	C ₂ H ₆ O ₃ S	METHYLMETHANE SULFONATE	66-27-3
0.8	36383.89	11265	125.2	424.9111	425.9184	-	-	-
0.8	300190.19	11279	8.7	946.7152	1895.445	C ₅₂ H ₁₀₁ NO ₁₃	LacCer(d18:0-22:0)	-
0.8	44009.58	11342	27.4	638.7735	639.7758	-	-	-
0.8	36689.9	11355	13.3	294.8928	295.9	-	-	-
1.4	55012.28	11356	25.3	100.9461	203.9065	-	-	-
12.1	64998.54	11425	16.2	207.1022	208.1094	C ₁₂ H ₁₆ O ₃	(Z)-3-Oxo-2-(2-pentenyl)-1-cyclopenteneacetic acid	120282-76-0
							beta-Asarone	5273-86-9
							Primin	15121-94-5
							Benzyl (2R,3S)-2-methyl-3-hydroxybutanoate	-
24.1	517788.34	11460	9.4	297.1516	298.1589	C ₁₉ H ₂₂ O ₃	4-(3-Hydroxy-7-phenyl-6-heptenyl)-1,2-benzenediol	158697-56-4
							5-Hydroxy-7-(4-hydroxyphenyl)-1-phenyl-3-heptanone	83161-96-0

							Gravelliferone	21316-80-3
1.6	50444.87	11473	9.9	228.0181	229.0254	-	-	-
0.9	83984.7	11506	9.2	548.7577	549.7649	-	-	-
1.2	39420.6	11626	4.9	170.9788	171.986	-	-	-
1	117694.27	11731	14.5	154.9177	155.925	-	-	-
0.9	30147.09	11748	8.1	412.7622	413.7694	-	-	-
0.8	44989.86	11750	99.6	554.8685	555.8758	-	-	-
0.8	38854.73	11919	6.9	706.7604	707.7677	-	-	-
0.8	42257.32	11972	133	814.7771	815.7844	-	-	-
0.9	160062.59	12159	4.4	608.6974	609.7047	-	-	-
10.8	60669.43	12231	20	193.0536	194.0609	C ₁₀ H ₁₀ N ₂	1-Benzylimidazole	4238-71-5
						C ₈ H ₁₀ N ₄ S	Benzaldehyde, p-amino-, thiosemicarbazone	6957-91-1
0.9	40089.82	12236	58.2	644.7904	645.7977	-	-	-

0.8	226632	12435	89.3	751.779	1505.5724	-	-	-
8	50906.56	12507	139	265.0924	266.0997	C ₁₁ H ₁₄ N ₄ O ₄	1-(3-Carboxypropyl)-3,7-dimethylxanthine	6493-07-8
1.2	51798.42	12514	38.2	94.9807	95.988	CH ₄ O ₃ S	Methanesulfonic acid	75-75-2
						H ₄ O ₄ Si	Silicic acid	10193-36-9
0.8	284590.59	12665	73.3	922.7481	1847.5108	-	-	-
11.9	66589.23	12806	21.8	149.0606	150.0679	C ₉ H ₁₀ O ₂	hydrocinnamic acid	501-52-0
							4-Ethoxybenzaldehyde	10031-82-0
							Phenyl glycidyl ether	122-60-1
							Tolylacetate	140-39-6
18.5	81279.27	12955	25.3	266.1022	267.1095	C ₈ H ₁₇ N ₅ O ₃	Glycyl-Arginine	-
11.9	95755.83	12995	39.4	182.0092	183.0165	C ₂ H ₅ N ₅ O ₃	N-Methyl-N'-nitro-N-nitrosoguanidine	70-25-7
0.8	39998.11	13091	44.5	768.7905	769.7977	-	-	-
13.1	83021.62	13111	24.5	133.0114	134.0187	-	-	-

0.9	174320.77	13181	5.8	706.661	707.6683	-	-	-
1.3	47060.04	13202	8.1	152.9862	153.9935	C ₄ H ₁₀ S ₃	2,4,6-Trithiaheptane	6540-86-9
						C ₁₄ H ₂₆ O ₆	1-Octen-3-yl glucoside	209863-00-3
15.6	75187.82	13257	18.7	325.1437	326.151		Dehydrodieugenol	4433-08-3
						C ₂₀ H ₂₂ O ₄	Uncinatone	99624-92-7
9.1	128021.18	13264	16.4	229.0173	230.0246	C ₁₃ H ₁₀ S ₂	5-(1-Propynyl)-5'-vinyl-2,2'-bithiophene	17257-06-6
0.9	96553.82	13406	4.3	434.8212	435.8285	-	-	-
0.9	46862.11	13462	15.6	532.7093	533.7166	-	-	-
							Phytuberin	37209-50-0
16.9	77762.77	13471	12.3	293.1747	294.182	C ₁₇ H ₂₆ O ₄	Gingerol	58253-27-3
							Embelin	550-24-3
						C ₁₆ H ₁₈ N ₂	NOMIFENSIN	32795-47-4
14.2	89280.72	13569	19.9	273.1158	274.1231	C ₁₆ H ₁₈ O ₄	Batatasin II	39354-56-8

							HETEROPEUCENIN, METHYL ETHER	26213-95-6
1	75472.52	13595	34.4	181.9373	182.9445	-	-	-
22.2	87706.95	13688	28.4	311.2003	312.2076	C ₂₁ H ₂₈ O ₂	Ethisterone	434-03-7
						C ₁₇ H ₂₄ N ₄ O ₈	Gly Ser Ser Tyr	-
18.5	112037.92	13763	34.1	447.1324	448.1397		Homobutein 4'-O-glucoside	-
						C ₂₂ H ₂₄ O ₁₀	5-Hydroxy-3,6,7,8,3',4',5'-heptamethoxyflavone	-
1.6	78006.38	13916	30	185.012	186.0193	C ₆ H ₁₀ CaO ₄	Calcium propionate	4075-81-4
0.9	64908.4	13927	30.8	516.7389	517.7462	-	-	-
20.2	100958.09	13979	22.1	267.1953	268.2026	C ₁₆ H ₂₈ O ₃	Methoprene acid	53092-52-7
						C ₁₃ H ₁₆ N ₂ O ₆	Val-Ala-OH	-
							3-Glucogallic acid	91984-84-8
7.7	64787.62	14024	7.1	331.0699	332.0772		4-Glucosyl gallate	84274-52-2
						C ₁₃ H ₁₆ O ₁₀	1-O-Galloyl-beta-D-glucose	554-37-0

9.8	71265.23	14042	27	441.1972	442.2044	C ₁₉ H ₃₀ N ₄ O ₈	Glu Pro Pro Thr	-
15.6	101180.7	14156	34.1	262.9755	263.9828	C ₁₃ H ₈ S ₂	Thiarubrine A	63543-09-9
1.5	87226.11	14162	24.5	182.9967	184.0039	C ₅ H ₁₂ OS ₃	Methyl 1-(methylsulfinyl)propyl disulfide	134018-95-4
16.2	108438.77	14218	12	243.1594	244.1667	C ₁₃ H ₂₄ O ₄	2-methyl-dodecanedioic acid	-
8.1	63333.16	14466	15.3	243.1234	244.1307	C ₁₂ H ₂₀ O ₅	Polyethylene, oxidized	68441-17-8
0.8	48614.53	14538	7.3	684.8267	685.8339	-	-	-
14.4	72312.5	14555	37.7	242.1755	243.1828	-	-	-
12.2	77974.04	14590	19.3	235.0639	236.0711	C ₁₂ H ₁₂ N ₂ O	4,4'-Diaminodiphenyl ether	101-80-4
						C ₁₀ H ₁₂ N ₄ OS	Thiacetazone	104-06-3
1.6	82736.31	14802	26.9	101.0242	102.0315	C ₄ H ₆ O ₃	Acetic anhydride	108-24-7
							Succinic acid semialdehyde	692-29-5
14.1	80148.45	14853	19.4	351.2168	352.224	C ₂₀ H ₃₂ O ₅	13,14-Dihydro-15-keto-PGE2	363-23-5
1.6	90508.59	14880	48	277.0284	278.0366	C ₁₄ H ₁₀ O ₄	hydrous benzoyl peroxide	94-36-0

							3-(2-Carboxyvinyl)naphthalene-2-carboxylic acid	-
							6,2'4'-Trihydroxy-2-phenylbenzofuran	-
							2-BENZOYL-5-METHOXYBENZOQUINONE	-
0.8	123999.37	14902	44.1	876.7511	877.7583	-	-	-
0.8	550134.13	14911	165.7	1084.6602	2171.335	C ₅₄ H ₉₉ NO ₁₈	Trihexosylceramide (d18:1-9Z-18:1)	-
9.6	72050.19	14922	35.4	199.0069	200.0142	-	-	-
15.3	88128.98	14945	31	197.02	198.0273	C ₇ H ₆ N ₂ O ₅	DNOC	534-52-1
8.7	69738.13	14953	166.1	309.1184	310.1257	C ₁₉ H ₁₉ ClN ₂	Descarboethoxyloratadine	100643-71-8
14.6	131486.22	15143	25.3	118.9924	119.9997	-	-	-
14.6	131970.2	15143	25.3	118.9924	119.9997	-	-	-
0.8	270860.44	15294	169.9	873.7475	1749.5095	-	-	-
7.2	83386.8	15405	27.7	199.007	200.0143	-	-	-
9.5	163682.45	15735	14.9	397.1705	398.1778	C ₁₇ H ₂₆ N ₄ O ₇	Ala Pro Asp Pro	-

14.2	89084.82	15748	11	299.0951	300.1024	C ₁₇ H ₁₆ O ₅	Methylnissolin	-
							Isosativanone	-
0.9	61728.64	15852	4.5	174.9379	175.9451	-	-	-
0.8	39470.94	15897	176.6	440.8281	441.8354	-	-	-
0.7	97706.04	15998	8.2	321.904	322.9113	-	-	-
1.2	65165.95	16019	36.1	292.8946	293.9019	-	-	-
16.2	90902.53	16494	34.2	197.02	198.0273	C ₇ H ₆ N ₂ O ₅	DNOC	534-52-1
1	112194	16541	25.4	170.8841	171.8914	C ₂ H ₂ BrClO ₂	Bromochloroacetic acid	5589-96-8
9.1	71480.49	16819	186.9	353.1444	354.1517	C ₁₄ H ₂₆ O ₁₀	Isopropyl apiosylglucoside	147742-24-3
							Naringenin trimethyl ether	-
14.8	229650.48	16881	18	313.1109	314.1182	C ₁₈ H ₁₈ O ₅	p-Hydroxyphenethyl trans-ferulate	84873-15-4
							2'-Hydroxy-4,4',6'-trimethoxychalcone	3420-72-2
1.3	175468	16892	15.1	136.9912	137.9985	-	-	-

0.9	26302.25	16901	375.6	390.8304	391.8377	-	-	-
1.5	131458.11	16931	33.2	225.007	226.0142	C ₁₀ H ₁₀ O ₂ S ₂	Bis(2-furanylmethyl) disulfide	4437-20-1
0.8	248153.44	17036	189.3	816.758	817.7653	-	-	-
0.8	47157.9	17389	193.2	638.8327	639.84	-	-	-
0.8	166826.53	17436	7.2	130.9665	131.9738	-	-	-
13.6	102520.66	17802	52.6	236.0957	237.103	-	-	-
1.5	149713	18137	11.1	152.9862	153.9935	C ₄ H ₁₀ S ₃	Ethyl (methylthio)methyl disulfide	183554-12-3
0.8	317809.03	18164	201.8	792.7901	1587.5947	-	-	-
							2',4'-Dihydroxy-4,6'-dimethoxychalcone	-
13.5	98679.98	18224	12.7	299.0949	300.1022	C ₁₇ H ₁₆ O ₅	(S)-3'-Hydroxy-4,4'-dimethoxydalbergione	-
							4-Methoxymedicarpin	-
0.8	36636.71	18252	30.5	508.876	509.8832	-	-	-
0.8	50458.38	18269	42.3	576.8026	577.8099	-	-	-

						C ₁₂ H ₂₆ N ₄ O ₃	Lysyl-Lysine	-
17.2	138281.34	18640	22.3	309.17	310.1772			
						C ₁₇ H ₂₆ O ₅	Valdiate	162232-32-8
0.8	252300.02	18679	19.6	130.9832	131.9904	-	-	-
5.7	24784440	18734	5.3	146.9644	147.9717	-	-	-
							(1R,2R,4R,8R)-p-Menthane-2,8,9-triol	212516-28-4
15.7	107939.25	18808	43.3	187.1334	188.1407	C ₁₀ H ₂₀ O ₃		
							2-hydroxy capric acid	-
1.2	102081.45	18867	10.5	215.0229	216.0302	C ₈ H ₈ N ₂ O ₃	Nicotinuric acid	583-08-4
6.4	135473.45	18889	33.9	199.0067	200.014	-	-	-
0.9	60099.32	19284	17.7	494.7571	495.7644	-	-	-
0.9	78959.05	19639	19.5	198.923	199.9303	-	-	-
0.8	47738.17	19674	28.2	508.8151	509.8224	-	-	-
1.3	194861.61	19936	32.2	98.9545	199.9238	-	-	-
0.9	63079.77	20000	51.3	446.8447	447.852	-	-	-

1.2	104995.71	20176	26.4	79.9572	80.9644	-	-	-
18.3	121046.42	20643	31.3	194.0817	195.089	C ₁₀ H ₁₃ NO ₃	alpha-Methyl-m-tyrosine	305-96-4
0.8	216968.59	20740	172.3	892.7329	1787.4803	-	-	-
0.9	70829.79	20740	33.6	390.78	391.7873	-	-	-
0.8	77398.07	20774	45.2	356.9236	357.9309	-	-	-
0.8	276897.5	21213	235.7	662.8323	663.8396	-	-	-
0.9	325129.03	21248	7.8	586.7124	587.7196	-	-	-
0.8	54203.23	21249	472.2	294.9533	295.9605	-	-	-
15.1	146285.61	21621	69.2	682.3633	683.3706	-	-	-
13.9	123606.09	22695	33.9	193.09	194.0972	-	-	-
							Hydroxyibuprofen	51146-55-5
15.7	151870.86	23041	39.9	221.1179	222.1251	C ₁₃ H ₁₈ O ₃	Isoamyl p-anisate	27739-29-3
							Dehydrovomifoliol	15764-81-5

0.8	95757.75	23312	66.6	830.7576	831.7649	-	-	-
0.9	229200.92	23780	8.5	570.7406	571.7479	-	-	-
0.9	97849.01	23884	66.9	358.8393	359.8466	-	-	-
0.8	99300.31	24002	533.4	746.7967	747.804	-	-	-
2	310752.88	24258	7.5	96.9599	97.9672	H ₂ O ₄ S	Sulfuric acid	7664-93-9
0.9	81293.27	24743	27.5	396.7902	397.7975	-	-	-
0.9	229886.67	25631	6.3	466.7628	467.7701	-	-	-
10.6	136079.16	25779	37.2	251.0589	252.0662	C ₁₂ H ₁₂ N ₂ O ₂	L-1,2,3,4-Tetrahydro-beta-carboline-3-carboxylic acid	42438--90-4
0.9	60644.37	25997	112.2	316.887	317.8942	C ₁₀ H ₇ C ₁₅ O	Tridipane	58138-08-2
0.9	211769.09	26455	9.7	488.7453	489.7526	-	-	-
0.8	68747.59	26906	109.1	310.9307	311.9373	C ₉ H ₁₄ Br ₂ O ₂	3,3-Dibromo-2-n-hexylacrylic acid	-
0.9	211085.48	27778	29.1	368.7963	369.8035	-	-	-
1.1	117136.84	27946	5.7	160.842	161.8492	-	-	-

1.1	169774.64	28295	4.9	162.8391	163.8464	-	-	-
1.3	167394.61	28689	9.9	210.9915	211.9988	C ₆ H ₄ N ₄ O ₃ S	2-Amino-5-(5-nitro-2-furyl)-1,3,4-thiadiazole	712-68-5
0.9	215621.78	29044	21.3	322.8435	323.8532	-	-	-
9.3	163104.45	29146	46.1	213.0223	214.0296	-	-	-
							Rubrofusarin	3567-00-8
11.7	200488.23	29231	15.4	271.0638	272.0711	C ₁₅ H ₁₂ O ₅	(±)-Naringenin	67604-48-2
							Butein	487-52-5
0.8	144062.45	30073	67.6	616.8393	617.8465	-	-	-
0.9	158016.84	30615	8.1	278.8796	279.8868	C ₆ H ₃ Cl ₃ O ₄	2,3,5-Trichloro-cis,cis-muconate	-
0.8	115626.27	31801	139	700.8023	701.8096	-	-	-
0.9	234337.67	31988	78.3	254.8577	511.7313	-	-	-
0.8	479683.28	32114	3.2	954.7027	1911.4199	-	-	-
0.9	242971.84	32569	16.8	314.8726	315.8799	-	-	-

0.9	160530.59	33570	45.7	238.8902	239.8975	-	-	-
8	193927.08	33936	81	178.0543	179.0616	C ₆ H ₁₃ NO ₃ S	Cyclohexylsulfamate	100-88-9
13.6	253528.11	34028	23.8	299.095	300.1023	C ₁₇ H ₁₆ O ₅	Sativanone	-
							Methylnissolin	-
0.9	304604.28	34310	13.1	472.7766	473.7839	-	-	-
9.9	173445.34	34555	31.6	257.0485	258.0557	C ₇ H ₁₅ N ₂ O ₄ P	cis-ACCP	777075-44-2
0.8	114206.34	34711	152.4	570.8455	571.8528	-	-	-
12.9	249686.14	36310	37.2	285.0793	286.0865	C ₁₆ H ₁₄ O ₅	Claussequinone	-
							Vesticarpan	-
							3'-Hydroxydihydroformononetin	-
							Brazilin	474-07-7
8.9	173929.3	36614	42.1	243.0329	244.0402	-	-	-
0.8	491230.63	36619	172.9	532.8746	533.8819	-	-	-

0.8	661358.81	36733	82.1	938.7255	1879.4655	-	-	-
0.9	110256.48	36882	89.6	260.873	261.8803	-	-	-
0.9	146708.59	37418	84.2	292.8948	293.9014	-	-	-
0.8	87132.89	37666	119.6	440.8886	441.8958	-	-	-
0.9	291122.88	39100	103.5	336.8572	337.8645	C ₁₂ H ₃ Cl ₅ O	1,2,3,7,8-Pentachlorodibenzofuran	57117-41-6
0.9	245351.27	39282	33.8	374.8079	375.8152	-	-	-
1.1	221153.03	39914	443.5	146.9657	147.973	-	-	-
1.6	212769.88	40392	119.5	261.0584	262.0657	C ₁₄ H ₁₄ O ₃ S	2-Thiopheneacetic acid, 5-(hydroxyphenylmethyl)- α -methyl-	54955-36-1
0.8	216385.81	40583	122.2	762.7742	763.7815	-	-	-
0.9	94810.45	40662	26.3	186.9293	187.9366	-	-	-
11.2	226199.33	42104	22.2	271.064	272.0713	C ₁₅ H ₁₂ N ₂ O	Glycosminine	4765-56-4
							2E,4E,8E,10E-Dodecatetraenedioic acid	-
12	218662.97	42730	44	221.0814	222.0887	C ₁₂ H ₁₄ O ₄	APIOLE	523-80-8

							Valeroyl Salicylate	64206-54-8
0.8	124528.48	42739	36.2	372.9011	373.9083	-	-	-
						C ₁₆ H ₁₄ N ₂ O	Methaqualone	72-44-6
							Melilotocarpin B	-
12.4	316017.06	43913	45	285.0795	286.0868			
						C ₁₆ H ₁₄ O ₅	Dihydrobiochanin A	-
							Brazilin	474-07-7
						C ₅ H ₁₀ S ₂	3,3-Dimethyl-1,2-dithiolane	58384-57-9
1.5	202470.86	44382	84	133.014	134.0213			
						C ₄ H ₆ O ₅	Velcorin	4525-33-1
							D-(+)-Malic acid	636-61-3
0.9	329769.13	46432	75.1	250.8848	251.8921	C ₅ H ₃ Cl ₃ O ₃	3-Chloro-4-(dichloromethyl)-5-hydroxy-2(5H)-furanone	77439-76-0
10.3	302011.94	47014	43.1	257.0485	258.0557	C ₇ H ₁₅ N ₂ O ₄ P	cis-ACCP	777075-44-2
0.8	122557.9	47971	30.7	310.8703	311.8776	-	-	-
1.2	372760.66	50516	106.9	232.8825	233.8897	-	-	-

0.8	674895.94	51671	292.4	402.9167	403.924	-	-	-
0.8	631690.44	52405	34.3	158.9786	159.9859	C ₇ H ₆ Cl ₂	2,4-Dichlorotoluene	95-73-8
0.9	177312.97	54063	600.7	226.9658	227.9731	C ₁₀ H ₅ ClO ₂	2-Chloro-1,4-naphthoquinone	1010-60-2
16.4	345701.06	56862	108.3	331.2478	332.2551	C ₁₈ H ₃₆ O ₅	9,10,13-Trihydroxystearic acid	50439-74-2
0.9	328022.59	57180	28.1	450.7916	451.7988	-	-	-
0.8	185945.13	61762	69.3	502.8591	503.8664	-	-	-
0.8	862540.44	62596	695.5	808.7678	1619.5502	-	-	-
14.6	620102.81	64507	70	184.984	185.9913	C ₄ H ₆ O ₆	Tartaric acid	87-69-4
0.8	235646.09	64569	86.1	632.8168	633.8241	-	-	-
0.9	158846.63	65630	94.8	248.8997	249.907	-	-	-
0.9	295809.78	67845	126.8	180.9125	181.9197	-	-	-
0.9	459223.97	68951	166.7	352.8262	353.8335	-	-	-
0.8	778203.25	75012	136.1	824.7453	825.7526	-	-	-

15.1	527731.75	76696	219.1	728.3687	729.376	-	-	-
0.8	883917.94	82410	1831.3	678.8101	679.8173	-	-	-
0.8	240697.59	87559	15	242.9434	243.9507	-	-	-
0.8	1464017.63	103337	4.6	272.9588	273.9661	C ₅ H ₁₁ AsO ₈	Ribose-1-arsenate	-
1.6	1619348.88	110443	34.2	96.9598	97.9671	H ₂ O ₄ S	Sulfuric acid	7664-93-9
13.7	668212.63	111240	165.5	183.0043	184.0116	C ₆ H ₄ N ₂ O ₅	2,4-DINITROPHENOL	51-28-5
0.8	1122843	112555	1250.6	694.7876	695.7948	-	-	-
0.8	1444724.13	122788	2728.6	548.8522	549.8595	-	-	-
0.9	914514.69	152340	270.3	330.8421	331.8488	-	-	-
0.8	1607299.75	152679	11.4	146.9612	147.9685	CH ₅ O ₄ P	Hydroxymethylphosphonate	-
0.8	1888754.25	160812	44.3	418.8943	419.9015	-	-	-
19	1150375.25	161910	238	313.2374	314.2447	C ₁₈ H ₃₄ O ₄	9,10-dihydroxy-12-octadecenoic acid	-
24.9	6320825	163064	134	297.1516	298.1588	C ₁₉ H ₂₂ O ₃	4-(3-Hydroxy-7-phenyl-6-heptenyl)-1,2-benzenediol	158697-56-4

							Doisynoestrol	15372-34-6
							Ostruthin	148-83-4
0.8	1803287.38	184236	696.4	564.8298	565.8371	-	-	-
0.9	429675.84	204162	78.2	112.9855	113.9928	C ₂ HF ₃ O ₂	trifluoroacetic acid	76-05-1
10.1	1058634.5	204693	587.5	213.9634	214.9707	-	-	-
1.2	975872.56	205514	124	194.9274	195.9347	-	-	-
0.8	2612348.5	260120	641	434.8718	435.8791	-	-	-
0.9	1933243.13	285005	344.4	216.9092	217.9165	-	-	-
0.8	3711385.25	301160	753.3	288.9364	289.9437	C ₇ H ₅ Cl ₂ FN ₂ O ₃	Fluroxypyr	69377-81-7
0.8	3519761.5	318565	30.4	174.9561	175.9634	C ₂ H ₅ O ₅ P	Acetyl phosphate	590-54-5
1.6	2249056.5	436984	765.5	119.0348	120.0421	C ₄ H ₈ O ₄	Glycolaldehyde dimer	23147-58-2
0.8	5060626.5	518820	187.6	304.9139	305.9212	-	-	-
0.9	20326802	2727154	843.7	96.9599	195.9339	H ₂ O ₄ S	Sulfuric acid	7664-93-9

Table S4. Compounds information of R1 in positive ionization modes.

Retention Time (min)	Area	Intensity	S/N	Max. <i>m/z</i>	Max. MW	Formula	Possible Name	CAS
0.9	556100.3	10005	24.8	702.6799	703.6871	C ₄₄ H ₈₉ NO ₃	Cer(d18:0-26:0)	-
0.9	64854.95	10005	3.4	387.8382	386.8318	-	-	-
9.5	49441.31	10022	11.2	453.2095	452.2023	C ₁₉ H ₂₈ N ₆ O ₇	Ala Glu His Pro	-
1.9	326387.2	10026	13	102.5311	101.5238	-	-	-
10.9	245078.8	10045	8	317.1931	315.1672	C ₁₆ H ₂₈ O ₆	Perilloside C	146763-94-2
							2-Methylpropyl 3-oxobutanoate	7779-75-1
							D-Linalool 3-glucoside	99096-59-0
							Ala Ala Arg	-
8.8	44015.93	10065	223.7	262.2016	261.1943	-	-	-

0.9	344739.2	10077	22.1	718.7125	719.7197	-	-	-
							Butyl formate	592-84-7
							(S)-2-Methylbutanoic acid	1730-91-2
7.1	51029.62	10093	13.2	103.0754	102.0681	C ₅ H ₁₀ O ₂	2,4-Dimethyl-1,3-dioxolane	3390-12-3
							Tetrahydro-2-furanmethanol	97-99-4
							Ethyl propionate	105-37-3
						C ₁₇ H ₂₆ N ₆ O ₄	Phe Gly Arg	-
21.6	164256.9	10127	2.7	401.1932	402.2005		Cortancyl	125-10-0
						C ₂₃ H ₂₈ O ₆	Gomisin L1 methyl ether	82467-51-4
0.8	54109.77	10144	225.4	211.9543	210.947	-	-	-
11.9	192149.3	10176	4.8	375.2351	373.2453	C ₁₅ H ₃₀ N ₆ O ₅	Arg Val Thr	-
0.9	64748.09	10182	11	251.9163	249.9128	-	-	-
22.2	172719.8	10231	13.1	590.4248	589.4175	-	-	-

							Amyl 2-furoate	4996-48-9
							Iridotrial	-
8	86641.47	10252	6.8	183.1012	182.0939	C ₁₀ H ₁₄ O ₃		
							3,4,5-Trimethoxytoluene	6443-69-2
							5-oxo-7-decynoic acid	-
							Valeric acid	109-52-4
							2,4-Dimethyl-1,3-dioxolane	3390-12-3
12.2	48293.57	10262	18.8	103.0754	102.0681	C ₅ H ₁₀ O ₂		
							2-Methylpropyl formate	542-55-2
							Ethyl propionate	105-37-3
							Anapear	189440-77-5
							xi-2,2,6-Trimethyl-1,4-cyclohexanedione	-
19.9	55794.36	10278	10.1	155.1068	462.3025	C ₉ H ₁₄ O ₂		
							4-oxo-2-Nonenal	103560-62-9
							2,6-nonadienoic acid	-
19.3	582554.3	10284	22.8	795.5414	796.5487	C ₄₁ H ₇₉ O ₁₂ P	PI(O-16:0-16:1(9Z))	-

0.8	117147.6	10294	5.2	200.9727	199.9655	-	-	-
0.9	121295.6	10332	14	578.7423	575.7042	-	-	-
11	88514.23	10343	25.6	729.3508	730.358	-	-	-
0.9	301320.7	10347	44.8	768.6166	769.6239	-	-	-
18.7	66818.54	10354	115	359.2387	358.2314	C ₁₅ H ₃₀ N ₆ O ₄	Arg Ile Ala	-
9.4	126936.6	10365	15.1	497.2562	496.2489	C ₂₂ H ₃₆ N ₆ O ₅ S	His Ile Met Pro	-
0.9	74935.69	10399	7.4	774.6194	1547.2242	-	-	-
22.4	75895.63	10425	8.5	228.2321	227.2249	C ₁₄ H ₂₉ NO	Halaminol A	-
0.9	120504.9	10458	21.2	796.6674	793.7025	C ₄₇ H ₈₉ NO ₈	GlcCer(d18:2-23:0)	-
							12-epi-LTB4	83709-73-3
						C ₂₀ H ₃₂ O ₄	PGF2α 1,11-lactone	62410-84-8
19	213333.2	10468	8	359.2186	358.2113		Piperoic acid	110979-04-9
						C ₂₂ H ₃₀ O ₄	tetramethyl Nordihydroguaiaretic Acid	24150-24-1

							CAFESTOL ACETATE	81760-48-7
20.1	70872.05	10493	8.3	259.1794	258.1722	-	-	-
9.4	49787.61	10525	9.3	134.0601	133.0528	C ₈ H ₇ NO	Oxindole	59-48-3
0.9	250375.2	10529	23.1	572.6812	565.7153	-	-	-
0.8	81335.03	10530	117	158.9276	157.9203	-	-	-
							Methyl acetyl ricinoleate	140-03-4
24.8	75202.57	10547	9.5	355.2809	354.2736	C ₂₁ H ₃₈ O ₄	2-Linoleoyl Glycerol	3443-82-1
							PGF2 α Alcohol methyl ether	143656-18-2
0.9	69405.46	10556	14.5	500.8348	499.8275	-	-	-
1.3	91959.92	10568	9.4	195.959	194.9518	-	-	-
11	54930.01	10576	10.3	188.0702	187.0629	C ₁₁ H ₉ NO ₂	3-amino-2-naphthoic acid	5959-52-4
11	71907.99	10576	10.3	188.0699	187.0626	C ₁₁ H ₉ NO ₂	Indoleacrylic acid	1204-06-4
0.9	48831.38	10602	117.8	434.8555	433.8482	C ₉ H ₈ I ₂ O ₄	3-(3,5-Diiodo-4-hydroxyphenyl)lactate	-

							1,1'-(Tetrahydro-6a-hydroxy-2,3a,5-trimethylfuro[2,3-d]-1,3-dioxole-2,5-diyl)bis-	
9.5	73002.05	10618	12.6	259.1154	258.1081	C ₁₂ H ₁₈ O ₆	ethanone	18114-49-3
9.1	162505.5	10622	19.1	495.1483	496.1556	C ₁₇ H ₂₄ N ₆ O ₁₀	Asp Asp His Ser	-
							5Z-Hexadecenyl acetate	-
22.5	175767.7	10641	3.3	283.2636	282.2563	C ₁₈ H ₃₄ O ₂	2Z-octadecenoic acid	-
0.9	212326.5	10664	8.9	330.8464	989.5587	-	-	-
21.8	55086.69	10673	11.1	307.1376	306.1303	C ₁₄ H ₁₈ N ₄ O ₄	Trimethoprim 1-N-oxide	27653-68-5
22.2	180238.7	10675	18.3	595.3801	594.3728	C ₄₀ H ₅₀ O ₄	7,8-Dehydroastaxanthin	19866-02-5
0.8	149788.8	10687	10.5	156.0139	155.0066	-	-	-
16.2	81861.36	10687	28.3	242.284	241.2767	C ₁₆ H ₃₅ N	1-Hexadecylamine	143-27-1
0.8	70919.84	10705	118.9	460.3668	459.3595	-	-	-
7.2	4567156	10712	6.1	209.9643	208.957	-	-	-
0.6	263658.3	10714	3.1	232.9799	231.9727	-	-	-

11	84893.15	10815	29.1	724.3957	723.3884	-	-	-
							Dimethyl succinate	106-65-0
0.7	143526.3	10825	5.7	169.0458	168.0385	C ₆ H ₁₀ O ₄	Mevaldate	541-07-1
							2-oxo-4-hydroxy-hexanoic acid	-
10.7	99393.97	10849	18.4	671.3453	672.3526	-	-	-
8	58940.25	10896	14.1	305.0602	304.053	C ₉ H ₁₈ N ₂ O ₄ S ₂	Homocysteine-penicillamine disulfide	22801-31-6
0.9	58698.52	10899	7.3	176.4937	175.4864			
							Ligustilide	4431-01-0
12.1	55781.7	10899	8.8	191.1067	190.0994	C ₁₂ H ₁₄ O ₂	Precocene I	17598-02-6
							3,5,7,9,11-dodecapentaenoic acid	-
14.4	52077.92	10902	11	173.1651	172.1579	-	-	-
8.6	53730.5	10916	242.6	190.1435	189.1363	-	-	-
1.7	116617.6	10928	24.4	314.0769	313.0696	C ₉ H ₁₆ ClN ₃ O ₇	Chlorozotocin	54749-90-5

0.8	143946.1	10952	24	275.9874	274.9801	C ₈ H ₁₀ AsNO ₅	ACETARSOL	97-44-9
10.9	150502.9	10975	12.9	362.223	722.4319	C ₂₁ H ₂₉ N ₃ O	Disopyramide	3737-09-5
11.9	77609.52	10990	15.7	306.2643	305.257	-	-	-
0.8	89102.49	10992	8.4	238.8871	237.8799	-	-	-
						C ₁₀ H ₁₀ O ₄	2E,4E,6E,8E-Decatetraenedioic acid	-
7.3	131961.8	11009	10.7	217.0474	216.0402		2,3-Naphthalenedicarboxylic acid	-
						C ₁₂ H ₈ O ₄	BERGAPTEN	484-20-8
						C ₁₇ H ₂₂ O ₃	Carbestrol	1755-52-8
17.9	276559.3	11035	6.2	297.1459	296.1387		(E)-Arachidin II	61517-87-1
						C ₁₉ H ₂₀ O ₃	Cryptotanshinone	35825-57-1
19.9	63677.96	11037	10.2	269.2106	268.2034	C ₁₆ H ₂₈ O ₃	Methoprene acid	53092-52-7
24.1	711991.9	11117	10.7	399.3074	398.3001	C ₂₃ H ₄₂ O ₅	1-Oleoyl-2-acetyl-sn-glycerol	86390-77-4
12.8	140160.3	11168	11.1	384.2949	383.2876	-	-	-

							Butyric acid	107-92-6
11.2	106920.5	11175	16.8	89.0598	88.0525	C ₄ H ₈ O ₂	1,4-Dioxane	123-91-1
							Ethyl acetate	141-78-6
0.8	159796.5	11225	23.9	348.8682	346.8479	-	-	-
17.7	253472.3	11238	12.2	457.2192	456.2119	C ₂₂ H ₂₈ N ₆ O ₅	Phe Gly His Pro	-
19	407576	11260	15.6	440.2769	439.2696	C ₁₈ H ₃₃ N ₉ O ₄	His Lys Arg	-
						C ₁₈ H ₃₀ O ₂	13Z-Hexadecen-11-ynyl acetate	-
22	81718.06	11266	7.8	279.2319	278.2246	C ₁₈ H ₃₀ O ₂	3E,9Z,12Z-octadecatrienoic acid	-
1.7	119002.5	11287	6.5	160.9897	159.9825	-	-	-
0.9	154227.8	11296	42.1	706.7418	1409.4567	-	-	-
20.7	73270.63	11306	13.1	443.2397	442.2324	C ₁₇ H ₃₀ N ₈ O ₆	Gly Asn Pro Arg	-
17.3	226253.1	11319	45.9	327.008	326.0013	C ₁₁ H ₁₃ Cl ₃ N ₂ O ₃	Fenuron-TCA	4482-55-7
0.8	84150.03	11325	7.9	334.9153	331.896	-	-	-

0.9	95344.32	11332	251.8	780.6799	781.6872	C ₄₉ H ₉₁ NO ₄	N-hexadecanoyl-35-aminobacteriohopane-32,33,34-triol	-
0.9	84653.58	11350	8.8	526.7722	524.7891	-	-	-
1.1	47808.3	11360	126.2	146.9967	145.9895	-	-	-
1.7	72369.52	11388	39.2	172.1699	171.1626	C ₁₀ H ₂₁ NO	N,2,3-Trimethyl-2-(1-methylethyl)butanamide	51115-67-4
10.7	62837.38	11407	20.9	666.3904	665.3831	-	-	-
9.5	60279.01	11413	8	353.1856	352.1783	C ₂₁ H ₂₄ N ₂ O ₃	Geissoschizine	439-66-7
0.8	127962.3	11415	12.1	132.9024	129.8989	-	-	-
0.9	108773.9	11423	16.7	430.7511	429.7443	-	-	-
8.5	52329.9	11429	10.1	335.1076	334.1003	C ₁₅ H ₂₀ O ₇	3-Hydroxychavicol 1-glucoside	-
15.5	106724.4	11437	3.3	229.0682	228.0609	C ₈ H ₁₄ O ₆	Diethyl tartrate	87-91-2
22.2	749767.4	11461	18.2	551.3547	552.362	C ₂₇ H ₄₆ N ₆ O ₆	Ile Lys Lys Tyr	-
16.4	69299.64	11462	4.5	315.2525	314.2452	C ₁₈ H ₃₄ O ₄	9,10-dihydroxy-12-octadecenoic acid	-
22.4	240642.8	11493	14.3	419.2763	420.2836	C ₂₅ H ₃₈ O ₅	Cavipetin D	128530-04-1

10.5	115154.9	11598	7.6	453.344	452.3367	C ₂₇ H ₄₆ N ₂ O ₂	Solanocapsine	639-86-1
1.5	60398.3	11617	4.8	186.0876	183.0885	C ₇ H ₁₁ N ₃ O ₃	(S)-N-(4,5-Dihydro-1-methyl-4-oxo-1H-imidazol-2-yl)alanine	176698-63-8
1.1	88295.23	11620	8.7	128.0194	127.0121	-	-	-
1.6	30363.73	11626	4.7	195.0179	194.0106	C ₇ H ₉ O ₃ P	Monomethyl phenylphosphonate	10088-45-6
7.3	53550.39	11629	16.7	103.0391	102.0319	C ₄ H ₆ O ₃	3-methyl pyruvic acid	600-18-0
1.6	216590.2	11635	14.9	277.0861	278.0934	C ₁₆ H ₁₄ O ₃	6-Methoxyflavanone	3034-04-6
9.2	107088.7	11650	5.9	448.2749	447.2676	C ₁₉ H ₃₇ N ₅ O ₇	Ile Ser Lys Thr	-
1.6	64399.04	11662	25.1	377.007	376.0007	-	-	-
15.3	176916.3	11664	6	503.3179	502.3107	C ₂₂ H ₄₂ N ₆ O ₇	Asp Ile Lys Lys	-
9.3	80013.44	11673	12	193.0841	192.0768	C ₁₁ H ₁₂ O ₃	Carpacin	23953-63-1
7.6	57134.85	11676	18	261.1314	260.1241	C ₁₂ H ₂₀ O ₆	ETHYL-p-COUMARATE	2979-06-8
13.1	209723.9	11685	8.1	403.2292	402.2219	C ₂₀ H ₃₄ O ₈	Glycerol tripropanoate	139-45-7
							Acetyl tributyl citrate	77-90-7

						C ₁₆ H ₃₀ N ₆ O ₆	Ala Ala Lys Asn	-
8	52257.99	11686	129.8	221.1018	220.0945	C ₁₀ H ₁₂ N ₄ O ₂	2,4-Diamino-6,7-dimethoxyquinazoline	60547-96-8
16.1	84003.47	11697	7.1	255.1588	254.1515	C ₁₄ H ₂₂ O ₄	C75	191282-48-1
							1,1-Dimethylethyl benzoate	774-65-2
17	59045.58	11701	10.8	179.107	178.0997	C ₁₁ H ₁₄ O ₂	4-t-Butylbenzoic acid	98-73-7
							Methyleugenol	93-15-2
0.9	90882.58	11719	7.4	197.9916	196.9843	-	-	-
18.9	71297.8	11729	6.7	170.0963	169.089	C ₁₂ H ₁₁ N	4-Biphenylamine	92-67-1
22.3	75614.52	11732	17.2	370.2004	369.1931	C ₁₅ H ₃₂ NO ₇ P	PC(7:0-0:0)	-
0.8	657716.1	11794	24.7	348.8682	695.7478	-	-	-
19	83549.34	11804	17.5	215.6272	429.2398	-	-	-
10.7	156161.7	11805	38	701.3923	700.3827	-	-	-
0.9	218704.4	11873	263.8	321.3986	640.7752	-	-	-

1.6	359058.6	11874	7.6	363.0277	364.035	-	-	-
0.9	33437.79	11884	23.7	458.7427	457.7354	-	-	-
0.9	76150.34	11909	51.5	814.7069	1624.3364	C ₄₈ H ₉₆ NO ₆ P	1-(2E-phytaenyl)-2-(2E-phytaenyl)-sn-glycero-3-phosphocholine	-
0.9	229481.4	11935	132.6	137.9817	136.9744	-	-	-
						C ₁₅ H ₂₂ N ₆ O ₈	Asp Gly His Ser	-
9.5	69681.11	11953	8	437.1402	436.133		Licoagroside F	-
						C ₂₁ H ₂₄ O ₁₀	Epiafzelechin 3-O-beta-D-glucopyranoside	-
							2-amino-octadecanoic acid	-
20.7	81578.85	11953	9.3	300.2894	299.2822	C ₁₈ H ₃₇ NO ₂	L-threo-Sphingosine C-18	25695-95-8
0.9	78712.79	11971	36.9	540.7426	537.7261	-	-	-
0.9	45772.94	11975	8.1	148.0972	147.0899	C ₆ H ₁₃ NO ₃	4-Hydroxyisoleucine	55399-93-4
0.8	44334.45	11984	266.3	218.4565	217.4492	-	-	-
10.6	79344.45	12019	9	287.1466	286.1393	C ₁₂ H ₂₄ O ₆	Hexyl glucoside	C12H24O6

0.8	271501.8	12025	133.6	336.4306	670.8466	-	-	-
0.8	85554.84	12045	267.7	191.4407	380.8668	-	-	-
							Toxyl angelate	106928-36-3
23.9	86027.05	12077	20.1	323.1239	322.1166	C ₁₈ H ₂₀ O ₄	2,2,4-Trimethyl-6-(1-oxo-3-phenylpropyl)-1,3,5-cyclohexanetrione	-
							4'-Hydroxy-5,7-dimethoxy-8-methylflavan	-
						C ₂₀ H ₃₂ N ₆ O ₄ S1	Phe Arg Met	-
9.2	135816.9	12137	13.4	453.231	452.2237	C ₂₇ H ₃₂ O ₆	DEOXYANDIROBIN	-
							1,4-Ipomeadiol	53011-73-7
8.7	80946.97	12174	11.6	171.0999	170.0926	C ₉ H ₁₄ O ₃	cis-3-Hexenyl pyruvate	68133-76-6
							Furfural diethyl acetal	13529-27-6
23.9	57474.32	12199	16.2	156.1382	155.1309	C ₉ H ₁₇ NO	3-(1-Pyrrolidinyl)-2-pentanone	97073-17-1
2.1	81507.55	12217	31	156.1383	155.1311	C ₉ H ₁₇ NO	3-(1-Pyrrolidinyl)-2-pentanone	97073-17-1
0.8	464008.1	12226	20.7	466.8455	465.8382	-	-	-

1.1	87043.76	12236	9.5	110.009	109.0017	-	-	-
8.1	88378.28	12256	10.9	192.0764	191.0692	C ₉ H ₉ N ₃ O ₂	Carbendazim	10605-21-7
16.5	74566.77	12291	15.6	215.6274	429.2402	-	-	-
2.4	2082240	12330	3.6	84.9598	83.9525	CH ₂ Cl ₂	Dichloromethane	75-09-2
1.2	80540.73	12365	274.8	280.9909	279.9836	C ₉ H ₁₁ BrN ₂ O ₂	Metobromuron	3060-89-7
13.2	60571.97	12369	14.3	225.0543	224.047	C ₁₂ H ₁₀ O ₃	Setarin	31005-07-9
							2-Napthylxyacetic acid	120-23-0
						C ₁₄ H ₈ O ₃	2,2',3-Trihydroxybiphenyl	91368-55-7
							Hydroxyanthraquinone	129-43-1
8.9	165585.7	12453	12.3	227.0903	226.083	C ₁₁ H ₁₄ O ₅	Dihydrosinapic acid	-
							ETHYL SYRINGATE	3943-80-4
0.7	163677	12456	6.1	179.0225	178.0153	C ₈ H ₉ ClO	chloroxlenol	88-04-0
0.8	48782.24	12459	138.4	170.9576	169.9504		-	-

10.9	118187.7	12467	9.3	287.1463	284.1244	C ₁₂ H ₂₄ O ₆	Hexyl glucoside	59080-45-4
10.8	74730.91	12496	19	142.1228	141.1155	C ₈ H ₁₅ NO	Trachelanthamidine	526-64-7
16.6	236886.7	12498	22.4	616.4617	615.4544	C ₃₂ H ₆₈ NO ₆ P	Hygrine	496-49-1
0.9	204379.7	12514	12.4	530.7496	531.7569		PC(O-12:0-O-12:0)	-
10.1	67501.24	12521	8.2	453.3436	452.3363	C ₂₇ H ₄₆ N ₂ O ₂	-	-
1.7	76143.02	12536	9	127.0731	126.0658	C ₃ H ₆ N ₆	Solanocapsine	639-86-1
18.3	71875.59	12536	13.1	429.1879	428.1806	C ₂₀ H ₂₄ N ₆ O ₅	Melamine	108-78-1
0.8	111315	12599	140	486.8117	485.8044	-	His Trp Ser	-
23	2328859	12610	7.8	160.9492	159.9419	-	-	-
0.8	55769.03	12651	281.1	386.3786	385.3713	-	-	-
0.9	47587.11	12652	140.6	702.741	700.7228	-	-	-
16.3	145343.5	12692	11.5	171.1379	170.1306	C ₁₀ H ₁₈ O ₂	2-Methyl-1,7-dioxaspiro[5.5]undecane	-

							2E-Octenyl acetate	-
							2-decylenic acid	-
17.5	162656.1	12704	24.9	302.3049	301.2976	C ₁₈ H ₃₉ NO ₂	Sphinganine	764-22-7
						C ₁₇ H ₂₄ N ₄ O ₇ S	Cys Gly Ser Tyr	-
8.7	57584.58	12711	9.3	451.1219	450.1146	C ₂₁ H ₂₂ O ₁₁	Okanin 3'-glucoside	-
0.5	271770.8	12747	4.6	106.9922	105.9849	-	-	-
0.8	1564957	12821	42.8	559.3395	560.3468	C ₂₇ H ₄₂ N ₈ O ₅	Phe His Lys Lys	-
9.1	123850.3	12829	36.6	393.1141	392.105	C ₁₇ H ₂₂ O ₉	Perilloside E	149380-62-1
14.3	81820.8	12882	25.7	360.3104	359.3031	-	-	-
8.8	113969.2	12895	8.3	404.2491	403.2418	C ₁₇ H ₃₃ N ₅ O ₆	Ala Lys Ser Val	-
						C ₉ H ₁₈ S ₃	2,2,4,4,6,6-Hexamethyl-1,3,5-trithiane	828-26-2
19.1	90722.07	12914	19.5	223.0635	222.0562	C ₈ H ₁₄ O ₅ S	2-(3'-Methylthio)propylmalic acid	-
0.8	55803.26	12918	143.5	256.4198	255.4126	-	-	-

14.1	75955.49	12947	9.3	213.1463	212.139	-	-	-
0.8	114138	12953	143.9	186.9224	185.9152	-	-	-
16.5	115125.5	12957	8.1	459.235	458.2277	C ₂₂ H ₃₀ N ₆ O ₅	Phe Gly His Val	-
19	74713.52	12957	6	201.1487	200.1414	C ₁₁ H ₂₀ O ₃	3-Nonanon-1-yl acetate	7779-54-6
							2R-hydroxy-10-undecenoic acid	-
0.9	248146.3	13008	289.1	826.692	1655.3985	-	-	-
12.1	54766.57	13031	289.6	251.1847	250.1775	-	-	-
							RETUSOQUINONE	-
11.9	135771.4	13159	14.2	183.0782	182.0709	C ₁₁ H ₁₂ O	3-Methyl-4-phenyl-3-buten-2-one	1901-26-4
							2-Phenyl-4-pental	24401-36-3
7.9	58405.63	13207	9.9	291.0819	290.0746	C ₁₃ H ₁₆ O ₆	Idebenone Metabolite (QS-4)	58186-01-9
							Isoamyl 2-furonpropionate	7779-67-1
9.4	61276.11	13224	9.8	211.133	210.1258	C ₁₂ H ₁₈ O ₃	1-Benzyloxy-1-(2-methoxyethoxy)ethane	7492-39-9

							(R)-8-Acetoxycarvotanacetone	56691-69-1
							(±)7-epi Jasmonic Acid	62653-85-4
14.5	124530.1	13276	10	316.2842	315.277	C ₁₈ H ₃₇ NO ₃	6-hydroxysphingosine	-
1.5	63244.32	13280	3.9	194.1388	192.1261	-	-	-
23.1	6053916	13329	7.7	126.9669	123.957	-	-	-
0.7	86013	13422	8	194.9998	193.9925	-	-	-
0.9	79103.04	13427	7.4	179.9817	178.9744	C ₆ H ₄ ClNO ₂	2-Chloronitrobenzene	88-73-3
9.3	136212.6	13484	16.4	340.2595	339.2524	C ₂₁ H ₃₅ NO	Amorolfine	78613-35-1
							Dehydrozingerone	1080-12-2
8.8	63042.09	13509	13.9	193.0844	192.0771	C ₁₁ H ₁₂ O ₃	Carpacin	23953-63-1
							ETHYL-p-COUMARATE	2979-06-8
14.1	70186.87	13583	8	317.2108	316.2035	C ₂₀ H ₂₈ O ₃	19-Hydroxy-13-cis-retinoic acid	-
2.2	628511.2	13587	8.3	107.0705	106.0632	C ₄ H ₁₀ O ₃	Diethylene glycol	111-46-6

0.9	97606.41	13646	12.1	491.8138	490.8065	-	-	-
14.1	99071.01	13688	7.8	335.2215	334.2142	C ₂₀ H ₃₀ O ₄	20-carboxy Arachidonic Acid	79551-84-1
0.8	156806.8	13859	8.9	259.9368	257.9248	-	-	-
15	76466.55	13871	18.4	216.1013	215.0941	C ₁₁ H ₁₅ NO ₂	p-Butylaminobenzoic acid	4740-24-3
1.6	76000.96	14012	21.7	221.1197	219.1146	-	-	-
0.8	751334	14024	311.6	507.1966	508.2039	C ₁₉ H ₃₀ N ₄ O ₁₂	Glu Glu Thr Glu	-
						C ₁₅ H ₂₂ O ₆	Sesamex	51-14-9
8.4	64160.85	14030	9	321.1304	320.1231	C ₁₇ H ₂₀ O ₆	Oleacein	149183-75-5
						C ₁₂ H ₂₀ N ₂ O ₈	Mugineic acid	69199-37-7
8.4	107442.1	14042	11.7	360.2227	359.2155	C ₁₅ H ₂₉ N ₅ O ₅	Ala Ala Ala Lys	-
1.6	109454.1	14047	20.2	349.1644	350.1717	C ₁₉ H ₂₄ O ₆	Onopordopicrin	19889-00-0
23.8	3085409	14083	9.7	118.9668	117.9595	-	-	-
1.5	59402.29	14105	15.3	179.1177	178.1105	C ₁₀ H ₁₄ N ₂ O	Glycine xylidide	18865-38-8

0.8	60000.45	14112	156.8	200.446	199.4387	-	-	-
17.4	221895.7	14113	27.2	346.3312	345.324	-	-	-
11.4	24853.5	14123	4.2	90.5261	89.5189	-	-	-
1.6	81022.16	14173	30.8	399.0812	398.0748	C ₁₂ H ₂₂ N ₄ O ₅ S ₃	Ala Cys Cys Cys	-
9.2	71698.85	14188	7.1	251.1256	250.1183	C ₁₂ H ₂₀ O ₄	Traumatic acid	-
						C ₁₄ H ₁₈ O ₄	Diisopropyl phthalate	605-45-8
						C ₁₄ H ₁₈ O ₄	δ-CEHC	1221504-67-
9	67069.95	14210	7.1	251.1257	250.1184			1
						C ₁₂ H ₂₀ O ₄	Traumatic acid	-
						C ₁₄ H ₁₈ O ₄	Diisopropyl phthalate	605-45-8
0.9	278205.4	14235	19.5	670.6479	671.6551	-	-	-
0.9	36690.15	14254	4	158.9654	631.8353	-	-	-
9.2	271514	14261	16.1	409.1829	408.1757	C ₂₀ H ₂₈ N ₂ O ₅ S	-	-

							Tamsulosin	106133-20-4
21.7	214350.8	14294	30.1	276.0526	275.0453	C ₁₂ H ₁₅ Cl ₂ NO ₂	Phenylacetic mustard	10477-72-2
							2-Pyridylacetaldehyde	54765-14-9
10.1	78675.38	14311	22.9	122.0603	121.053	C ₇ H ₇ NO		
							Benzamide	55-21-0
19.3	155888.3	14325	12.7	317.21	316.2027	C ₂₀ H ₂₈ O ₃	all-trans-4-hydroxyretinoic acid	66592-72-1
1.1	59572.63	14334	17.4	133.0718	132.0645	C ₃ H ₈ N ₄ O ₂	Methylenediurea	-
0.8	309292.2	14336	7.4	366.8778	364.8583	-	-	-
1.6	80420.82	14371	4.4	145.0475	144.0403	C ₄ H ₁₀ O ₄	D-Threitol	2418-52-2
9.6	152863.4	14376	8.6	209.0786	207.0533	C ₉ H ₁₄ O ₄	cis-2-Carboxycyclohexyl-acetic acid	14715-37-8
14.2	177831.1	14432	8.6	445.2767	444.2694	C ₁₉ H ₃₆ N ₆ O ₆	Ala Ile Lys Asn	-
0.9	118862.9	14436	21.2	314.8736	312.8602	-	-	-
10.5	92094.85	14472	17.6	622.3647	621.3574	-	-	-
8.1	217285.8	14496	25.6	227.1755	226.1688	C ₁₅ H ₂₄	α-Humulene	6753-98-6

						C ₁₂ H ₂₂ N ₂ O ₂	1,8-Diazacyclotetradecane-2,9-dione	-
15.7	277154.6	14510	11.4	558.4201	557.4128	C ₃₃ H ₅₉ D ₅ O ₅	DG(15:0-0:0-15:0) (d5)	-
0.8	245521.4	14527	322.8	310.4313	308.4078	-	-	-
1.5	185379.5	14598	4.3	129.066	130.0732	C ₅ H ₈ N ₂ O ₂	4-amino-4-cyano-butanoic acid	-
23.6	4964573	14735	20.4	154.9668	153.9595	C ₂ ClF ₅	Chloropentafluoroethane	76-15-3
0.9	50343.5	14804	164.5	350.8314	349.8241	C ₆ H ₄ Cl ₆ O ₄	TCA-ethadyl	2514-53-6
25	375788.8	14850	10.9	90.5071	89.4999	-	-	-
0.8	82708.43	14865	330.3	478.8245	476.8083	-	-	-
						C ₁₅ H ₁₀ N ₂ O ₄	N-(p-Nitrobenzyl)phthalimide	62133-07-7
1.6	87207.66	14924	17.6	283.0701	282.0629	C ₁₃ H ₉ F ₃ N ₂ O ₂	Niflumic Acid	4394-00-7
1.5	79148.44	14928	10.6	199.1059	198.0986	C ₉ H ₁₄ N ₂ O ₃	Metharbital	50-11-3
						C ₂₃ H ₄₄ N ₆ O ₅	Ile Lys Lys Pro	-
22.3	715552.3	14934	18	507.3279	506.3207	C ₂₉ H ₄₆ O ₇	2-deoxy-20-hydroxy-5alpha-ecdysone 3-acetate	-

9.9	70016.49	14973	166.4	143.1178	142.1105	-	-	-
7.5	82603.09	15042	13.3	171.0631	170.0558	C ₆ H ₁₂ O ₄	Glycerol 1-propanoate	624-47-5
							Mevalonic acid	-
12	275631	15078	4	345.1881	344.1809	C ₂₄ H ₂₄ O ₂	6,9,12,15,18,21-Tetracosahexaynoic acid	-
18.4	427368.5	15090	29.9	737.5005	736.4932	-	-	-
10	164629.1	15092	15.8	273.1311	272.1238	C ₁₁ H ₂₂ O ₆	Isopentyl beta-D-glucoside	-
16.7	912552.6	15172	16.8	331.1143	332.1216	C ₁₆ H ₂₀ O ₆	Monocerin	30270-60-1
8.8	64954.65	15220	11.8	365.1565	364.1492	C ₁₇ H ₂₆ O ₇	Jasmolone glucoside	-
						C ₁₉ H ₂₄ O ₇	Gibberellin A79	132043-65-3
15.6	90055.2	15241	8.3	277.1893	276.182	C ₁₆ H ₂₄ N ₂ O ₂	Carolinianine	36101-39-0
19	236011.2	15363	22.4	685.4177	686.425	-	-	-
1.7	168601.5	15416	11.7	177.0344	176.0271	C ₈ H ₁₀ OS	1-(2-Thienyl)-1-butanone	5333-83-5
0.8	75205.05	15417	6.2	404.8624	806.7612	-	-	-

1.6	172105.2	15463	10.9	163.0277	162.0205	-	-	-
14	215478.5	15509	8.4	277.135	274.1192	C ₁₈ H ₁₆ N ₂ O	SC-66	871361-88-5
22.8	4883323	15588	12.1	178.9594	179.9667	-	-	-
24.5	120337.8	15680	21.2	367.1882	366.1809	C ₂₁ H ₂₈ O ₄	4-[4-(3,4-Dimethoxyphenyl)-2,3-dimethylbutyl]-2-methoxyphenol	-
							21-Deoxycortisone	1882-82-2
							2,2-Dimethyl-3-(4-methoxyphenyl)-4-propyl-2H-1-benzopyran-7-ol acetate	-
							2,2-Dimethyl-3-(4-methoxyphenyl)-4-propyl-2H-1-benzopyran-7-ol acetate	-
11.2	149068.3	15717	15.3	134.0714	133.0641	C ₁₈ H ₂₆ N ₂ O ₆	Bufotenine O-glucoside	64656-15-1
							2-Aminobenzimidazole	934-32-7
							(all-E)-6'-Apo-γ-caroten-6'-al	22255-36-3
24.3	266070.5	15731	15.5	443.3333	442.3261	C ₃₂ H ₄₂ O	(all-E)-6'-Apo-γ-caroten-6'-al	22255-36-3
0.9	274961	15745	41	556.7134	553.7164	-	-	-
13.7	137164.9	15770	12.8	379.1748	378.1676	C ₁₃ H ₂₆ N ₆ O ₅ S	Cys Arg Thr	-
						C ₂₀ H ₂₆ O ₇	Niveusin C	75680-27-2
0.9	293956.8	15776	66.4	746.7223	747.7296	-	-	-

19	214190.5	15777	13.7	371.2105	370.2039	-	-	-
							trans-O-Hydroxybenzylidenepyruvate	-
11.2	71292.23	15790	12.9	193.0498	192.0425	C ₁₀ H ₈ O ₄	Naphthazarin	475-38-7
							4-METHYLDAPHNETIN	2107-77-9
1.6	134302.6	15869	176.3	186.0662	187.0734	C ₁₀ H ₇ N ₃ O	Cyometrinil	78370-21-5
0.9	195985.5	15960	38.5	446.8272	447.8345	-	-	-
							2,4,6-Triethyl-1,3,5-trioxane	2396-42-1
12.2	68527.34	15972	177.5	175.1328	174.1255	C ₉ H ₁₈ O ₃	2-hydroxy pelargonic acid	-
0.9	144231.1	16014	27.7	628.7387	627.7314	-	-	-
0.8	389524.1	16082	39.8	403.9114	400.8594	-	-	-
0.8	95523.38	16125	179.2	284.9373	283.93	-	-	-
						C ₁₃ H ₁₆	1,2-Dihydro-1,1,6-trimethylnaphthalene	30364-38-6
1.5	65879.2	16227	13	195.1136	194.1063	C ₁₀ H ₁₄ N ₂ O ₂	Laccarin	175669-28-0

1.5	403298.6	16277	5.4	158.003	156.0038	C ₇ H ₅ NS	Benzothiazole	95-16-9
1.6	358321.7	16277	5.4	158.003	156.9958	C ₇ H ₅ NS	Benzothiazole	95-16-9
10.7	130476.7	16304	28.9	696.4369	695.4308	C ₃₇ H ₆₁ NO ₁₁	Mycinamicin IV	73684-71-6
0.9	72096.71	16350	28.6	572.7987	571.7914	-	-	-
10.5	133454.1	16395	17.5	627.3194	628.3267	C ₂₄ H ₄₀ N ₁₄ O ₅	His His Arg Arg	-
21.8	111888.9	16411	38.1	658.2524	657.2451	C ₃₂ H ₃₇ N ₅ O ₉	Gln Tyr Tyr Tyr	-
0.8	178336.7	16437	18.8	277.9473	276.94	-	-	-
1.5	116468.1	16475	19	130.0871	129.0798	C ₆ H ₁₁ NO ₂	NIPECOTIC ACID	498-95-3
0.9	125967.8	16506	26.1	318.8449	635.6733	-	-	-
2.2	6261889	16507	4.6	125.9864	124.9791	-	-	-
21.7	195686.3	16551	15	297.0647	298.072	C ₁₆ H ₁₅ ClO ₂	PDM 11	-
21.8	177917.1	16604	16.5	297.2423	296.2354	C ₁₈ H ₃₂ O ₃	(±)9-HODE	98524-19-7
16.2	101142.3	16627	20.7	327.1418	326.1345	C ₁₆ H ₂₂ O ₇	4-(4-Hydroxyphenyl)-2-butanone glucoside	38963-94-9

						C ₁₂ H ₁₈ N ₆ O ₅	Gly Gly Gly His	-
							6-Methylcoumarin	92-48-8
12.2	100807.1	16631	14.8	161.06	160.0527	C ₁₀ H ₈ O ₂	2-Formyl-1-indanone	56794-24-2
							Naphthalene-1,2-diol	574-00-5
6.7	125450.7	16640	13.8	157.0839	156.0766	C ₆ H ₁₄ O ₃	Polypropylene glycol (m w 1,200-3,000)	25322-69-4
0.9	170712.8	16655	25.8	498.7876	497.7823		-	-
0.8	232273.6	16701	17	252.9708	251.9635	CH ₃ ClHg	Methylmercury chloride	115-09-3
						C ₁₉ H ₂₈ N ₄ O ₆	Ala Gly Tyr Val	-
8.8	163902.8	16713	23.7	409.2046	408.1973	C ₂₅ H ₂₈ O ₅	Paratocarpin D	-
12.1	89327.56	16778	10.3	171.1489	170.1417	C ₉ H ₁₈ N ₂ O	3-Acrylamidopropyl trimethylammonium	45021-77-0
21.8	145395.9	16794	30.2	579.2921	578.2848	C ₂₅ H ₃₈ N ₈ O ₈	Glu Phe Gln Arg	-
0.8	210356.5	16844	3.4	218.9833	217.976	-	-	-
0.9	122083.1	16857	8.4	290.8551	288.8654	-	-	-

0.8	231189.8	16869	54.4	690.7734	689.7661	-	-	-
10.9	109894.3	16899	31.9	680.3698	679.3625	-	-	-
1.2	129827.3	16926	22.9	158.9125	157.9052	-	-	-
18.4	349558.3	16968	13.7	251.1278	250.1205	C ₁₂ H ₂₀ O ₄	Traumatic Acid	6402-36-4
							Helinorbisabone	201288-95-1
							Diisopropyl phthalate	605-45-8
						C ₁₄ H ₁₈ O ₄	Ubiquinone-1	727-81-1
								1221504-67-
							δ-CEHC	1
0.9	102636.7	17027	189.2	248.8822	495.7558	-	-	-
23.4	4434227	17069	10.2	138.9797	137.9725	-	-	-
1.7	262766.3	17176	14.1	209.0334	208.0261	C ₁₀ H ₆ N ₂ O ₂	AG-18	118409-57-7
11.2	175681.1	17196	30.6	101.0962	100.0889	C ₆ H ₁₂ O	1-Hexen-1-ol	-

							4-Methylpentanal	-
							Caproaldehyde	-
0.9	144936.2	17236	13.8	386.8519	1157.5343	-	-	-
0.6	442455.8	17249	5.4	113.9638	112.9565	-	-	-
1.7	760054.6	17264	22.3	206.9951	203.9942	C ₅ H ₄ N ₄ O ₂ S	6-Thiouric acid	2002-60-0
1.1	166652.7	17265	6.4	143.997	142.9897	-	-	-
13.9	104972.2	17309	13	316.2845	315.2772	C ₁₈ H ₃₇ NO ₃	6-hydroxysphingosine	-
1.2	186783.1	17331	12.6	177.9484	530.8241	-	-	-
15.4	88608.23	17336	12.4	283.1809	282.1736	C ₁₈ H ₂₂ N ₂ O	2-Hydroxydesmethyylimipramine	-
0.8	384371.4	17471	14.7	409.8546	817.6947	-	-	-
13.2	113612.5	17546	11.2	290.2686	289.2613	-	-	-
24	152810.9	17574	15.3	482.4043	481.397	-	-	-
1.6	114581.6	17613	23.7	221.0336	220.0268	C ₆ H ₉ N ₂ O ₅ P	3-(Imidazol-4-yl)-2-oxopropyl phosphate	99979-59-6

1.6	84031.77	17640	46	294.0038	292.9966	-	-	-
0.9	90114.86	17661	48.7	576.7838	573.7689	-	-	-
0.9	122407.1	17670	25	518.7538	519.7611	-	-	-
4.4	402085.3	17682	20.1	157.0474	156.0403	C ₅ H ₁₀ O ₄	2-Deoxy-alpha-D-ribose	36792-85-5
							2,3-Dihydroxy-3-methylbutanoate	-
24	293639.4	17718	20.2	487.3593	486.352	C ₂₃ H ₄₆ N ₆ O ₅	Ile Lys Lys Val	-
14.8	316005.1	17738	16.9	500.3786	499.3713	-	-	-
0.9	119434.6	17754	14.5	284.8721	851.5845	-	-	-
0.8	226558.7	17761	28.2	223.9889	222.9816	-	-	-
11.3	194778.4	17769	9.6	277.1909	276.1836	C ₁₉ H ₂₆	18-Nor-4(19),8,11,13-abietatetraene	22478-62-2
						C ₁₆ H ₂₄ N ₂ O ₂	Carolinianine	36101-39-0
2.1	791981.4	17786	10	191.0229	190.0156	-	-	-
21.8	107789.6	17822	22.2	248.2009	247.1936	C ₁₆ H ₂₅ NO	alpha-Sanshool	504-97-2

15.1	129197.7	17827	45.6	370.6727	739.3308	-	-	-
0.8	465366.9	17830	14.4	185.0232	184.0159	C ₆ H ₁₀ O ₃ S	1-(Methylsulfanyl)-1-oxopropan-2-yl acetate	74586-09-7
						C ₅ H ₁₀ Cl ₂ N ₂ O	N,N'-bis(2-chloroethyl)- Urea (Carmustine Metabolite)	2214-72-4
20.2	176461.7	17859	16.6	269.2108	268.2036	C ₁₆ H ₂₈ O ₃	Methoprene acid	53092-52-7
17.7	103110.6	17862	18.7	429.1875	428.1802	C ₂₀ H ₂₄ N ₆ O ₅	His Trp Ser	-
1.9	800197.3	18006	11.8	145.0257	144.0184	C ₇ H ₆ O ₂	Benzoic acid	65-85-0
							4-Hydroxybenzaldehyde	123-08-0
15.9	108651.5	18039	4.5	219.1488	218.1415	C ₁₃ H ₁₈ N ₂ O	Eseroline	469-22-7
0.7	80754.34	18103	5.5	176.9885	175.9813	-	-	-
21.8	170767.7	18170	24.6	197.581	393.1531	-	-	-
4	145736.5	18193	45.5	264.1806	263.1733	C ₁₃ H ₂₁ N ₅ O	Pinacidil	85371-64-8
13	97980.67	18220	12.4	333.1308	332.1235	C ₁₆ H ₂₂ O ₆	tetranor-PGAM	52510-53-9
						C ₁₈ H ₂₀ O ₆	3,3'-Dihydroxy-4',5,7-trimethoxyflavan	105330-59-4

							BYSSOCHLAMIC ACID	743-51-1
						C ₁₃ H ₂₀ N ₂ O ₈	Mytilin A	73112-73-9
22.1	164518.7	18284	10.3	149.0234	148.0161	-	-	-
0.6	349935	18345	6.5	186.9566	185.9493	-	-	-
							1-O-p-Coumaroyl-beta-D-glucose	7139-64-2
8.7	145799.8	18387	27.2	349.0871	348.0781	C ₁₅ H ₁₈ O ₈	Bilobalide	33570-04-6
23.3	547956.3	18551	9.3	328.2841	327.2773	C ₁₉ H ₃₇ NO ₃	N-palmitoyl alanine	-
1.5	75248.34	18653	29.6	192.1597	191.1524	-	-	-
11.2	434759.7	18719	4.2	361.2194	341.1641	C ₁₄ H ₂₈ N ₆ O ₅	Val Arg Ser	-
8	82939.55	18722	208	284.134	283.1267	C ₁₁ H ₁₇ N ₅ O ₄	Ala His Gly	-
								1357160-72-
9.5	91372.45	18726	14	377.1457	376.1384	C ₂₀ H ₂₂ N ₂ O ₄	URB937	5
						C ₁₇ H ₂₀ N ₄ O ₆	Gly Asp Trp	-

						C ₁₆ H ₂₄ O ₁₀	(1x,2x)-Guaiacylglycerol 3-glucoside	7094-73-7
1.1	90919.04	18779	7	141.9588	563.8073	-	-	-
	2038167							
7.5		18869	5.9	113.9638	112.9565	-	-	-
	8							
	2042553							
10.1		18869	5.9	113.9638	112.9565	-	-	-
	4							
1.4	742905	18923	5.3	158.9617	157.9544	-	-	-
						C ₉ H ₉ N ₂	4-Aminomethylindole	3468-18-6
1.5	89580.2	19082	16.6	168.066	167.0587		p-Aminosalicylic acid methyl ester	4136-97-4
						C ₈ H ₉ NO ₃	2-Amino-3-methoxy-benzoic acid	3177-80-8
0.8	110173.9	19153	425.6	265.4246	528.8347	-	-	-
0.8	93850.73	19154	32.9	412.8688	823.7231	-	-	-
0.9	67234.07	19176	26.6	554.7944	553.7871	-	-	-

	1314395							
2		19188	6.4	158.003	156.9957	C ₇ H ₅ NS	Benzothiazole	95-16-9
	0							
	1322125							
3.1		19188	6.4	158.003	156.9957	C ₇ H ₅ NS	Benzothiazole	95-16-9
	6							
9	155037.2	19194	15.4	229.1054	228.0981	C ₁₁ H ₁₆ O ₅	Propyl propane thiosulfonate	1113-13-9
10	98493.55	19202	8.4	303.178	302.1707	C ₁₁ H ₂₂ N ₆ O ₄	Gamma-glutamyl-Arginine	-
0.8	220592.6	19219	6.2	114.9874	226.9416	-	-	-
0.8	140398.9	19280	8	498.8611	993.6924	-	-	-
						C ₃₀ H ₅₀ O ₅	Meliantriol	25278-95-9
0.8	345272.5	19356	215.1	513.357	510.3487		Ganoderic acid X	86377-53-9
						C ₃₂ H ₄₈ O ₅		
							11a,12a-Epoxy-3b-hydroxy-28,13-oleananolide 3-acetate	35738-25-1
0.9	118407.2	19375	58.2	634.7677	1265.5065	-	-	-
0.9	158649.4	19472	28.2	310.8531	311.8603	-	-	-

0.9	180360.2	19525	7.3	146.9753	145.968	C ₆ H ₄ Cl ₂	1,2-Dichlorobenzene	95-50-1
0.6	403423.8	19557	4.2	98.5123	97.5051			
1.4	394870.6	19659	5.7	84.9598	83.9525	CH ₂ Cl ₂	Dichloromethane	75-09-2
0.8	68924.07	19674	6.2	274.4302	273.4229	-	-	-
13.1	248487	19695	9.7	387.2349	386.2276	C ₂₀ H ₃₄ O ₇	Oleandolide	-
1.6	126312.5	19735	12.1	247.0491	244.0199	-	-	-
23.1	135126.3	19819	10	328.2842	327.2769	-	-	-
0.8	1068694	19837	46.5	679.7949	677.7788	-	-	-
0.9	123493.7	19860	124	684.7508	685.7581	-	-	-
1.1	104405	19904	18.5	155.0538	154.0465	C ₃ H ₈ N ₄ O ₂	Methylenediurea	-
						C ₈ H ₁₀ OS	1-(5-Methyl-2-thienyl)-1-propanone	59303-13-8
14.1	87524.68	19970	221.9	299.1999	298.1926	C ₁₈ H ₂₈ O ₂	Moroctic acid	-
						C ₂₀ H ₂₆ O ₂	Juvocimene 2	75539-63-8

							(5E)-(24R)-24,25-dihydroxy-[6,19,19-trideutrio]vitamin D3 - (5E)-(24R)-24,25-	
13.8	305168.5	20031	11.5	442.3367	441.3295	C ₂₇ H ₄₁ D ₃ O ₃	dihydroxy-[6,19,19-trideutrio]cholecalciferol	-
0.9	130486.7	20050	21.3	155.9804	154.9731	-	-	-
						C ₁₁ H ₁₈ N ₄ O ₃	His Val	-
7.2	153851	20062	30.5	277.126	276.1188	C ₁₄ H ₂₂ O ₂ S	2,6-Dimethyl-3-[(2-methyl-3-furanyl)thio]-4-heptanone	61295-51-0
						C ₁₂ H ₂₀ O ₇	Triethyl citrate	77-93-0
17.6	779724.5	20076	25.4	679.4588	680.4661	C ₃₅ H ₆₇ O ₁₀ P	PG(12:0-17:1(9Z))	-
						C ₄ H ₁₀ O ₄	D-Threitol	2418-52-2
1.5	84749.8	20083	6.2	145.0483	144.0411	C ₆ H ₈ O ₄	2,3-Dimethylmaleate	488-21-1
1.1	141390	20094	3.6	90.5261	89.5188	-	-	-
23.4	142318.3	20445	18.9	429.3175	428.3102	C ₂₄ H ₄₄ O ₆	Glyceryl lactooleate	30283-16-0
21.7	145998.2	20468	24.8	437.2088	872.403	C ₁₇ H ₃₂ N ₄ O ₇ S	Cys Ile Thr Thr	-
0.8	57819.05	20478	455.1	220.9576	219.9503	-	-	-

							4-formyl Indole	1074-86-8
8.1	118036.6	20580	19.1	146.0601	145.0528	C ₉ H ₇ NO	2(1H)-Quinolinone	59-31-4
0.8	208935.6	20667	28.7	459.8592	457.8222	-	-	-
0.9	53464.7	20683	48.9	242.9253	241.918	C ₆ H ₅ IO	2-Iodophenol	-
0.9	154380.9	20724	30.6	294.8329	293.8263	-	-	-
0.8	70116.41	20737	48.5	209.4513	208.4441	-	-	-
10.4	106571.9	20879	10	578.3382	577.3309	C ₃₂ H ₄₃ N ₅ O ₅	Phe Ile Ile Trp	-
0.8	94258.73	20977	466.2	395.383	394.3757	-	-	-
						C ₁₄ H ₂₆ O ₂	8Z-Dodecenyl acetate	-
20.5	152604.4	20988	13.8	249.1849	248.1776	C ₁₆ H ₂₄ O ₂	4,7,10,13-hexadecatetraenoic acid	-
							Furfuryl pentanoate	36701-01-6
7.6	168753.1	21380	14.3	183.1001	182.0928	C ₁₀ H ₁₄ O ₃	3,4,5-Trimethoxytoluene	6443-69-2
							2-Oxo-delta3-4,5,5-trimethylcyclopentenylacetate	1130-49-0

						C ₆ H ₁₀ N ₆ O	Dacarbazine	4342-03-4
21.7	254397.8	21443	27.3	398.1119	397.1037	C ₁₅ H ₁₉ N ₅ O ₆ S	S-Adenosyl-4-methylthio-2-oxobutanoate	22365-11-3
8.5	180954.9	21447	12.3	365.1782	364.171	C ₁₅ H ₂₆ N ₄ O ₅	Ala Gly Pro Val	-
23.5	195315	21598	16.9	341.266	342.2733	C ₂₀ H ₃₆ O ₄	15(S)-HpEDE	145375-41-3
0.8	85220.93	21672	481.6	330.4042	329.3969	-	-	-
14.4	119018.5	21675	41.2	226.1801	225.1729	-	-	-
10.1	150234.7	21742	9.5	303.1779	302.1707	C ₁₁ H ₂₂ N ₆ O ₄	Glutaminy-Arginine	-
13.2	154920.5	21749	4.3	299.2187	298.2114	C ₁₇ H ₃₀ O ₄	Plakortc acid	87803-10-9
0.9	135410.3	21776	8.6	389.8752	388.8679	-	-	-
11.9	113258.4	21954	20	177.0548	176.0475	C ₁₀ H ₈ O ₃	1,4,5-Naphthalenetriol	481-40-3
							4-Methylumbelliferone	90-33-5
1.2	144418.2	22085	21.1	174.8865	173.8792	-	-	-
0.9	107719	22124	26.4	392.7944	391.7871	-	-	-

11.5	100985.5	22130	8.2	304.2481	303.2409	-	-	-
0.9	232184.6	22135	34.1	534.7278	535.7351	-	-	-
1.6	187848.2	22138	29.9	118.0554	234.0966	-	-	-
21.7	168500.1	22139	44	320.0803	319.0737	C ₁₆ H ₁₅ N ₃ OS	L-Menthone 1,2-glycerol ketal	977178-02-1
16.6	121909.8	22151	246.1	313.1619	312.1546	C ₁₄ H ₂₆ O ₆	1-Octen-3-yl glucoside	209863-00-3
15.5	121976.8	22183	5.5	207.044	206.0367	C ₉ H ₁₂ O ₂ S	(+--)-3-[(2-methyl-3-furyl)thio]-2-butanone	61295-44-1
10.6	189761.7	22333	28.5	657.367	658.3742	C ₃₅ H ₅₄ O ₁₀	Digitoxigenin bisdigitoxoside	16479-50-8
1.8	123594.3	22366	7.7	139.0504	138.0431	C ₆ H ₆ N ₂ O ₂	2-Pyrimidine Acetic Acid	66621-73-6
0.9	43342.75	22391	497.6	430.7922	429.7849	C ₁₂ H ₃ Cl ₇ O	2,2',3,3',4',5,5'-Heptachloro-4-biphenylol	158076-64-3
10.6	425547.1	22452	25.1	229.1415	228.1343	C ₁₂ H ₂₀ O ₄	Traumatic acid	-
10.9	174449.7	22509	49.7	685.3249	686.3322	C ₃₂ H ₅₃ NaO ₁₂ S	Evasterioside B	-
0.9	148015.2	22551	48.9	560.8101	559.804	-	-	-
8.8	136631.8	22589	9.4	245.1363	244.1312	C ₁₂ H ₂₀ O ₅	Polyethylene, oxidized	68441-17-8

							L-Arabinono-1,4-lactone	51532-86-6
1.1	71978.5	22593	19.5	171.0279	170.0206	C ₅ H ₈ O ₅	D- α -Hydroxyglutaric acid	103404-90-6
						C ₇ H ₆ O ₅	2,4,6-Trihydroxybenzoic acid	83-30-7
5.9	178043.2	22594	16.1	102.128	101.1208	C ₆ H ₁₅ N	Hexylamine	111-26-2
0.9	117270.6	22603	8.9	256.8729	255.8656	-	-	-
0.9	102099.6	22727	33.8	376.8219	375.8146	-	-	-
4.3	175514.3	22857	19.5	99.0443	98.037	C ₅ H ₆ O ₂	β -vinyl acrylic acid	-
		22881		279.2317		C ₁₆ H ₃₂ O ₂	Dodecyl butyrate	3724-61-6
16.4	145537.4		15.9		278.2245	C ₁₈ H ₃₀ O ₂	3E,9Z,12Z-octadecatrienoic acid	-
1.7	229255	22975	29.7	102.5311	101.5239	-	-	-
							Epinepetalactone	17257-15-7
10.8	568075.3	22981	18.2	167.1068	166.0995	C ₁₀ H ₁₄ O ₂	2-tert-Butyl-1,4-benzenediol	1948-33-0
							bornane-2,3-dione	-

							dolichodial	-
							2E,6Z,8E-decatrienoic acid	-
0.9	131932.2	22992	40	420.7891	419.7819	-	-	-
0.9	171093.6	23028	31.8	236.9854	235.9781	C ₆ H ₁₁ Cl ₃ O ₃	1,2,3-Tris(chloromethoxy)propane	38571-73-2
23.5	222826.8	23057	21.7	385.2917	386.299	C ₂₂ H ₄₀ O ₅	17,20-dimethyl Prostaglandin F1 α	-
8	230997.6	23110	5.5	321.1521	320.1437	C ₁₄ H ₂₄ O ₈	Valproic acid glucuronide	60113-83-9
0.8	249743.3	23117	36	457.3833	456.376	-	-	-
0.9	110969	23149	54.9	504.8156	503.8084	-	-	-
10.4	249431.4	23210	42.9	583.2939	564.3772	C ₂₈ H ₃₈ N ₈ O ₆	Phe Phe Asn Arg	-
1.4	438860.9	23226	6.5	125.9864	124.9791	-	-	-
							($\pm$)-threo-Anethole glycol	94497-49-1
8.6	247825.7	23235	15.5	183.1015	182.0942	C ₁₀ H ₁₄ O ₃	Amyl 2-furoate	4996-48-9
							Bis(2,3-epoxycyclopentyl)ether	2386-90-5

							Iridotrial	-
							5-oxo-7-decynoic acid	-
						C ₁₀ H ₁₆ O ₄	Decenedioic acid	-
8.6	160212.1	23323	13.8	223.0945	222.0872		APIOLE	523-80-8
						C ₁₂ H ₁₄ O ₄	Valeroyl Salicylate	64206-54-8
9.4	245448.9	23419	18.7	229.1037	228.0964	C ₁₅ H ₁₃ FO	CAY10512	139141-12-1
1.5	157456	23522	26.9	138.0553	139.0626	C ₇ H ₇ NO ₂	3-Aminobenzoic acid	-
1.7	279410.8	23757	14.8	179.0004	177.9931	C ₆ H ₁₀ S ₃	Diallyl Trisulfide	2050-87-5
19.3	467884.6	23863	43.8	330.3362	329.3289	C ₂₀ H ₄₃ NO ₂	N,N-dimethyl-Safingol	-
14.1	181461.7	23903	17.2	213.1098	212.1025	-	-	-
10.8	379426.9	23992	17.9	287.1468	284.124	C ₁₂ H ₂₄ O ₆	Hexyl glucoside	59080-45-4
0.9	99801.66	24135	23.2	134.1177	131.0946	C ₆ H ₁₅ NO ₂	Bis (2-hydroxypropyl) amine	110-97-4
10.7	183240.4	24288	44.6	636.344	635.3367	-	-	-

							4-Acetyl-1-methylcyclohexene	6090-09-1
14.1	150229.8	24340	15.9	139.1118	138.1046	C ₉ H ₁₄ O	2-Pentylfuran	3777-69-3
							(Z,Z)-3,6-Nonadienal	21944-83-2
21.8	191648.9	24651	17.1	279.232	278.2247	C ₁₈ H ₃₀ O ₂	3E,9Z,12Z-octadecatrienoic acid	-
0.8	644428.3	24742	9.2	505.368	506.3753	-	-	-
0.9	264459.2	25143	8.1	410.8041	409.7963	C ₁₂ H ₂ Cl ₆ O ₂	1,2,3,4,7,8-Hexachlorodibenzodioxin	39227-28-6
1.6	238052.1	25236	26.7	124.097	246.1739	-	-	-
15.8	189591.1	25333	30.5	223.0638	222.0565	C ₈ H ₁₄ O ₅ S	2-(3'-Methylthio)propylmalic acid	-
14	149944.6	25389	32.2	170.1175	169.1103	C ₉ H ₁₅ NO ₂	Homoarecoline	28125-84-0
24.1	215583	25604	25.3	443.3333	442.326	C ₃₂ H ₄₂ O	(all-E)-6'-Apo-y-caroten-6'-al	22255-36-3
0.9	136186.6	25679	12.1	262.888	261.8807	-	-	-
1	132004.1	25712	4.8	160.9871	159.9798	-	-	-
19	141917	25767	47.2	332.2791	331.2718	-	-	-

16.7	910080.3	25843	34.5	621.4172	622.4244	C ₃₂ H ₆₀ O ₁₁	Butyl 4'-O-hexadecanoyl-neohesperidoside	-
8.3	746283.1	25876	21.5	225.1101	224.1028	C ₁₀ H ₁₈ O ₄	Diethyl adipate	141-28-6
						C ₁₂ H ₁₆ O ₄	3',4',5'-Trimethoxycinnamyl alcohol	30273-62-2
5.7	201020.5	25879	21.5	157.0837	156.0764	C ₆ H ₁₄ O ₃	Polypropylene glycol (m w 1,200-3,000)	25322-69-4
0.9	138388.3	25917	54.7	368.8304	367.8231	-	-	-
1.2	185155.8	26091	23.2	195.959	194.9517	-	-	-
2.1	1151549	26223	28.5	179.1178	176.095	C ₁₀ H ₁₄ N ₂ O	6-Hydroxynicotine (R)	22956-40-7
9.3	3136839	26399	5.7	98.5123	192.0141	-	-	-
	4							
15.2	497982.7	26667	20.7	361.1621	362.1693	C ₂₀ H ₂₄ O ₆	Dibenzo-18-crown-6	14187-32-7
11.9	284441.6	26778	15.9	329.1933	328.186	C ₁₃ H ₂₄ N ₆ O ₄	Arg Pro Gly	-
19	477555.1	26841	19.2	195.1143	388.2149	C ₁₀ H ₁₄ N ₂ O ₂	3-Hydroxy-N-glycyl-2,6-xylidine (3-Hydroxyglycinexylidide)	112606-87-8
12.6	148964.7	26875	38.6	288.2532	287.2459	C ₁₆ H ₃₃ NO ₃	Lauroyl diethanolamide	120-40-1

0.9	260939.8	26978	299.8	378.8436	1511.3823	-	-	-
10.8	326257	27144	24.7	239.0893	240.0965	C ₁₂ H ₁₄ O ₅	Trans-2, 3, 4-Trimethoxycinnamate	33130-03-9
0.9	78434.68	27149	27.3	113.1073	112.1001	C ₆ H ₁₂ N ₂	2-Imino-4-methylpiperidine	165383-72-2
21.7	516284.5	27378	33.7	383.2037	384.211	C ₁₆ H ₂₆ N ₆ O ₅	Ala Gly His Val	-
16.5	326932.8	27396	22.1	333.2631	332.2561	C ₁₈ H ₃₆ O ₅	Phloionolic acid	-
4	3738302	27437	7.6	158.9614	157.9542	-	-	-
	4							
0.9	54555.09	27772	18.4	384.7962	383.7889	-	-	-
1.3	219390.9	27989	32	138.0551	137.0478	C ₇ H ₇ NO ₂	Anthranilic acid	118-92-3
24.3	253958.2	28054	29.1	345.2564	344.2495	C ₂₁ H ₃₂ N ₂ O ₂	16β-Hydroxystanozolol	125590-76-3
0.8	614401	28099	624.4	375.4104	746.7709	-	-	-
0.8	240651.9	28145	29.4	480.8563	479.8552	-	-	-
0.9	252164.1	28212	20.8	414.779	413.9198	-	-	-

1.5	140923.9	28219	34.2	133.0724	132.0652	C ₃ H ₈ N ₄ O ₂	Methylenediurea	-
12.3	156707.9	28259	18.1	290.2692	289.2619	-	-	-
1.9	270667.9	28384	22.1	94.0653	93.058	C ₆ H ₇ N	Aniline	62-53-3
1.8	137857.2	28389	18.6	121.0402	120.0329	-	-	-
10.5	368244	28453	17.2	271.1521	270.1448	-	-	-
0.9	175746.6	28575	55	164.9856	163.9783	C ₄ H ₈ Cl ₂ O	Bis(2-chloroethyl)ether	-
20.2	192811.4	28595	21.7	251.2004	250.1932	C ₁₆ H ₂₆ O ₂	4,7,10-hexadecatrienoic acid	-
12.8	218367.1	28981	18.6	290.2689	289.2616	-	-	-
8.8	270202.6	29247	21	213.1101	212.1028	-	-	-
0.9	115208.5	29305	19	152.9472	151.9399	C ₂ H ₄ Cl ₂ O ₂	2,2-Dichloro-1,1-ethanediol	-
0.9	264113.9	29367	12.6	374.859	375.8663	-	-	-
10.1	158176.9	29501	22.4	534.3115	533.3042	C ₂₂ H ₄₃ N ₇ O ₆ S	Lys Lys Met Gln	-
0.9	173365	29879	20.5	154.9324	153.9251	-	-	-

							D-Threose	95-43-2
11.8	139168.6	29971	9.2	121.0497	120.0424	C ₄ H ₈ O ₄	4-deoxy-erythronic acid	-
10.6	163207.9	30118	52.7	652.4115	651.4042	-	-	-
15.7	899501.1	30126	19.3	563.3752	564.3825	C ₂₉ H ₅₅ O ₈ P	PA(14:1(9Z)-12:0)	-
1.7	279326.3	30216	35	349.0479	348.0407	-	-	-
0.8	960799.8	30281	62.9	484.8558	482.8328	-	-	-
10.1	227107.8	30410	42	539.2674	540.2747	C ₂₄ H ₃₈ N ₆ O ₆ S	Phe Lys Met Asn	-
1.6	112625.5	30417	35.5	179.0757	356.1368	-	-	-
							Confertifoline	1811-23-0
							Helminthosporal	723-61-5
20.5	227079.5	30418	19.5	235.1689	234.1616	C ₁₅ H ₂₂ O ₂	Curmadione	-
							Macrophyllic acid A	-
							1,13-Dihydroxy-herbertene	-

13.8	203960.5	31174	14.6	318.3001	317.2928	C ₁₈ H ₃₉ NO ₃	Phytosphingosine	-
0.8	411606.6	31288	695.3	318.4203	634.8261	-	-	-
19	1364544	31391	35.6	206.6222	411.2282	-	-	-
14.8	189628	31574	33.7	200.1281	199.1208	C ₁₀ H ₁₇ NO ₃	Tussilagine	80151-77-5
1.4	579881.9	32396	12	141.9587	140.9515	-	-	-
10.7	352855.4	32830	69.1	641.2989	642.3061	-	-	-
						C ₁₀ H ₁₆ O ₃	(3R)-3-isopropenyl-6-oxoheptanoic acid	-
10.8	459636.4	32872	25.1	207.0997	208.107		(2RS,5RS)-(E)-2-(2-Phenylethenyl)-1,3-dioxan-5-ol	87562-73-0
						C ₁₂ H ₁₄ O ₃	p-Methoxycinnamic acid ethyl ester	1929-30-2
							3-Dimethylallyl-4-hydroxybenzoate	-
1	172301.1	32909	5.1	142.9765	141.9692	C ₃ H ₄ O ₃ S	3-mercaptopyruvate	10255-67-1
21.7	205130.1	32933	34.1	307.138	612.2615	C ₁₄ H ₁₈ N ₄ O ₄	Trimethoprim 3-N-oxide	27653-67-4
0.9	320338.4	33040	44.7	158.9122	789.5446	-	-	-

11.7	154127.6	33689	374.3	207.1591	206.1519	-	-	-
9.1	152241.9	33722	19.2	289.1259	288.1186	-	-	-
0.9	201188.5	33781	27.7	136.922	135.9147	-	-	-
1.7	136570.9	33862	26	155.0679	154.0606	C ₆ H ₁₂ O ₃	DL-3-hydroxy caproic acid	-
16.4	208590.4	34269	34	297.2421	296.2348	-	-	-
0.9	405024.2	35051	14.1	394.8304	393.8231	-	-	-
10.1	226886.3	35580	96.9	215.9786	214.9718	-	-	-
14.7	383785.5	35613	33.9	227.1253	228.1325	C ₁₀ H ₂₀ O ₄	3,7-Dimethyl-3-octene-1,2,6,7-tetrol	261949-44-4
15.7	555237.3	35628	60.9	362.3261	361.3188	-	-	-
13.1	240796.6	35718	42.1	332.279	331.2717	-	-	-
3.4	1122988 3	35821	13.3	141.9587	140.9515	-	-	-
0.9	85627.99	36460	45.4	424.8359	423.8286	-	-	-

1.9	259140.4	36569	39.5	220.1545	219.1472	C ₁₀ H ₂₁ NO ₄	Miglustat	72599-27-0
0.9	318968.8	36602	110	278.8601	277.8529	-	-	-
0.8	1386968	36744	816.5	558.8394	1679.5399	-	-	-
	1							
8.5	238489.7	36804	81.2	314.1808	313.1735	-	-	-
6.4	367275.1	36869	30.6	157.0839	156.0766	C ₆ H ₁₄ O ₃	Polypropylene glycol (m w 1,200-3,000)	25322-69-4
6.8	467369	36989	8.9	245.0635	244.0562	C ₁₀ H ₁₂ O ₇	1-O-Galloylglycerol	87087-60-3
10.5	236067.9	37056	57.6	592.3179	591.3107	C ₃₂ H ₄₁ N ₅ O ₆	Nummularine B	53947-96-9
10.4	320098.2	37188	27.7	613.3403	614.3476	C ₃₀ H ₄₄ N ₈ O ₆	Phe Lys Arg Tyr	-
14	255263.7	37355	26.7	216.1595	215.1522	C ₁₁ H ₂₁ NO ₃	Ethyl 3-(N-butylacetamido)propionate	52304-36-6
0.8	473318.2	37382	57.1	398.9066	397.8993	-	-	-
0.8	800093.6	37447	56.4	418.866	835.7199	-	-	-
10.8	243612.2	37964	19.8	273.1674	272.1616	C ₁₃ H ₄ D ₁₀ N ₂ O ₄	DMABA-d10 NHS ester	1175002-05-

								7
14.8	1039402	38075	24.8	505.3339	506.3412	C ₂₇ H ₄₄ N ₄ O ₅	Phe Ile Ile Ile	-
0.9	697167.8	38266	35.5	204.9088	815.579	-	-	-
0.9	145904.9	38527	12.7	220.9347	221.9419	-	-	-
1	211601.4	38546	13.4	101.95	100.9427	-	-	-
1.6	201969.5	38583	33	385.1017	384.0938	C ₂₂ H ₁₈ O ₅	Chamanetin	-
15.5	353632.3	38610	78.6	230.2477	229.2404	C ₁₄ H ₃₁ NO	Xestoaminol C	-
0.8	486056.9	38918	65	328.8977	327.8904	C ₆ H ₁₂ Br ₂ O ₄	Mitobronitol	488-41-5
18	654748.8	39508	51.3	415.2109	414.2041	C ₂₂ H ₃₂ O ₆	Dihydrofukinolide	41059-95-4
						C ₁₇ H ₃₀ N ₆ O ₄ S	Lys Met His	-
							Eplerenone	107724-20-9
						C ₂₄ H ₃₀ O ₆	Magnoshinin	86702-02-5
0.8	384752	39549	878.9	327.4257	652.8368	-	-	-

10.4	224926.6	39648	48	608.3847	607.3775	C ₃₃ H ₅₃ NO ₉	Malyngamide J	-
15.5	306609.4	40438	28.6	225.0546	224.0476	C ₁₄ H ₈ O ₃	Hydroxyanthraquinone	129-43-1
0.9	89395.55	40661	59.6	304.896	303.8887	-	-	-
1.1	332195.4	40952	11.9	84.9598	83.9525	CH ₂ Cl ₂	Dichloromethane	75-09-2
							(-)-Viburnitol	488-76-6
3.5	465639.3	41088	46.8	187.058	186.0507	C ₆ H ₁₂ O ₅	2-Deoxy-D-galactose	1949-89-9
							Digitoxic acid	-
0.9	130241	41246	42.4	226.8911	225.8839	-	-	-
12.7	232913.2	41679	56.5	246.2428	245.2355	-	-	-
20.2	362558	41769	29.6	282.2788	281.2715	C ₁₈ H ₃₅ NO	Oleamide	301-02-0
19	453120.9	42125	86.7	667.444	666.4381	C ₃₇ H ₆₂ O ₁₀	Notoginsenoside T2	343962-54-9
9.9	321529.4	42509	51.2	495.2413	496.2486	C ₂₃ H ₃₄ N ₄ O ₈	Ala Glu Ile Tyr	-
9.9	236134.3	42638	30.3	490.2857	489.2785	C ₂₁ H ₃₉ N ₅ O ₈	Glu Ile Lys Thr	-

0.8	603378.8	42692	42.4	241.9993	240.992	C ₈ H ₁₀ ClNO ₂ S	4-AMINO-3- (5-CHLOROTHIEEN-2-YL)BUTANOIC ACID	-
13.9	255152.8	42725	32.7	359.2035	358.1962	C ₁₄ H ₂₆ N ₆ O ₅	Arg Pro Ser	-
1.7	281187.5	42998	21.3	113.0362	224.0579	-	-	-
8.5	388165.1	43000	21.3	201.1101	202.1174	-	-	-
0.8	630456.1	43092	478.8	383.3993	382.392	-	-	-
8.9	235838.7	43103	24.2	215.1255	214.1182	-	-	-
0.8	133420.9	43182	33.1	282.9049	281.8977	-	-	-
0.8	463717.6	43592	484.4	392.4046	782.7947	-	-	-
18.2	309472.5	43874	57.4	182.1175	181.1102	C ₁₀ H ₁₅ NO ₂	beta-O-Methylnephine	60094-92-0
1.1	409954.1	44656	12.5	125.9863	124.979	-	-	-
1.5	329672.8	44821	32.9	152.0708	149.048	C ₈ H ₉ NO ₂	2-Phenylglycine	2835-06-5
0.8	584613.2	44919	36.3	430.8723	429.8651	-	-	-
17.2	586899	45590	89.5	302.3052	301.2979	C ₁₈ H ₃₉ NO ₂	Sphinganine	764-22-7

13.7	348741	45920	29.4	290.2689	289.2616	-	-
0.8	633770.3	46153	512.8	448.3781	447.3708	C ₂₆ H ₅₁ NO ₃	C-8 Ceramide 74713-59-0
20.5	294632	46231	32.7	282.2789	281.2717	C ₁₈ H ₃₅ NO	Oleamide 301-02-0
0.8	5388698	46765	19.2	622.7998	1247.6141	-	-
0.9	89559.55	47133	69.3	226.9512	225.9445	C ₆ H ₄ Cl ₂ O ₅	2,5-Dichloro-4-oxohex-2-enedioate -
11.2	446208.1	47626	39.8	107.0704	106.0632	C ₄ H ₁₀ O ₃	Diethylene glycol 111-46-6
21.7	290787.4	47741	110.9	658.2525	657.2452	C ₃₂ H ₃₇ N ₅ O ₉	Gln Tyr Tyr Tyr -
10.2	415424.5	47964	74.2	569.3142	570.3215	C ₂₆ H ₄₄ N ₆ O ₆ S	Lys Lys Met Tyr -
0.9	302914.8	48139	77.4	142.9386	141.9313	-	-
1.7	919087.4	48141	27.2	191.0229	190.0157	-	-
1.5	358052.2	48207	97.3	283.1402	282.133	C ₁₀ H ₂₀ N ₄ O ₄	Lys Asn -
10.5	368180.3	48457	71.2	597.273	598.2803	C ₃₂ H ₃₈ N ₄ O ₆	Phe Phe Val Tyr -
0.8	1605693	48640	540.4	440.3893	441.3966	-	-

10.2	266004	49811	23.6	564.3588	563.3515	-	-	-
1.6	456086.2	50021	137.7	281.0317	279.0176	C ₁₀ H ₁₁ ClN ₂ O ₄	2-(4-amino-5-chloro-2-methoxybenzamido)acetic acid	-
13.8	1214668	50225	21.3	447.2922	448.2995	C ₁₉ H ₃₈ N ₆ O ₆	Ala Lys Lys Thr	-
7.3	223987.5	50267	8.3	133.0861	132.0788	C ₆ H ₁₂ O ₃	4,4-Dimethoxy-2-butanone	5436-21-5
							DL-4-hydroxy caproic acid	-
0.9	61714.37	50416	1120.4	362.8664	361.8591	C ₁₂ H ₅ Cl ₅ O	2-Hydroxy-2',3',4',5,5'-pentachlorobiphenyl	67651-36-9
0.9	226967.1	51770	49.4	294.8797	1469.3681	-	-	-
10.3	284214.9	51868	94.3	548.2914	547.2841	C ₂₂ H ₄₁ N ₇ O ₇ S	Glu Ile Met Arg	-
							13-Nor-6-cremophilene-8,11-dione	348119-85-7
21.8	379318.5	52017	50.1	243.1355	242.1283	C ₁₄ H ₂₀ O ₂	3-Phenylpropyl isovalerate	5452-07-3
							2,6-di-tert-butylbenzoquinone	719-22-2
						C ₁₁ H ₁₈ N ₂ O ₄	Hydroxypentobarbital	4241-40-1
0.9	139184.4	52105	578.9	90.9766	89.9693	-	-	-

9.6	271444.8	52556	46.4	446.2593	445.252	C ₁₉ H ₃₅ N ₅ O ₇	Ala Asp Ile Lys	-
10.3	391283.9	53269	130.6	182.1906	181.1833	C ₁₂ H ₂₃ N	Dicyclohexylamine	101-83-7
14.1	340809.4	53503	40.3	316.2844	315.2772	C ₁₈ H ₃₇ NO ₃	Dehydrophytosphingosine	-
1.7	639262	53591	77.9	297.086	296.0787	C ₁₄ H ₁₁ F ₃ N ₂ O ₂	flunixin	-
						C ₁₂ H ₂₀ O ₄	Traumatic acid	-
							Diisopropyl phthalate	605-45-8
9.4	313991.4	53774	26.8	251.1255	252.1328	C ₁₄ H ₁₈ O ₄	Ubiquinone-1	727-81-1
							δ-CEHC	1221504-67-1
8.4	233069	54746	20.7	300.2019	299.1946	-	-	-
0.8	547720.6	56753	96.4	102.9702	101.9629	-	-	-
18.2	398917.7	57124	37.2	275.175	274.1678	C ₁₆ H ₂₂ N ₂ O ₂	Allyxycarb	6392-46-7
0.9	188308.7	57498	56.9	350.8937	349.8868	-	-	-

20.3	380032.2	57954	41	282.2788	281.2715	C ₁₈ H ₃₅ NO	Elaidamide	4303-70-2
							3-Acetyldihydro-2(3H)-furanone	-
0.8	660348.4	58327	25.4	151.0353	150.028	C ₆ H ₈ O ₃	2-Oxo-4E-hexenoic acid	-
11.7	371180	58513	129.2	262.2377	261.2304	-	-	-
8.7	297480.6	58748	107	328.1602	327.1529	C ₁₃ H ₂₁ N ₅ O ₅	Ala Thr His	-
9.6	531813.2	59218	54.7	451.215	429.7607	C ₂₁ H ₃₀ N ₄ O ₇	Ala Asp Val Phe	-
9	294905.4	59495	97.1	358.2074	357.2001	C ₁₅ H ₂₇ N ₅ O ₅	Gly Gly Lys Pro	-
19	472714.5	59916	154.5	651.4786	652.4859	-	-	-
							Acetic anhydride	108-24-7
11.8	290706	60319	86.4	103.0391	102.0318	C ₄ H ₆ O ₃	4-hydroxy-crotonic acid	-
0.8	1035958	60559	38.9	130.9652	127.9572	C ₂ H ₄ Cl ₂ O ₂	2,2-Dichloro-1,1-ethanediol	16086-14-9
						C ₁₄ H ₂₄ O ₄	5-Nonyltetrahydro-2-oxo-3-furancarboxylic acid	-
21.8	956933.8	60626	32	279.1591	278.152	C ₁₆ H ₂₂ O ₄	Dibutyl phthalate	84-74-2

	2310746							
23.3		60791	18.4	108.5177	107.5104	-	-	-
	8							
1.6	919929	60820	50.9	251.0753	248.0718	C ₈ H ₁₂ N ₄ O ₄	Decitabine	2353-33-5
0.8	1348532	60922	71.2	501.8506	500.8448	-	-	-
1.6	270423.8	61023	86.9	279.0389	278.0324	C ₁₀ H ₁₂ N ₂ O ₄ S	N1,N4-Diacetylsulfanilamide	5626-90-4
12.5	462733.2	61324	85.3	187.0396	186.0323	C ₁₁ H ₆ O ₃	Psoralen	66-97-7
8.2	384923.9	61467	45.6	231.1204	232.1277	-	-	-
9.3	312898.5	62008	84.4	402.2332	401.2259	C ₁₇ H ₃₁ N ₅ O ₆	Ala Ala Ile Gln	-
10.3	462104.2	62370	94.7	553.2469	554.2542	C ₂₄ H ₃₆ N ₆ O ₇ S	Phe Met Gln Gln	-
7.8	413093.9	62551	39.6	114.0916	113.0843	C ₆ H ₁₁ NO	2-Acetylpyrrolidine	60026-20-2
3.5	627075.9	62692	34.4	173.0786	174.0859	-	-	-
1.5	250966	63071	63	182.0814	181.0742	C ₉ H ₁₁ NO ₃	DL-o-Tyrosine	2370-61-8
12.6	427116.8	63141	6.9	287.1464	288.1537	C ₁₂ H ₂₄ O ₆	Hexyl glucoside	59080-45-4

	2150058							
23		63327	20.4	115.9641	114.9568	-	-	-
	6							
0.9	420720.1	64075	76.5	213.9694	212.9622	C ₆ H ₆ ClNO ₂ S	p-Chlorobenzenesulfonylamide	98-64-6
0.9	345354.6	64285	68.3	300.9143	299.907	-	-	-
16.3	339605.6	65525	728.1	299.1825	298.1752	C ₁₆ H ₂₆ O ₅	13,14-dihydro-15-keto-tetranor PGE2	20675-85-8
23.1	451481.5	65774	46.6	282.2787	281.2714	C ₁₈ H ₃₅ NO	Elaidamide	4303-70-2
10	540566.7	66088	59.1	525.2883	526.2956	C ₂₄ H ₄₀ N ₆ O ₅ S	Cys Phe Lys Lys	-
12.8	1461992	66478	23.7	389.2505	390.2578	C ₁₆ H ₃₂ N ₆ O ₅	Gly Gly Lys Lys	-
23.3	499113.1	68143	48.3	282.2787	281.2714	C ₁₈ H ₃₅ NO	Elaidamide	4303-70-2
1	690870.5	69114	49.4	127.0728	126.0656	C ₃ H ₆ N ₆	Melamine	108-78-1
23.9	500126.6	69145	84	300.2892	299.2819	C ₁₈ H ₃₇ NO ₂	12-amino-octadecanoic acid	-
9.3	513398.7	69962	76.3	407.1886	408.1959	C ₁₉ H ₂₆ N ₄ O ₆	Phe Gly Ser Pro	-
0.9	474661.5	70697	51.4	177.9482	176.9409	-	-	-

19	488255.1	70797	69.2	356.2792	355.2719	-	-	-
9.1	362922.6	71895	118.9	372.1864	371.1791	C ₁₅ H ₂₅ N ₅ O ₆	Ala Ala Asn Pro	-
1.6	335500.5	71899	72.6	237.0916	236.0843	C ₁₆ H ₁₂ O ₂	trans-4,5-Dihydroxy-4,5-dihdropyrene	-
						C ₈ H ₁₆ N ₂ O ₄ S	Methionyl-Serine	-
0.9	178840.9	71963	86.3	164.1282	163.1209	-	-	-
12.8	482174	72222	100	334.2948	333.2875	-	-	-
0.8	1029340	72516	39.1	167.0127	166.0054	-	-	-
10	369538.9	72634	128.1	520.3327	519.3254	-	-	-
10.1	405711.9	74170	133.6	504.2651	503.2578	C ₂₈ H ₃₃ N ₅ O ₄	Trp Trp Leu	-
0.9	193335.3	74354	171.2	180.8945	359.7757	-	-	-
9.2	493246.5	75378	42.2	215.1258	214.1185	C ₁₁ H ₁₈ O ₄	2,2'-(3-methylcyclohexane-1,1-diyl)diacetic acid	-
15.6	890423.9	78813	66	271.1878	272.1951	C ₁₅ H ₂₆ O ₄	Ethylene brassylate	105-95-3
9	308183.2	79606	884.5	195.088	194.0807	C ₁₁ H ₁₂ N ₂	NORELEAGNINE	16502-01-5

						C ₇ H ₁₄ O ₆	QUEBRACHITOL	642-38-6
1.5	345908.8	79610	144.5	158.1541	157.1468	-	-	-
0.8	2582030	79766	130.8	436.8704	435.8632	-	-	-
8.7	470324.8	80496	65.5	215.0892	216.0964	C ₈ H ₁₆ O ₅	5(S),6(R)-7-trihydroxymethyl Heptanoate	-
9.8	449021.7	81070	112.6	460.2388	459.2315	C ₁₉ H ₃₃ N ₅ O ₈	Ala Glu Ile Gln	-
11.7	1320205	81418	91	229.1415	226.1202	C ₁₂ H ₂₀ O ₄	Traumatic acid	-
10.1	562434.7	81504	104.8	509.2207	510.228	C ₁₉ H ₃₆ N ₆ O ₆ S ₂	Cys Lys Met Gln	-
15.2	468347.1	82156	99.3	192.1384	191.1312	C ₁₂ H ₁₇ NO	diethyltoluamide	134-62-3
11.8	1523652	82325	40.6	331.209	332.2163	C ₁₃ H ₂₆ N ₆ O ₄	Gly Val Arg	-
2.4	8024239	83509	41	129.0525	128.0452	C ₄ H ₁₀ O ₃	Diethylene glycol	111-46-6
0.7	1196082	83829	16.5	99.5311	98.5238	-	-	-
16	450921	84161	61.8	225.196	224.1887	C ₁₃ H ₂₄ N ₂ O	Anapheline	19519-53-0
0.8	1361632	84343	35.2	162.0073	160.0048	-	-	-

						C ₁₄ H ₁₈ O ₇	Picein	530-14-3
14	854706.9	84345	58.2	299.11	298.1028			
						C ₁₂ H ₂₀ O ₇	Triethyl citrate	77-93-0
								1175002-05-
10.6	1187954	84435	44	273.1675	250.6181	C ₁₃ H ₄ D ₁₀ N ₂ O ₄	DMABA-d10 NHS ester	7
9.5	440185.7	84798	246.4	416.2126	415.2053	C ₁₇ H ₂₉ N ₅ O ₇	Ala Pro Gln Thr	-
0.8	1012602	85761	43.5	146.0297	145.0225	-	-	-
0.8	1059292	88230	28.5	81.5205	161.0265	-	-	-
9	584477.2	90015	90.5	363.1626	364.1699	C ₁₅ H ₂₄ N ₄ O ₅	Ala Gly Pro Pro	-
17.2	900535.6	90846	34.1	311.185	310.1781	C ₁₇ H ₂₆ O ₅	Valdiate	162232-32-8
0.9	290833.2	91130	53.3	288.9216	287.9143	-	-	-
9.8	484775.9	91876	113.2	481.2617	480.2545	C ₂₃ H ₃₆ N ₄ O ₇	Phe Ile Thr Thr	-
9.8	638369.8	92190	69.2	465.1941	466.2014	C ₂₁ H ₂₈ N ₄ O ₈	Ala Asp Pro Tyr	-
1.6	461827.3	93443	140.2	89.0599	88.0526	C ₄ H ₈ O ₂	Isobutyric acid	79-31-2

							Propyl formate	110-74-7
							1-Hydroxy-2-butanone	5077-67-8
							Ethyl acetate	141-78-6
9.8	487837.8	93967	50.4	476.3062	475.299	C ₂₁ H ₄₁ N ₅ O ₇	Netilmicin	-
						C ₁₄ H ₂₄ N ₆ O ₉	Ser Asn Ser Asn	-
9.5	636120.7	99519	53.5	421.1681	422.1754	C ₂₅ H ₂₄ O ₆	Pomiferin	572-03-2
0.9	373909.3	103126	59.3	164.9205	327.826	-	-	-
8	887823.6	105771	104.1	130.1591	129.1519	C ₈ H ₁₉ N	Octylamine	111-86-4
1.6	369611.3	106141	19	213.1336	212.1263	-	-	-
0.9	687910.4	108003	96	195.9588	194.9516	-	-	-
7.1	806968.8	112813	113.9	187.0944	188.1017	C ₈ H ₁₂ N ₄	1-(2-Pyrimidyl)piperazine	20980-22-7
15.1	1347444	113220	106.8	684.3787	683.3719	-	-	-
8.4	611070	114280	78.7	245.0998	246.1071	C ₉ H ₁₈ O ₆	Isopropyl beta-D-glucoside	5391-17-3

						C ₁₁ H ₁₆ O ₆	threo-Syringoylglycerol	121748-11-6
21.8	1066416	115197	82.9	205.086	204.0787	C ₁₂ H ₁₂ O ₃	Anofinic acid	34818-56-9
6.4	965866.9	116887	75	217.105	218.1123	-	-	-
9.1	679734.1	117866	87.9	377.142	378.1493	C ₁₆ H ₂₄ O ₁₀	(1x,2x)-Guaiacylglycerol 3-glucoside	7094-73-7
9.5	667964.3	122964	115.1	437.2357	436.2284	C ₂₁ H ₃₂ N ₄ O ₆	Ala Ala Ile Tyr	-
8.7	728668.8	123354	98.9	333.1155	334.1228	C ₁₉ H ₃₇ N ₅ O ₆	Ala Lys Thr Ile	-
9.5	639935.3	123764	159.7	432.2802	431.273	-	-	-
20.7	839195.3	125441	88.8	282.2788	281.2715	-	-	-
8.8	589032.3	125479	69	344.2278	343.2206	-	-	-
6.6	845853.5	125514	136.6	231.0843	232.0916	C ₈ H ₁₆ O ₆	Ethyl beta-D-glucopyranoside	3198-49-0
8.5	858610.2	126721	179	319.1364	320.1437	-	-	-
0.8	1491326	129806	133.6	239.9664	238.9591	-	-	-
15.8	825088.7	132561	80.1	158.1539	157.1467	-	-	-

19	938343.3	133688	132.6	297.2421	296.2357	C ₁₈ H ₃₂ O ₃	(±)9-HODE	98524-19-7
8	649009.2	135925	217.6	289.0895	288.0822	C ₁₂ H ₁₆ O ₈	Glucosylisomaltol	85559-61-1
21.7	1633252	137708	72.8	279.1592	278.1522	C ₁₆ H ₂₂ O ₄	Diisobutyl phthalate	84-69-5
1.6	641950	141312	67.1	371.1226	370.1153	C ₂₂ H ₂₀ O ₄	Erybraedin E	-
23.6	5117199 2	141442	23.1	99.5124	197.0103	-	-	-
9.6	894574.1	141843	61.1	212.1184	211.1111	C ₁₃ H ₁₃ N ₃	Varenicline	249296-44-4
1.6	2202618	144930	312	265.0595	264.053	C ₁₅ H ₈ N ₂ O ₃	Necatorine	89915-35-5
7.9	873764.8	146145	134.8	275.1104	276.1177	C ₁₀ H ₂₀ O ₇ C ₁₀ H ₁₆ N ₃ O ₆	2,3-Butanediol glucoside Glutamyl-Glutamine	146763-54-4 -
11.5	854886.8	147895	226.1	218.2116	217.2043	-	-	-
13	968912.8	150689	216.4	288.2532	287.246	C ₁₆ H ₃₃ NO ₃	Lauroyl diethanolamide	120-40-1
21.7	890356.3	150713	108.4	205.0861	204.0788	C ₁₂ H ₁₂ O ₃	Anofinic acid	34818-56-9

0.8	2769459	151648	95.5	474.833	473.8258	-	-	-
9.2	731907.4	152436	159.2	388.2541	387.2468	C ₁₇ H ₃₃ N ₅ O ₅	Ala Ala Lys Val	-
19	1138074	161953	112.3	279.2317	278.2244	C ₁₈ H ₃₀ O ₂	8Z,10E,12Z-octadecatrienoic acid	-
9.2	1185052	167344	205.7	393.2095	394.2167	C ₁₉ H ₂₈ N ₄ O ₅	Phe Gly Ile Gly	-
0.8	2325609	170044	288.3	344.8752	343.8689	C ₈ HCl ₄ F ₃ N ₂	4,5,6,7-Tetrachloro-2-trifluoromethylbenzimidazole	2338-29-6
1.6	1029600	171296	245.3	103.0392	102.0319	C ₄ H ₆ O ₃	Acetoacetic acid	541-50-4
15.5	1936969	172159	168.7	318.3	317.2927	C ₁₈ H ₃₉ NO ₃	Phytosphingosine	-
0.8	2053439	173406	4	198.9399	197.9326	-	-	-
25	1506536	175873	76.6	256.2632	255.2559	C ₁₆ H ₃₃ NO	Palmitic amide	629-54-9
7.8	1314946	176466	271.4	261.1311	262.1383	C ₁₂ H ₂₀ O ₆	Glycerol tripropanoate	139-45-7
0.8	2132191	179542	38.7	234.961	233.9541	C ₇ H ₇ IO	2-Iodophenol methyl ether	-
8.8	1458519	180195	160.4	349.1835	326.266	C ₁₂ H ₂₄ N ₆ O ₆	Ser Ser Arg	-
0.7	2744159	187204	34	90.5259	179.0373	-	-	-

21.7	1228681	190873	107.6	149.0235	148.0163	-	-	-
8.4	1454345	193176	166.2	305.1574	306.1646	-	-	-
0.8	3589091	195073	265.8	492.8435	983.6722	-	-	-
0.8	2459631	199462	91	257.9769	256.9697	-	-	-
0.8	2552113	202058	627	380.8964	358.9138		-	-
9.4	979060.4	205070	187.1	120.0558	119.0485		-	-
0.8	2788027	209945	87.6	362.8858	361.8789	C ₁₂ H ₈ Cl ₆	ALDRIN	309-00-2
0.8	2574937	230041	26.8	216.9505	215.9437	-	-	-
0.9	432786.2	231364	82.1	150.1125	149.1052	C ₆ H ₁₅ NO ₃	Trolamine	102-71-6
11.8	1587336	232008	164.7	199.0942	200.1014	C ₈ H ₁₆ O ₄	6,8-dihydroxy-octanoic acid	-
12.2	1582500	247895	232.9	243.1205	244.1278	-	-	-
24.1	1914786	288910	196.5	398.232	397.2247	C ₁₇ H ₃₆ NO ₇ P	PE(12:0-0:0)	-
1.6	1994391	297293	318	143.0317	144.039	C ₄ H ₈ O ₄	a,b-Dihydroxyisobutyric acid	21620-60-0

12.6	1747992	299822	192	290.269	289.2617	-	-	-
0.8	2936727	303086	173.5	255.944	253.9243	-	-	-
19	2271015	306870	188.8	337.2346	314.4636	C ₂₀ H ₃₂ O ₄	15-epi-PGA1	20897-92-1
15.4	3336940	371088	592.3	274.274	273.2667	C ₁₆ H ₃₅ NO ₂	C16 Sphinganine	-
0.8	3537059	376868	428.7	273.9545	272.9473	-	-	-
7.3	2130709	396953	310.8	201.0736	202.0809	C ₇ H ₁₄ O ₅	Digitalose	4481-08-7
11.2	6811981	455184	212.5	185.115	186.1223	C ₈ H ₁₈ O ₃	(3R,7R)-1,3,7-Octanetriol	217650-11-8
0.8	6738036	569761	426.2	128.0192	127.0119	-	-	-
0.8	5400843	572761	306.7	250.9386	249.9314	-	-	-
0.8	6308986	606314	225	143.9968	142.9895	-	-	-
1.6	3489648	629791	267.9	126.0441	250.0736	-	-	-
0.8	7774674	670276	520.8	110.0087	109.0014	-	-	-
0.8	8565710	878668	422.3	232.9281	231.9208	C ₇ H ₅ Cl ₃ O	2,4,6-Trichloroanisole	87-40-1

		102827						
0.8	9936981		601.1	214.9175	213.9102	-	-	-
		7						
	1455209	119180						
1.6			729.8	107.0705	106.0636	C ₄ H ₁₀ O ₃	Diethylene glycol	111-46-6
	3	9						
	1843313	161329						
0.8			453.4	125.9862	124.9789	-	-	-
	8	4						
	1736909	170769						
0.8			495.4	84.9596	83.9523	-	-	-
	8	9						

Table S5. Compounds information of C1 in negative ionization modes.

Retention Time (min)	Area	Intensity	S/N	Max. <i>m/z</i>	Max. MW	Formula	Possible Name	CAS
						C ₂₁ H ₂₀ O ₁₄ S	Orientin 7-O-sulfate	-
10.6	51312.84	10234	39.6	527.0489	528.0561		dTDP-3,4-dioxo-2,6-dideoxy-L-glucose	-
						C ₁₆ H ₂₂ N ₂ O ₁₄ P ₂	dTDP-2,6-dideoxy-D-glycero-hex-2-enos-4-ulose	321847-68-1
1.5	51843.18	10302	16.9	151.0069	152.0141	C ₅ H ₄ N ₄ S	6-Mercaptopurine	50-44-2
1.2	36602.38	10338	9.2	110.9753	111.9826	CH ₄ O ₄ S	Monomethyl sulfate	75-93-4
0.8	29818	10379	230.6	910.7737	911.781	-	-	-
1.1	59760.65	10380	22.9	154.9183	155.9255	-	-	-
19	190031.3	10426	22.3	381.2249	382.2322	C ₁₇ H ₃₀ N ₆ O ₄	His Lys Val	-
18.7	91441.77	10475	19.5	349.1679	350.1752	C ₁₄ H ₂₆ N ₄ O ₄	Ala Pro Lys	-

						C ₁₉ H ₂₆ O ₆	Arctiopirin	19889-01-1
							Benzoic acid	65-85-0
7.2	66639.23	10497	16.1	121.0294	122.0367	C ₇ H ₆ O ₂	Tropolone	533-75-5
							4-Hydroxybenzaldehyde	123-08-0
15.1	59300.36	10697	51.7	554.243	555.2503	C ₂₃ H ₃₇ N ₇ O ₇ S	Met Arg Ser Tyr	-
0.9	61385.42	10716	13	608.6995	609.7068	-	-	-
0.8	291471.3	10826	3.9	1076.672	2155.358	-	-	-
0.8	140882.4	10908	43.5	464.8348	1863.413	-	-	-
1.6	50934.54	10923	16.2	228.0177	229.025	-	-	-
0.9	69433.09	11206	12.1	668.7075	669.7148	-	-	-
0.9	27048.77	11246	52	446.8443	447.8516	-	-	-
0.8	182232.2	11372	252.7	1003.704	2009.422	-	-	-
0.8	202217.1	11387	253	792.7896	793.7969	-	-	-

0.9	27895.62	11403	36.9	458.8781	459.8849	-	-	-
							cis-p-Coumaric acid	4501-31-9
9.2	54977.65	11619	15.8	163.0399	164.0472	C ₉ H ₈ O ₃	9-hydroxy-7Z-Nonene-3,5-dienoic acid	-
							Caffeic aldehyde	-
							3',4'-(Methylenedioxy)acetophenone	-
0.9	51541.13	11631	11.1	538.7236	539.727	-	-	-
8	86409.94	11749	23.2	165.0191	166.0264	C ₈ H ₆ O ₄	Phthalate	88-99-3
1.5	106466.3	11824	12.9	225.0065	226.0138	C ₉ H ₆ N ₂ O ₃	Nitroxoline	4008-48-4
						C ₁₀ H ₁₀ O ₂ S ₂	Bis(2-furanylmethyl) disulfide	4437-20-1
0.9	90563.7	12473	10.4	554.7725	555.7798	-	-	-
0.9	220608.7	12515	24.4	712.6765	713.6837	-	-	-
1	192133.2	12649	5.9	466.7634	467.7727	-	-	-
1.2	62924.32	12786	284.1	250.9354	251.9427	-	-	-

0.8	144177.3	12897	12.2	759.7667	1521.548	-	-	-
20.2	83214.16	13043	27.6	267.1957	268.203	C ₁₆ H ₂₈ O ₃	Methoprene acid	53092-52-7
0.8	40860.69	13061	39.6	492.898	493.9049	-	-	-
0.8	202527.3	13088	145.4	873.7466	1749.508	-	-	-
1.2	51040.69	13346	21.7	170.9785	171.9858	-	-	-
1.4	152723.1	13414	3.3	146.9647	147.9719	-	-	-
1.5	118624.8	13447	22.7	194.9964	196.0036	-	-	-
							18-hydroxypregna-1,4,20-trien-3-one	-
22.2	88276.64	13508	19.3	311.2003	312.2076	C ₂₁ H ₂₈ O ₂	Levonorgestrel	797-63-7
15.5	94805.14	13828	29.3	262.9753	263.9826	C ₁₃ H ₈ S ₂	Thiarubrine A	63543-09-9
0.9	44148.46	13934	27	520.8482	521.8583	-	-	-
18.5	73163.35	14055	28.4	266.1028	267.1101	C ₈ H ₁₇ N ₅ O ₃	Gly Arg	-
12.3	84291.72	14171	83.3	108.0215	109.0287	C ₃ H ₇ NO	3-Aminopropanal	352-92-1

						C ₆ H ₅ O ₂	p-Benzosemiquinone	-
0.8	335810.8	14172	2	946.7139	1895.442	C ₅₂ H ₁₀₁ NO ₁₃	LacCer(d18:0-22:0)	-
							4-(3-Hydroxy-7-phenyl-6-heptenyl)-1,2-benzenediol	158697-56-4
24.8	520459.8	14561	19.6	297.1516	298.1589	C ₁₉ H ₂₂ O ₃	5-Hydroxy-7-(4-hydroxyphenyl)-1-phenyl-3-heptanone	83161-96-0
							Gravelliferone	21316-80-3
							Caffeate	501-16-6
10.8	89782.49	14574	23.9	179.0348	180.0421	C ₉ H ₈ O ₄	Monomethyl phthalate	4376-18-5
0.8	157166.9	14631	10.6	130.9829	131.9902	-	-	-
7.2	113652.1	14639	28.9	165.0193	166.0266	C ₈ H ₆ O ₄	Terephthalic acid	100-21-0
0.8	155329.6	14679	163.1	662.8317	663.839	-	-	-
0.8	146476.6	14766	328.1	876.7514	1755.517	-	-	-
14.4	75617.32	15104	59.6	242.1756	243.1829	-	-	-
0.9	31472.58	15124	50.3	500.7697	501.777	-	-	-

0.8	60964.31	15285	14	814.7833	1631.581	-	-	-
1	61480.41	15359	19.9	225.926	226.9333	-	-	-
0.9	142582	15439	5.6	586.7134	587.7207	-	-	-
0.8	247878.2	15472	343.8	1022.69	1023.698	-	-	-
1.2	106451.7	15600	35.2	138.9705	139.9778	C ₃ H ₈ S ₃	Methyl (methylthio)methyl disulfide	42474-44-2
0.9	58917.07	15686	19.6	164.9465	165.9538	-	-	-
10.2	89100.82	16075	37.9	507.2072	508.2144	C ₁₉ H ₃₆ N ₆ O ₆ S ₂	Cys Lys Met Gln	-
9.9	101654.9	16474	104.6	689.1015	690.1087	C ₂₇ H ₃₀ O ₁₉ S	Kaempferol 3-(6"-sulfatogetiobioside)	-
0.9	48525.19	16482	95.5	452.8613	453.8686	C ₁₆ H ₈ Br ₂ N ₂ O ₂	6,6'-Dibromoindigotin	19201-53-7
0.8	193925.3	16577	184.2	751.7782	1505.571	-	-	-
0.8	130164	16606	184.5	898.7478	1799.498	-	-	-
14.3	87471.84	16925	40.1	152.0349	153.0422	C ₇ H ₇ NO ₃	2-Nitroanisole	91-23-6
							3-Aminosalicylic acid	570-23-0

0.8	185907	17129	11.8	130.9662	131.9735	-	-	-
1.3	81888.85	17277	8.3	198.9913	199.9986	C ₇ H ₅ ClN ₂ O ₃	AKLOMIDE	3011-89-0
0.9	41669.74	17326	35.4	276.8469	277.8542	-	-	-
0.9	44003.5	17339	13.2	322.8433	323.8506	-	-	-
1.1	50512.68	17535	194.8	199.8047	200.812	-	-	-
0.9	47342.68	17597	54.6	390.8909	391.8982	-	-	-
							Ethyl (±)-3-hydroxyoctanoate	7367-90-0
15.6	103855.1	17681	40	187.1331	188.1404	C ₁₀ H ₂₀ O ₃	7-Methyl-3-methylene-1,6,7-octanetriol	240495-78-7
							2-hydroxy capric acid	-
0.8	57740.3	17710	11.4	684.8266	685.8339	-	-	-
0.9	120173.5	17783	8.2	488.7471	489.7544	-	-	-
1.3	184407.3	18026	15.1	136.991	137.9983	-	-	-
0.9	207397.9	18179	20.4	690.69	691.6973	-	-	-

							Acitretin	55079-83-9
18.7	839186.4	18270	17.2	325.1832	326.1905	C ₂₁ H ₂₆ O ₃		
							Moxestrol	34816-55-2
0.8	324519.5	18422	18.7	1084.66	2171.334	C ₅₄ H ₉₉ NO ₁₈	Trihexosylceramide (d18:1-9Z-18:1)	-
9.9	117702.3	18603	43.9	507.2075	508.2148	C ₁₉ H ₃₆ N ₆ O ₆ S ₂	Cys Lys Met Gln	-
0.9	39365.27	18732	116.7	452.922	453.9292	-	-	-
0.9	41652.9	19124	5.9	516.7405	1035.495	-	-	-
1.5	124586.6	19176	44.2	182.9964	184.0037	C ₅ H ₁₂ OS ₃	Methyl 1-(methylsulfinyl)propyl disulfide	134018-95-4
						H ₄ O ₄ Si	Silicic acid	10193-36-9
1.2	102502.9	19548	43.5	94.9805	95.9878			
						CH ₄ O ₃ S	Methanesulfonic acid	75-75-2
						C ₁₂ H ₂₆ N ₄ O ₃	Lysyl-Lysine	-
17.2	258124.4	19656	24.4	309.1699	310.1772			
						C ₁₇ H ₂₆ O ₅	3-Hydroxy-6,8-dimethoxy-7(11)-eremophilen-12,8-olide	162613-65-2
0.8	260213.5	19805	220.1	816.7571	1635.529	-	-	-
0.9	131549.7	20200	25.4	576.756	577.7633	-	-	-

						C ₄ H ₆ ClF ₃ O	2-Chloro-1,1,2-trifluoroethyl ethyl ether	310-71-4
1	105896.5	20758	3.8	196.9757	197.983			
						C ₄ H ₆ O ₇ S	(±)-Sulfobutanedioic acid	-
0.8	81576.59	20930	232.6	554.8681	555.8754	-	-	-
0.9	57809.23	20932	66.2	478.7885	479.7966	-	-	-
0.9	172138.2	21598	24.6	592.7279	593.7352	-	-	-
0.9	138818.6	21681	19.8	254.8582	511.732	-	-	-
1	118723	21839	52.2	181.9372	182.9445	-	-	-
1.2	139502.4	21942	40.6	79.9571	80.9643	-	-	-
15.1	154272.5	22345	90.6	682.3632	683.3705	-	-	-
							L-Tyrosine methyl ester	1080-06-4
18.3	126387.2	22378	33.6	194.0817	195.0889	C ₁₀ H ₁₃ NO ₃	O-BENZYL-L-SERINE	4726-96-9
0.8	121526.6	22585	250.9	746.7964	747.8044	-	-	-
0.9	56220.89	23065	256.3	316.887	317.8943	C ₁₀ H ₇ Cl ₅ O	Tridipane	58138-08-2

16.2	140037.9	23164	61.6	197.0196	198.0269	C ₇ H ₆ N ₂ O ₅	DNOC	534-52-1
1.1	65959.39	23340	25.9	162.8388	163.8461	-	-	-
1.2	118207.5	23348	27.7	215.0227	216.0299	C ₈ H ₈ N ₂ O ₃	Nicotinuric acid	583-08-4
0.8	140962.5	23425	25.7	836.7777	837.785	-	-	-
1.6	82260.44	23625	11.9	119.0346	120.0419	C ₄ H ₈ O ₄	a,b-Dihydroxyisobutyric acid	21620-60-0
							D-Erythrose	583-50-6
0.9	52688.96	23707	85.9	328.86	329.8673	-	-	-
1.1	67285.21	23783	28.2	160.8417	161.849	-	-	-
1.2	137244.1	23944	24	314.8753	315.8826	-	-	-
0.8	100194.5	23976	69.7	356.9233	357.9306	-	-	-
0.9	86699.43	24003	83.2	494.7584	495.7657	-	-	-
0.8	270879	24056	267.3	532.874	533.8812	-	-	-
13	30676608	24833	6.2	146.9646	147.9719	-	-	-

							Hydroxyibuprofen	51146-55-5
15.7	145633.7	25377	55.7	221.1173	222.1246	C ₁₃ H ₁₈ O ₃	Isoamyl p-anisate	27739-29-3
							Annuionone B	211183-73-2
0.8	76208.42	25527	283.6	424.9108	425.9181	-	-	-
0.9	136234.4	25658	9.4	434.8241	435.8313	-	-	-
0.9	138634.6	26366	36.9	180.9122	181.9195	-	-	-
0.9	52407.58	26660	72.4	380.8215	381.8288	-	-	-
0.8	108875.6	26764	3.6	486.8809	487.8882	-	-	-
14.6	245865.9	26951	33.9	184.9838	185.9911	C ₈ H ₆ OS	2-(2-Thienyl)furan	27521-80-8
0.8	148155.8	26979	299.8	892.7314	893.7386	-	-	-
0.9	157293.1	27003	49.9	79.9571	80.9643	-	-	-
							3-Vinylcatechol	-
10.8	136049	27518	60.4	135.045	136.0523	C ₈ H ₈ O ₂	Toluate	99-94-5

							Phenyl acetate	122-79-2
							4-Hydroxyphenylacetaldehyde	7339-87-9
1.1	82957.05	27899	310	195.8105	196.8177	-	-	-
10.1	186898.5	28983	68.1	213.9634	214.9707	-	-	-
0.8	450835	30140	18.5	158.9784	159.9857	C ₇ H ₆ Cl ₂	2,4-Dichlorotoluene	95-73-8
0.8	145752.7	31432	349.2	616.8384	617.8457	-	-	-
0.8	463982.3	31439	6.3	938.7246	1879.464	-	-	-
0.9	242918.9	31465	7.9	570.7417	571.749	-	-	-
0.8	124803.2	31573	350.8	768.7902	769.7975	-	-	-
0.9	230131.1	32643	42.8	250.8847	251.8919	C ₅ H ₃ Cl ₃ O ₃	3-Chloro-4-(dichloromethyl)-5-hydroxy-2(5H)-furanone	77439-76-0
0.9	74333.87	34311	11.4	322.9036	323.9108	-	-	-
1.5	171398.1	34871	33	152.9859	153.9932	C ₄ H ₁₀ S ₃	Methyl propyl trisulfide	17619-36-2
0.9	155687.5	37033	66.5	374.8083	375.8156	-	-	-

1.1	105773.3	37374	415.3	197.8074	198.8147	-	-	-
0.8	95246.93	38689	134.1	576.8626	577.8699	-	-	-
0.8	359588.6	39279	3.2	954.7015	1911.418	-	-	-
0.8	148289.9	39301	873.4	830.7608	831.7679	-	-	-
0.8	119156.4	41552	923.4	294.9532	295.9605	-	-	-
0.9	298931.3	41951	47.1	472.778	473.7831	-	-	-
1.2	411987.5	42222	47.8	232.8825	233.8898	-	-	-
0.9	162085	42440	79.9	358.8395	359.8468	-	-	-
1.1	219776.8	42919	10.7	146.9657	147.9729	-	-	-
1	252789.6	44658	100.7	138.9704	139.9776	C ₃ H ₈ S ₃	Methyl (methylthio)methyl disulfide	42474-44-2
0.9	272432.8	45575	137	456.8067	457.814	-	-	-
0.9	213941.9	47935	99.2	238.8908	239.8975	-	-	-
0.9	272501.4	48352	48.5	314.875	315.8823	-	-	-

						$C_{10}H_5ClO_2$	2-Chloro-1,4-naphthoquinone	1010-60-2
0.8	194617.7	49487	549.9	226.9657	227.973	$H_8N_2O_8S_2$	Ammonium peroxydisulfate	7727-54-0
0.8	222859.3	49916	11.6	762.7742	763.7815	-	-	-
0.9	262511.7	51505	20.5	292.8944	293.9017	-	-	-
0.8	186700.6	54413	18.9	700.8037	701.811	-	-	-
0.9	323721.1	54622	35.4	450.7921	451.7994	-	-	-
0.8	145591.5	54678	50.9	638.8334	639.8407	-	-	-
0.8	647273.6	55597	1235.5	808.7672	1619.549	-	-	-
1.9	3495792	58797	16.9	96.9599	97.9672	H_2O_4S	Sulfuric acid	7664-93-9
16.4	358864.8	59717	147.2	331.248	332.2553	$C_{18}H_{36}O_5$	9,10,13-Trihydroxystearic acid	50439-74-2
0.9	159423.8	59851	11.6	180.9728	181.9801	-	-	-
0.9	133609.5	62716	94.2	316.9473	317.9546	$C_{14}H_{10}C_{14}$	Mitotane	53-19-0
0.9	418241.5	64037	83.6	352.8269	353.8342	-	-	-

0.8	697928.7	66020	149.5	678.8093	679.8164	-	-	-
0.8	167569.8	67325	124.4	508.8756	509.8829	-	-	-
1.2	797601	79222	109.1	216.909	217.9163	-	-	-
15.1	526113.9	79477	213.7	728.3682	729.3754	-	-	-
0.9	166553	79882	158.7	186.9292	187.9365	-	-	-
0.9	523689.3	80187	70.1	336.8578	337.8651	C ₁₂ H ₃ Cl ₅ O	1,2,3,7,8-Pentachlorodibenzofuran	57117-41-6
0.8	245204.5	80522	97.9	570.8459	571.8532	-	-	-
0.8	281629.6	85011	944.6	632.8165	633.8237	-	-	-
0.8	788969	85665	12.7	824.7447	825.752	-	-	-
0.8	251737.2	87967	78.1	372.9009	373.9082	-	-	-
0.9	202501.4	89001	988.9	248.9601	249.9673	-	-	-
0.8	333102.9	96021	24.2	502.8585	503.8658	-	-	-
0.8	1106301	101641	4.8	548.8516	549.8588	-	-	-

0.9	677505.8	110798	98.4	330.842	331.8493	-	-	-
0.8	255690.7	121061	2690.2	440.8883	441.8956	-	-	-
0.8	1105075	125695	69.7	694.787	695.7943	-	-	-
13.7	808677.8	133736	219.7	183.0043	184.0116	C ₆ H ₄ N ₂ O ₅	2,4-DINITROPHENOL	51-28-5
0.8	1449297	134296	8.4	418.8939	419.9012	-	-	-
0.8	1560404	150164	16.3	146.9611	147.9683	CH ₅ O ₄ P	Hydroxymethylphosphonate	-
0.8	463532.1	152722	34.6	242.9433	243.9505	-	-	-
12.3	891721.3	157457	234.9	138.0195	139.0267	C ₆ H ₅ NO ₃	2-Nitrophenol	88-75-5
							3-Hydroxypicolinic acid	874-24-8
							Dibutyl decanedioate	109-43-3
19	1134373	163886	287.1	313.2374	314.2446	C ₁₈ H ₃₄ O ₄	9,10-dihydroxy-12-octadecenoic acid	-
0.8	2819738	255365	223.3	288.9362	289.9435	-	-	-
0.8	2610534	270301	375.9	434.8714	435.8787	-	-	-

0.9	752685.3	306092	110	112.9855	113.9928	C ₂ HF ₃ O ₂	trifluoroacetic acid	76-05-01
0.8	3420062	318449	25.6	174.956	175.9627	C ₂ H ₅ O ₅ P	Acetyl phosphate	590-54-5
0.9	2538500	348456	479.9	216.909	217.9163	-	-	-
0.8	4995733	521614	41.5	304.9137	305.921	-	-	-
1.2	21506516	3134946	899.6	96.9598	195.9337	H ₂ O ₄ S	Sulfuric acid	7664-93-9

Table S6. Compounds information of C1 in positive ionization modes.

Retention Time (min)	Area	Intensity	S/N	Max. <i>m/z</i>	Max. MW	Formula	Possible Name	CAS
23.9	52119.75	10070	14.1	156.1382	155.1309	C ₉ H ₁₇ NO	2-(1-Pyrrolidinyl)-3-pentanone	97073-16-0
1	75793.97	10074	223.9	132.0767	129.0793	C ₄ H ₉ N ₃ O ₂	Creatine	57-00-1
						C ₁₃ H ₂₆ N ₆ O ₄ S	Met Gly Arg	-
							12-Dehydroporson	171438-25-8
18.2	75960.72	10076	12.5	385.1615	384.1563		Kanzonol N	156250-71-4
						C ₂₂ H ₂₄ O ₆	Benzyl acetoacetate	5396-89-4
							Schizandrin C	61301-33-5
0.9	97869.77	10120	25.3	640.7063	1277.398	-	-	-
1.9	296810.3	10139	9.3	145.0258	144.0185	C ₇ H ₆ O ₂	Benzoic acid	65-85-0

							3-Hydroxybenzaldehyde	100-83-4
0.8	100814.4	10144	11.1	133.0344	132.0271	-	-	-
0.8	109293.3	10165	112.9	336.4309	335.4236	-	-	-
1.2	97578.94	10179	8.9	100.0394	98.0368	C ₄ H ₅ NO ₂	Succinimide	123-56-8
21.7	102979.9	10187	11.4	219.9895	218.9822	C ₆ H ₅ NO ₆ S	4-Nitrophenyl sulfate	1080-04-2
16.3	77810.98	10233	30.6	242.2842	241.277	C ₁₆ H ₃₅ N	1-Hexadecylamine	143-27-1
20.2	4831338	10235	4.1	101.9498	100.9425	-	-	-
0.9	29466.65	10259	16.3	182.892	181.8847	-	-	-
0.9	69452.16	10305	6.1	155.9804	309.9466	-	-	-
1.6	50882.54	10312	5.3	160.9892	159.982	-	-	-
0.9	129944.8	10323	5.3	627.7374	626.7302	-	-	-
							6-Methylcoumarin	92-48-8
12.2	71447.38	10380	14.2	161.0595	160.0523	C ₁₀ H ₈ O ₂	2-Formyl-1-indanone	56794-24-2

							Naphthalene-1,2-diol	574-00-5
0.9	70738.75	10414	10	486.8584	485.8511	-	-	-
0.9	81032.6	10433	17.3	497.8305	498.8378	-	-	-
10.1	54012.96	10467	8.4	534.3118	533.3045	C ₂₂ H ₄₃ N ₇ O ₆ S	Lys Lys Met Gln	-
19.9	73166.04	10473	6.6	149.023	147.0116	-	-	-
0.9	24665.51	10503	18.4	242.8646	241.8573	-	-	-
1.1	34943.56	10511	116.8	146.9967	145.9894	-	-	-
19	86024.75	10516	9	186.1089	185.1017	-	-	-
8.5	45357.12	10524	23.2	314.1813	313.174	-	-	-
0.9	274364.2	10548	28.8	780.6292	1557.2	C ₄₄ H ₈₈ NO ₆ P	PC(O-18:1(9E)-O-18:1(9E))[U]	-
9.6	81009.38	10548	7.6	209.0785	207.0537	C ₉ H ₁₄ O ₄	cis-2-Carboxycyclohexyl-acetic acid	14715-37-8
						C ₂₂ H ₂₇ NO ₄	Corydaline	518-69-4
22.3	167184.1	10586	17.7	370.2014	369.1941	C ₁₅ H ₃₂ NO ₇ P	PC(7:0-0:0)	-

							3-(3,4-Methylenedioxyphenyl)propenal	14756-00-4
							7-Hydroxy-6-methyl-2H-1-benzopyran-2-one	53811-56-6
12	120241.4	10634	12.9	177.0546	176.0487	C ₁₀ H ₈ O ₃		
							1,4,5-Naphthalenetriol	481-40-3
							HERNIARIN	531-59-9
1.2	74860.76	10674	9	294.8353	293.828	-	-	-
0.7	128160.1	10686	24.5	223.989	222.9817	-	-	-
0.9	110720.3	10722	20.8	297.8972	298.9045	-	-	-
2	2114574	10723	3.1	84.9597	83.9524	-	-	-
0.9	149318.5	10724	11.1	714.7147	1421.357	-	-	-
0.9	62253.98	10748	18	606.8073	605.8	-	-	-
14.7	131874.7	10751	36.3	284.9612	283.9539	C ₆ H ₁₂ Cl ₃ O ₄ P	Tris(2-chloroethyl)phosphate	115-96-8
24.1	102907.5	10758	11.6	399.3068	398.2996	C ₂₃ H ₄₂ O ₅	1-Oleoyl-2-acetyl-sn-glycerol	86390-77-4
0.9	54874.33	10759	3.3	133.0279	132.0206	C ₈ H ₄ O ₂	2,4,6-Octatriynoic acid	51193-80-7

9.9	302262.9	10782	21.6	509.2229	508.2159	C ₁₉ H ₃₆ N ₆ O ₆ S ₂	Cys Lys Met Gln	-
0.7	137038	10864	10.4	252.971	251.9637	CH ₃ ClHg	Methylmercury chloride	115-09-3
0.9	115832.1	10906	242.4	894.564	891.5395	-	-	-
							12-amino-octadecanoic acid	-
20.7	142149.1	10914	9.2	300.2892	299.2822	C ₁₈ H ₃₇ NO ₂	Sphingosine	123-78-4
						C ₃₁ H ₄₆ O ₂	Phylloquinone	84-80-0
23.3	361524.4	10929	11.8	473.3436	472.3363	C ₂₂ H ₄₄ N ₆ O ₅	Lys Lys Val Val	-
0.9	62089.95	10967	121.9	576.7844	1147.537	-	-	-
11	155647.8	10974	8.7	384.2358	766.4566	C ₂₁ H ₂₉ N ₅ O ₂	CAY10598	346673-06-1
						C ₁₇ H ₃₀ N ₆ O ₄ S	Lys Met His	-
							Estra-1,3,5(10)-triene-3,6beta,17beta-triol triacetate	-
22.1	118338.8	10979	15.6	415.2093	416.2166	C ₂₄ H ₃₀ O ₆	Eplerenone	107724-20-9
							Magnoshinin	86702-02-5

0.7	122962.1	11037	4.9	179.0223	178.0151	C ₈ H ₉ ClO	chloroxylenol	88-04-0
							Isobutyric acid	79-31-2
							Isopropyl formate	625-55-8
11.2	111108.5	11055	13.7	89.0598	88.0525	C ₄ H ₈ O ₂	1,4-Dioxane	123-91-1
							Ethyl acetate	141-78-6
						C ₁₆ H ₃₂ O ₂	2-Octanone	111-13-7
22.1	81218.39	11055	14.1	279.2321	278.2248		10E,12E,14Z-Hexadecatrienyl acetate	-
						C ₁₈ H ₃₀ O ₂	3E,9Z,12Z-octadecatrienoic acid	-
1	92913.73	11086	23.2	180.8944	179.8872	-	-	-
							Ketoprofen	22071-15-4
							Chalepensin	13164-03-9
1.6	72932.42	11105	8.9	277.0858	275.0816	C ₁₆ H ₁₄ O ₃	4'-Hydroxy-2'-methoxychalcone	-
							Dalbergichromene	-

							4-METHOXYDALBERGIONE	4646-86-0
						C ₁₅ H ₁₃ FO ₄	3',4'-dihydroxyflurbiprofen	66067-41-2
						C ₁₂ H ₁₈ Cl ₂ N ₂ O	Clenbuterol	37148-27-9
10.5	84180.12	11130	28.4	597.2732	598.2805	C ₃₂ H ₃₈ N ₄ O ₆	Phe Phe Val Tyr	-
19	80749.23	11144	23.7	215.627	429.2394	-	-	-
							4-(Ethoxymethyl)-2-methoxyphenol	13184-86-6
							Amyl 2-furoate	4996-48-9
							3,4,5-Trimethoxytoluene	6443-69-2
						C ₁₀ H ₁₄ O ₃		
7.6	93163.69	11164	8.5	183.1	182.0928		MEPHENESIN	59-47-2
							Iridotrial	-
							5-oxo-7-decynoic acid	-
						C ₆ H ₁₀ N ₆ O	Dacarbazine	4342-03-4
1.5	83006.12	11174	13.5	182.0811	183.0883	C ₉ H ₁₁ NO ₃	DL-o-Tyrosine	2370-61-8

0.8	1930128	11239	249.8	559.3398	560.347	C ₂₇ H ₄₂ N ₈ O ₅	Phe His Lys Lys	-
							Toxyl angelate	106928-36-3
						C ₁₈ H ₂₀ O ₄		
23.9	70586.39	11261	18.3	323.124	322.1167		TMS	24144-92-1
						C ₁₅ H ₁₈ N ₂ O ₆	Binapacryl	485-31-4
8.1	90820.04	11269	9.2	192.0767	191.0694	C ₁₂ H ₁₁ N	4-Biphenylamine	92-67-1
0.9	139730.7	11313	23.2	731.7122	730.705	-	-	-
0.9	58218.59	11365	17.4	532.7461	531.7388	-	-	-
0.9	134622.1	11401	36.3	698.6411	1399.297	C ₄₄ H ₈₅ NO ₃	Ceramide (d18:1-26:1(17Z))	-
						C ₁₇ H ₁₆ N ₄ O	SB 206553	-
						C ₁₂ H ₁₆ N ₆ O ₃	His His	-
18.8	77731.05	11430	15.8	315.1199	314.1126		2'-Hydroxy-4,4',6'-trimethoxychalcone	3420-72-2
						C ₁₈ H ₁₈ O ₅		
							DEOXSAPPANONE B 7,3'-DIMETHYL ETHER	-
						C ₁₄ H ₁₄ N ₆ O ₃	Dihydropteroic acid	2134-76-1

0.9	120404.2	11434	11.6	432.7863	1295.331	-	-	-
18	70141.41	11448	10.5	337.2346	336.2273	C ₂₀ H ₃₂ O ₄	8,12-iso-iPF2 α -VI 1,5- lactone	-
							15-epi-PGA1	20897-92-1
0.4	381083.3	11499	6.6	97.9689	95.9539	-	-	-
24.5	1047663	11542	7.6	172.9812	171.9739	-	-	-
0.9	48732.41	11640	24.1	554.7979	552.7653	-	-	-
1.9	290301.1	11695	9.8	107.0704	106.0631	C ₄ H ₁₀ O ₃	Diethylene glycol	111-46-6
22.5	175579.2	11719	4.2	283.264	282.2567	C ₁₈ H ₃₄ O ₂	Palmitoleic Acid ethyl ester	56219-10-4
							2Z-octadecenoic acid	-
17.7	91361.89	11738	14	387.193	386.1865	C ₂₄ H ₂₈ O ₃	3-(1,1-Dimethyl-2-propenyl)-8-(3-methyl-2-butenyl)xanthyletin	30310-55-5
22.4	69537.35	11745	12.2	228.2321	227.2249	C ₁₄ H ₂₉ NO	Halaminol A	-
0.6	249957.6	11834	6.1	106.9921	105.9849	-	-	-
0.8	257067.3	11856	131.7	310.4311	308.4079	-	-	-

							(E)-Urocanic acid	3465-72-3
1.8	55447.92	11874	5.8	139.0503	138.043	C ₆ H ₆ N ₂ O ₂	methyl 2-Pyrimidine Carboxylate	34253-03-7
							2-Pyrimidine Acetic Acid	66621-73-6
0.9	34523.38	11897	8.7	458.7423	457.7351	-	-	-
21.8	81169.95	11938	26.8	307.1381	612.2616	C ₁₄ H ₁₈ N ₄ O ₄	Trimethoprim 1-N-oxide	27653-68-5
11.7	93854.6	11952	10.3	229.1409	230.1482	-	-	-
							Norecasantalic acid	59300-52-6
							(+)-Myrtenyl formate	72928-52-0
15.4	75302.44	11953	12.5	181.1224	180.1151	C ₁₁ H ₁₆ O ₂	Dihydroactinidiolide	15356-74-8
							2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]nona-3,8-diene	15129-55-2
0.8	12530.89	11975	239.5	310.8523	309.845	C ₆ H ₆ Cl ₆	Lindane	58-89-9
0.5	284576.5	12011	3.9	128.9509	127.9437	C ₂ H ₂ Cl ₂ O ₂	Dichloroacetate	79-43-6
14.2	77657.91	12013	23.5	163.0391	162.0318	C ₉ H ₆ O ₃	3-HYDROXYCOUMARIN	939-19-5

7.1	75618.8	12016	11.6	187.0944	188.1017	C ₅ H ₁₀ N ₆ O ₂	Dinitrosopentamethylenetetramine	101-25-7
19	213191.5	12039	18.7	685.4178	686.425	-	-	-
0.9	25813.63	12049	267.8	708.6967	707.6868	-	-	-
0.9	57747.57	12111	269.1	448.7832	445.7589	-	-	-
0.9	121491.6	12114	21.1	646.7274	1291.44	-	-	-
0.9	90156.55	12166	27.6	516.7721	517.7794	-	-	-
14	71565.95	12169	17.2	329.0993	328.0935	C ₁₈ H ₁₆ O ₆	7-Hydroxy-2',4',5'-trimethoxyisoflavone	-
							ISOTECTORIGENIN, 7-METHYL ETHER	-
14	66029.06	12172	17.1	575.2299	574.2226	C ₂₇ H ₃₄ N ₄ O ₁₀	Glu Thr Tyr Tyr	-
10.3	169771	12184	30.9	583.2936	584.3008	C ₂₈ H ₃₈ N ₈ O ₆	Phe Phe Asn Arg	-
0.8	198453.4	12196	271	522.3626	521.3554	-	-	-
18.3	531461.5	12237	16.5	442.283	441.2758	C ₂₅ H ₃₃ D ₄ NO ₄	17-phenyl trinor Prostaglandin F2 α ethyl amide-d4	-
0.8	157625.5	12282	136.5	866.7439	2592.172	-	-	-

0.9	38883.85	12389	137.7	566.8868	565.8795	-	-	-
0.9	56126.06	12427	17.1	498.7801	497.769	-	-	-
3.5	87703.77	12441	16	187.0578	186.0506	C ₇ H ₁₆ S ₂	Butyl isopropyl disulfide	72437-53-7
						C ₆ H ₁₂ O ₅	Alpha-D-Fucose	3615-37-0
0.9	51657.3	12470	32.7	764.8235	763.8162	-	-	-
0.9	79923.22	12471	16.5	752.6379	751.6306	-	-	-
23.9	386929.3	12488	14	526.4305	525.4232	C ₃₄ H ₅₅ NO ₃	ICI 164384	98007-99-9
							4-[4-(3,4-Dimethoxyphenyl)-2,3-dimethylbutyl]-2-methoxyphenol	-
24.5	285735.4	12618	15	367.1885	366.1812	C ₂₁ H ₂₈ O ₄	Bisphenol A bis(2-hydroxypropyl) ether	116-37-0
							21-Deoxycortisone	-
						C ₁₈ H ₂₆ N ₂ O ₆	Bufotenine O-glucoside	64656-15-1
0.9	122602.1	12773	33.4	860.7419	858.7134	C ₅₀ H ₁₀₂ NO ₇ P	PC(O-16:0-26:0)[U]	-
19.1	96204.25	12785	16.3	223.0635	222.0563	C ₁₃ H ₁₃ P	Diphenylmethylphosphine	1486-28-8

						C ₉ H ₁₈ S ₃	1-(1-Propenylthio)propyl propyl disulfide	143193-11-7
10.1	73406.01	12816	22.4	504.2652	503.2579	C ₂₈ H ₃₃ N ₅ O ₄	Trp Trp Leu	-
0.8	127570.9	12919	23.8	186.9225	185.9152	-	-	-
							Anthranilic acid	118-92-3
1.7	73212.15	12957	12.3	138.055	137.0478	C ₇ H ₇ NO ₂	3-Nitrotoluene	99-08-1
							Salicylamide	-
1.2	154699.9	12977	14.2	177.9484	176.9411	-	-	-
0.9	113075.7	12984	15.2	616.7165	617.7237	-	-	-
						C ₁₂ H ₁₈ O ₁₁	L-Ascorbic acid-2-glucoside	129499-78-1
9.9	76930.27	13039	20.5	339.0926	338.0853	C ₁₉ H ₁₅ ClN ₂ O ₂	Inabenfide	82211-24-3
0.9	161843.7	13048	14.6	530.7523	527.7795	-	-	-
1.2	137448.7	13061	13.6	142.9387	141.9314	-	-	-
10.9	177881.1	13080	17	373.2135	744.4126	C ₂₁ H ₃₁ FO ₃	5alpha-Androstane-2beta-fluoro-17beta-ol-3-one acetate	-

						C ₁₉ H ₃₀ N ₂ O ₄	Perindopril lactam	129970-98-5
							Succinylacetone	51568-18-4
6.2	84779.7	13135	17.5	181.0472	180.0399	C ₇ H ₁₀ O ₄	2-Isopropylmaleate	44976-69-4
							Laurencione monoacetate	-
0.9	26668.88	13143	25	172.0945	171.0872	C ₆ H ₁₅ NO ₃	Trolamine	102-71-6
0.7	179236.7	13145	15.3	442.8792	441.8719	-	-	-
10.3	100481	13186	55.2	553.2469	554.2541	C ₂₄ H ₃₆ N ₆ O ₇ S	Phe Met Gln Gln	-
0.9	134963.7	13251	11.3	747.6837	746.6764	-	-	-
							3,5-Dihydroxy-1,4-naphthoquinone	-
9.2	70716.72	13255	14.4	191.0342	190.0269	C ₁₀ H ₆ O ₄	8H-1,3-Dioxolo[4,5-h][1]benzopyran-8-one	4361-93-7
							Coumarin-4-carboxylic acid	27393-46-0
6.8	94895.35	13282	6	245.0632	244.056	C ₁₀ H ₁₂ O ₇	1-O-Galloylglycerol	87087-60-3
1.7	74842.79	13287	11.6	118.0553	234.0987	-	-	-

0.9	42651.65	13297	25	434.8541	433.8469	-	-	-
1.8	67717.75	13301	12.6	121.0395	120.0322	-	-	-
8.7	60423.35	13347	34.8	328.1606	327.1533	C ₁₃ H ₂₁ N ₅ O ₅	Ala Thr His	-
0.9	231002.8	13385	19.4	594.7161	595.7234	-	-	-
0.9	62542.83	13456	30.2	578.6939	577.6866	-	-	-
							1,6-Dihydroxycyclohexa-2,4-diene-1-carboxylate	60463-06-1
14	73211.68	13460	33.3	157.0495	154.0219	C ₇ H ₈ O ₄	3-Methylmuconolactone	-
							IRETOL	487-71-8
9.9	70327.36	13500	10.4	490.2863	489.279	C ₂₁ H ₃₉ N ₅ O ₈	Glu Ile Lys Thr	-
						C ₁₂ H ₂₄ N ₆ O ₄ S	Ala Arg Cys	-
1.6	53453.27	13522	7.4	349.1646	347.1606	C ₁₉ H ₂₄ O ₆	Gibberellin A63	63351-80-4
17.4	223425.6	13589	29.7	346.3311	345.3238	-	-	-
10.7	93481.66	13650	151.7	351.2004	700.3862	C ₁₇ H ₂₆ N ₄ O ₄	Gly Phe Lys	-

						C ₁₆ H ₃₀ O ₈	trans-p-Menthane-1,7,8-triol 8-glucoside	217962-29-3
23	3796242	13650	6.7	133.9739	132.9666	C ₃ H ₃ NOS ₂	Rhodanine	141-84-4
1.2	161240.6	13695	18.9	213.9693	425.9247	C ₆ H ₆ ClNO ₂ S	p-Chlorobenzenesulfonylamide	98-64-6
21.9	157477	13704	14.3	297.242	296.2352	C ₁₈ H ₃₂ O ₃	(±)13-HODE	73804-64-5
1.1	44494.5	13790	3.8	125.9864	124.9792	-	-	-
0.9	25632.28	13835	14.8	378.8997	377.8924	-	-	-
0.9	135672.2	13907	23.9	611.7632	610.7559	-	-	-
1.2	113371.2	14083	15.8	174.8865	173.8792	-	-	-
9.6	76898.19	14084	24.5	446.26	445.2527	C ₁₉ H ₃₅ N ₅ O ₇	Ala Asp Ile Lys	-
							Phenylpropionic acid	637-44-5
							Coumarin	91-64-5
10.5	72701.89	14103	22	147.0442	146.037	C ₉ H ₆ O ₂	2-Benzofurancarboxaldehyde	4265-16-1
							Chromone	491-38-3

0.9	93651.39	14117	15.9	174.8864	173.8791	-	-	-
1.6	79004.99	14173	17.9	143.0322	568.1022	C ₄ H ₈ O ₄	D-Threose	95-43-2
							4-deoxy-erythronic acid	-
10.7	127969.3	14199	38.2	701.393	702.4003	-	-	-
20.2	140465.5	14217	16.3	269.2105	268.2035	C ₁₆ H ₂₈ O ₃	Methoprene acid	53092-52-7
0.8	3497046	14222	8.3	1000.681	2003.376	-	-	-
23.5	4219037	14263	21.9	154.9667	152.9516	C ₂ ClF ₅	Chloropentafluoroethane	76-15-3
0.8	142894.6	14286	12.2	132.9025	129.899	-	-	-
9.9	122663.9	14320	35.5	495.2413	496.2486	C ₂₃ H ₃₄ N ₄ O ₈	Ala Glu Ile Tyr	-
0.9	33211.09	14322	318.3	656.7424	655.7351	-	-	-
0.8	148433.4	14334	20.4	366.8782	365.871	-	-	-
4.3	105641.6	14364	13.8	99.0442	98.0369	C ₅ H ₆ O ₂	5-Methyl-2(3H)-furanone	591-12-8
							2-Furanmethanol	98-00-0

							β-vinyl acrylic acid	-
0.7	121009.1	14377	9.7	194.9996	193.9923	-	-	-
0.9	46877.87	14412	11.9	356.8488	355.8415	-	-	-
19	77768.03	14435	25	332.2789	331.2716	-	-	-
1.5	327262.7	14486	6.6	159.9689	158.9616	-	-	-
9	67835.56	14546	24.5	358.2074	357.2002	C ₁₅ H ₂₇ N ₅ O ₅	Gly Gly Pro Lys	-
0.8	736117.8	14578	162	432.3987	433.406	-	-	-
0.8	69421.01	14601	3.3	284.9376	283.9303	-	-	-
							2-Methyl-3'-hydroxyphenylpropionic acid	46207-82-3
							1-(2,4-Dihydroxyphenyl)-1-butanone	4390-92-5
8.3	170963.7	14601	13.4	181.0847	180.0775	C ₁₀ H ₁₂ O ₃	4-Ethoxy-3-methoxybenzaldehyde	120-25-2
							Isopeopyl Paraben	4191-73-5
							Coniferyl alcohol	458-35-5

							5(S),12(S)-DiHETE	73151-67-4
18.1	91724.92	14643	13.4	337.2349	336.2276	C ₂₀ H ₃₂ O ₄	8S,15S-DiHETE(Z,E,E,E)	80234-66-8
							11-deoxy-PGE2	35535-53-9
9.6	69526.36	14736	15.4	135.0442	134.0369	C ₈ H ₆ O ₂	6E-Octene-2,4-dienoic acid	-
0.8	134975	14776	19.8	464.8719	463.8646	-	-	-
0.8	6338282	14788	328.6	507.1966	508.2039	C ₁₉ H ₃₀ N ₄ O ₁₂	Glu Glu Glu Thr	-
0.9	54248.55	14805	29.7	452.8437	451.8374	-	-	-
0.8	151563.9	14813	20.9	460.8571	459.8498	-	-	-
11.9	439551.5	14862	7	185.1149	184.1076	C ₈ H ₁₈ O ₃	(3R,7R)-1,3,7-Octanetriol	217650-11-8
10.1	136822.2	14880	35	539.2673	540.2746	C ₂₄ H ₃₈ N ₆ O ₆ S	Phe Lys Met Asn	-
22.5	3154420	14950	10	160.9491	159.9418	-	-	-
0.9	103166.4	14957	22.2	287.9368	285.9449	-	-	-
23.1	6147481	14967	8	126.9666	123.9569	-	-	-

							Dehydrozingerone	1080-12-2
9.3	126998.4	14970	18	193.084	192.0767	C ₁₁ H ₁₂ O ₃	Carpacin	23953-63-1
							ETHYL-p-COUMARATE	2979-06-8
							2-Hydroxy-3,4,6-trimethoxydihydrochalcone	-
17	81492.38	14983	12.7	317.1359	316.1286	C ₁₈ H ₂₀ O ₅	Combrestatin A4	117048-59-6
9.1	130353.6	14988	48.9	372.1864	371.1791	C ₁₅ H ₂₅ N ₅ O ₆	Ala Ala Asn Pro	-
							2-Napthyloxyacetic acid	120-23-0
13.2	72893	14992	23.9	225.0544	224.0472	C ₁₂ H ₁₀ O ₃	2,2',3-Trihydroxybiphenyl	91368-55-7
						C ₁₄ H ₈ O ₃	Hydroxyanthraquinone	129-43-1
1.6	104931.4	15037	37.6	100.9911	99.9838	-	-	-
0.8	6086042	15079	167.5	544.5124	545.5197	C ₃₆ H ₆₅ NO ₂	1-[1,4-Dihydro-4-nonyl-5-(1-oxodecyl)-3-pyridinyl]-1-dodecanone	158528-01-9
0.9	62695.45	15178	31.1	758.6497	1512.325	C ₄₄ H ₈₈ NO ₆ P	PC(O-18:1(9E)-O-18:1(9E))[U]	-
18.4	143307.1	15208	13.3	251.1277	250.1208	C ₁₂ H ₂₀ O ₄	Traumatic acid	-

							Diisopropyl phthalate	605-45-8
						C ₁₄ H ₁₈ O ₄	Ubiquinone-1	727-81-1
							δ-CEHC	1221504-67-1
0.6	567338.6	15224	4.9	113.9638	112.9565	-	-	-
0.9	117863.1	15247	9.1	632.6916	1263.369	-	-	-
0.8	228391.1	15278	5.8	334.9145	335.9218	-	-	-
21.7	193445.1	15280	39.4	276.0528	275.0455	C ₁₂ H ₁₅ Cl ₂ NO ₂	Phenylacetic mustard	10477-72-2
0.8	155361	15315	170.2	114.9876	113.9803	-	-	-
0.6	283455.8	15497	3.6	98.5122	195.0104	-	-	-
24	142814.5	15529	18.2	482.4038	481.3965	-	-	-
1.4	300680.6	15563	4.5	84.9597	83.9524	-	-	-
15.3	72620.8	15584	9.8	149.0232	148.0159	-	-	-
9.3	76970.09	15593	33.2	402.2339	401.2266	C ₁₇ H ₃₁ N ₅ O ₆	Ala Ala Ile Gln	-

0.9	154542.4	16202	23.6	514.7792	512.7961	-	-	-
2	4395619	16256	7.4	159.9689	158.9616	-	-	-
2	4398478	16256	7.4	159.9689	158.9616	-	-	-
							cis-3-Hexenyl pyruvate	68133-76-6
8.7	158547.9	16312	19.6	193.0836	192.0763	C ₉ H ₁₄ O ₃	1,4-Ipomeadiol	53011-73-7
							Furfural diethyl acetal	13529-27-6
9.6	185047.9	16344	44.7	451.2154	431.6816	C ₂₁ H ₃₀ N ₄ O ₇	Ala Asp Phe Val	-
						C ₂₇ H ₃₀ O ₆	sofalcone	64506-49-6
9.8	176282.7	16352	27.5	460.239	459.2317	C ₁₉ H ₃₃ N ₅ O ₈	Ala Glu Ile Gln	-
0.8	231507.2	16437	365.3	291.9652	289.9624	-	-	-
1.7	241769.2	16490	18.1	163.1232	162.116	C ₁₀ H ₁₄ N ₂	Anabesine	494-52-0
0.9	127710.6	16505	33.9	368.9061	365.9021	-	-	-
0.8	61605.28	16543	183.8	170.9575	169.9502	-	-	-

0.9	42703	16565	368.1	430.792	429.7847	C ₁₂ H ₃ Cl ₇ O	4-Hydroxy-2,2',3,4',5,5',6-heptachlorobiphenyl	158076-68-7
10	163072.2	16580	33.2	509.2205	510.2278	C ₁₉ H ₃₆ N ₆ O ₆ S ₂	Cys Lys Met Gln	-
23	10849284	16713	10.5	138.9796	137.9723	-	-	-
0.9	112363.7	16791	12.2	236.9851	235.9788	C ₆ H ₁₁ Cl ₃ O ₃	1,2,3-Tris(chloromethoxy)propane	38571-73-2
1.2	150867.7	16793	23.8	158.9125	157.9052	-	-	-
							3E-Hexen-1-ol	-
11.2	175697.3	16801	35.3	101.0962	100.0889	C ₆ H ₁₂ O	4-Methylpentanal	-
							Caproaldehyde	-
0.9	86323.02	16821	42.5	458.7995	457.7922	-	-	-
22.9	6847901	16882	12.2	178.9594	179.9667	-	-	-
1.6	390994.6	17003	5	158.003	156.9957	C ₇ H ₅ NS	Benzothiazole	95-16-9
						C ₆ H ₁₀ O ₃ S	1-(Methylsulfanyl)-1-oxopropan-2-yl acetate	74586-09-7
0.8	171853.6	17083	4.6	185.0233	184.0166	C ₃ H ₁₀ Cl ₂ N ₂ O	N,N'-bis(2-chloroethyl)- Urea (Carmustine Metabolite)	2214-72-4

						C ₁₂ H ₂₀ O ₄	Traumatic acid	-
							Diisopropyl phthalate	605-45-8
9.3	90246.17	17114	14.3	251.1258	250.1186	C ₁₄ H ₁₈ O ₄	Ubiquinone-1	727-81-1
							δ-CEHC	1221504-67-1
15.8	157824.6	17118	26.9	272.2585	271.2512	C ₁₆ H ₃₃ NO ₂	2S-aminohexadecanoic acid	-
0.8	224606.2	17243	47.6	403.9117	402.9044	-	-	-
1.6	98167.6	17268	20.1	124.0968	123.0895	-	-	-
0.9	52330.86	17270	24	318.8453	317.8381	-	-	-
10.7	146450	17380	44.8	696.4377	695.4313	C ₃₇ H ₆₁ NO ₁₁	Mycinamicin IV	73684-71-6
9.5	93701.89	17471	51.4	416.2128	415.2055	C ₁₇ H ₂₉ N ₅ O ₇	Ala Pro Gln Thr	-
						C ₁₀ H ₁₈ O ₄	Sebacic acid	111-20-6
8.3	450399.8	17539	18.1	225.1101	224.1028		3',4',5'-Trimethoxycinnamyl alcohol	30273-62-2
						C ₁₂ H ₁₆ O ₄	Vanillin 1,2-butylene glycol acetal	63253-24-7

							Dhelwangin	23800-56-8
							Aspidinol	519-40-4
9.3	116883.3	17568	20.9	407.1892	408.1965	C ₁₉ H ₂₆ N ₄ O ₆	Gly Ala Tyr Pro	-
19.8	90365.91	17584	26.2	167.0339	166.0266	C ₈ H ₆ O ₄	Phthalate	88-99-3
0.9	53661.76	17613	391.4	578.7454	577.7381	-	-	-
0.7	84570.65	17655	196.2	176.9886	175.9814	-	-	-
							3-Keto-beta-D-galactose	-
13.2	128696	17701	29.2	201.0368	200.0299	C ₆ H ₁₀ O ₆	2-Deoxy-5-keto-D-gluconic acid	-
							L-Galactono-1,4-lactone	1668-08-2
0.8	2625380	17737	31.2	932.6962	1867.407	-	-	-
23.3	111448	17801	9.3	328.284	327.2767	C ₁₉ H ₃₇ NO ₃	N-palmitoyl alanine	-
							Ethyl 2,4-dioxohexanoate	13246-52-1
8.1	101673.4	17806	20.6	195.0631	194.0558	C ₈ H ₁₂ O ₄	3-Isopropenylpentanedioic acid	6839-75-4

						C ₆ H ₆ N ₆ O ₂	Temozolomide	85622-93-1
0.8	155674.8	17816	12.6	277.9474	276.9401	-	-	-
10.8	78906.89	17991	3.6	157.1337	156.1264	-	-	-
24	569253.8	18126	21.9	487.3592	486.3519	C ₂₃ H ₄₆ N ₆ O ₅	Ile Lys Lys Val	-
19	510319.4	18190	22.7	371.2101	740.4055	C ₁₉ H ₃₀ O ₇	5-Megastigmen-7-yne-3,9-diol 3-glucoside	62512-27-0
1.6	108190.4	18200	28.2	314.0761	313.0688	C ₁₈ H ₁₃ NO ₃	Naptalam	132-66-1
							exo-2-Methyl-3-methylenebicyclo[2.2.1]heptan-2-ol	59300-40-2
14.1	121895.2	18272	12.7	139.1118	138.1045	C ₉ H ₁₄ O	(2E,6Z)-nona-2,6-dienal	-
							2,6-nonadienal	-
9.8	96737.3	18303	34.6	465.1948	464.1875	C ₂₁ H ₂₈ N ₄ O ₈	Asp Ala Pro Tyr	-
12.4	131736.6	18305	64.4	172.0159	171.0086	-	-	-
23.4	180570	18305	17.7	429.3177	430.325	C ₂₄ H ₄₄ O ₆	Sorbitan oleate	1338-43-8
21.7	117803.8	18485	28	383.204	382.1967	C ₁₆ H ₂₆ N ₆ O ₅	Ala Gly His Val	-

1.6	75243.85	18582	25.9	265.0594	263.0423	C ₁₃ H ₁₀ N ₂ O ₃	2-Amino-5-nitrobenzophenone	1775-95-7
23.5	176437.8	18651	17.5	341.2659	342.2732	C ₂₀ H ₃₆ O ₄	15(S)-HpEDE	145375-41-3
0.8	396872.4	18766	45.1	419.8767	418.8694	-	-	-
23.1	231959.1	18783	9.8	328.2842	327.2773	C ₁₉ H ₃₇ NO ₃	N-palmitoyl alanine	-
21.8	142265.4	18839	25.8	197.5808	393.147	-	-	-
20.5	141556.3	18942	16.1	249.1846	248.1773	C ₁₄ H ₂₆ O ₂	Rhodinyl butyrate	141-15-1
						C ₁₆ H ₂₄ O ₂	4,7,10,13-hexadecatetraenoic acid	-
1.1	139695.5	18951	5.5	84.9597	83.9524	-	-	-
21.8	178721.2	18985	43	398.1121	397.1048	C ₁₅ H ₁₉ N ₅ O ₆ S	S-Adenosyl-4-methylthio-2-oxobutanoate	22365-11-3
0.9	69945.87	18988	55.5	442.8286	441.8213	-	-	-
0.9	399205.7	18991	28.6	676.6562	677.6635	C ₄₄ H ₈₅ NO ₃	Ceramide (d18:1-26:1(17Z))	-
16.4	107929.3	19039	24.3	279.2321	278.2249	C ₁₈ H ₃₀ O ₂	3E,9Z,12Z-octadecatrienoic acid	-
1.6	133222.4	19139	21.2	134.0305	264.0523	-	-	-

2.4	13405873	19169	5.6	158.003	156.9957	C ₇ H ₅ NS	Benzothiazole	95-16-9
15.1	196634.8	19178	69.4	370.6725	739.3304	-	-	-
21.7	166313.6	19320	22.7	437.209	872.4035	C ₁₇ H ₃₂ N ₄ O ₇ S	Cys Ile Thr Thr	-
7.3	168464	19426	32.8	193.0134	192.0061	C ₈ H ₁₀ S ₂	Benzyl methyl disulfide	699-10-5
0.9	138231.6	19508	8.6	410.8036	409.7971	-	-	-
9.5	187382.3	19862	37.1	421.1683	400.6219	C ₁₉ H ₂₄ N ₄ O ₇	Ser Trp Glu	-
						C ₂₅ H ₂₄ O ₆	Pomiferin	572-03-2
							2',6'-Dihydroxy-3,4,4'-trimethoxydihydrochalcone	-
13	144381.3	19868	20.8	333.1305	334.1378	C ₁₈ H ₂₀ O ₆	Catechin 5,7,3'-trimethyl ether	-
							BYSSOCHLAMIC ACID	743-51-1
							DUARTIN (-)	52305-04-1
0.8	215559.8	19872	5.7	440.8842	439.877	C ₁₆ H ₈ Br ₂ N ₂ O ₂	6,6'-Dibromoindigotin	19201-53-7
0.9	162840.5	19895	14.8	491.8138	490.8065	-	-	-

21.8	112682.6	19914	16.9	248.2006	247.1934	C ₁₆ H ₂₅ NO	1-(5-Methyl-3-pyridinyl)-1-decanone	194345-50-1
0.9	144014.9	20026	43.2	269.9262	267.9345	-	-	-
0.8	352433.2	20066	32.6	409.8547	817.6949	-	-	-
0.9	44378.2	20122	31.4	390.8137	388.8275	-	-	-
1	113693.5	20179	10.4	160.987	159.9797	-	-	-
1.1	127910.6	20179	10.4	160.987	158.9614	-	-	-
0.9	123423.8	20213	22.5	154.9322	153.925	-	-	-
13.8	156846.7	20678	35	290.2689	289.2617	-	-	-
16.4	255858.9	20717	9.4	333.2636	332.2567	C ₁₈ H ₃₆ O ₅	9,10,13-Trihydroxystearic acid	50439-74-2
						C ₁₃ H ₁₈ O ₄	1,2,3,4-Tetramethoxy-5-(2-propenyl)benzene	15361-99-6
							Wyerol	20450-52-6
1.6	100302.4	20847	40.9	261.1119	260.1047	C ₁₅ H ₁₆ O ₄	Cyperine	33716-82-4
							PEUCENIN	578-72-3

0.9	160191	20850	38.3	377.8807	378.888	-	-	-
0.9	84684.66	21038	80.3	572.7866	571.7794	-	-	-
0.9	95703.72	21053	15.1	496.77	495.7627	-	-	-
1.6	136044.8	21103	13.7	179.0003	177.993	C ₆ H ₁₀ S ₃	Diallyl Trisulfide	2050-87-5
23	5082770	21360	11.5	140.9514	139.9441	CH ₃ AsO ₃	Methylarsonate	124-58-3
10.7	168983.3	21400	27.1	271.0792	270.0719	-	-	-
0.9	139642	21454	25.1	654.6731	653.6658	-	-	-
0.9	137397.7	21481	48.9	442.7707	441.7671	-	-	-
21.8	148846.7	21590	55.4	658.253	657.2457	C ₃₂ H ₃₇ N ₅ O ₉	Gln Tyr Tyr Tyr	-
14.4	111151.3	21593	47	226.1804	225.1731	-	-	-
0.9	75321.24	21634	4.1	416.8115	415.8055	-	-	-
0.9	119503.1	21663	5.5	137.9827	684.8767	-	-	-
21.7	191276.4	22018	45.4	320.0804	319.0731	C ₁₁ H ₁₅ N ₅ O ₃ S	5'-Deoxy-5'-(methylthio)adenosine	2457-80-9

1.7	812958.1	22195	19.6	209.0333	210.0406	C ₁₀ H ₆ N ₂ O ₂	Pyrocoll	484-73-1
23.5	7243772	22244	8.3	90.507	178.9995	-	-	-
0.9	253967.5	22287	18.2	556.7101	557.7174	-	-	-
1.6	68755.45	22437	249.3	213.1333	212.126	-	-	-
20.2	131397.3	22622	23.5	251.2003	250.193	C ₁₄ H ₂₈ O ₂	3-Methylbutyl nonanoate	7779-70-6
						C ₁₆ H ₂₆ O ₂	4,7,10-hexadecatrienoic acid	-
9	148409.9	22854	43	363.163	364.1703	C ₁₇ H ₂₂ N ₄ O ₅	Ser Trp Ala	-
7.7	112398.9	22875	19.2	199.058	198.0507	C ₇ H ₁₂ O ₅	(±)-Glycerol 1,2-diacetate	101364-64-1
							3-propylmalic acid	-
15.8	186998.4	22893	29.2	223.0641	222.0568	C ₉ H ₁₈ S ₃	(E)-1-Propenyl 1-(propylthio)propyl disulfide	137363-95-2
0.8	954417.9	23012	255.7	375.4101	752.8348	-	-	-
14.7	298987.4	23088	47.9	411.1624	412.1696	C ₁₄ H ₂₄ N ₆ O ₇	Ala Ala Asn Asn	-
9.1	271643.8	23230	18.8	215.1256	214.1183	-	-	-

						C ₂₂ H ₃₂ O ₆	Dihydrofukinolide	41059-95-4
18	255970.8	23301	33.2	415.2109	414.2045	C ₁₇ H ₃₀ N ₆ O ₄ S	His Lys Met	-
						C ₂₄ H ₃₀ O ₆	Eplerenone	107724-20-9
23.5	656447.1	23324	27.2	385.2918	386.2991	C ₂₁ H ₄₀ N ₂ O ₂ S	Kalkitoxin thioamide alcohol	-
8.4	109453.8	23461	51.2	300.2016	299.1943	-	-	-
						C ₆ H ₈ N ₄	Tetrahydropteridine	-
11.5	135367.7	23491	20.1	159.0653	158.0581		2-Isopropylmaleate	44976-69-4
						C ₇ H ₁₀ O ₄	Laurencione monoacetate	-
							3-Carboxy-2,4,4-trimethyl-2-cyclohexenone	51823-74-6
							3,4,5-Trimethoxytoluene	6443-69-2
8.7	143347.5	23928	18.2	183.1017	182.0945	C ₁₀ H ₁₄ O ₃	2-Oxo-delta3-4,5,5-trimethylcyclopentenylacetate	1130-49-0
							MEPHENESIN	59-47-2
15.5	220102.8	23974	47.5	230.2479	229.2406	C ₁₄ H ₃₁ NO	Xestoaminol C	-

0.9	146008.6	24036	25	389.875	388.8677	-	-	-
15.4	110598	24047	15.2	149.0234	148.0161	-	-	-
0.9	108386.8	24257	24.9	534.728	533.7215	-	-	-
14.1	196096.1	24726	21.3	213.1098	212.1026	-	-	-
0.9	95827.07	24784	51.7	424.836	423.8287	-	-	-
24.1	206802.3	24995	24	443.3334	442.3261	C ₃₂ H ₄₂ O	(all-E)-6'-Apo-y-caroten-6'-al	22255-36-3
19	414417.1	25108	17.5	195.1142	192.0887	C ₁₃ H ₁₆	1,2-Dihydro-1,1,6-trimethylnaphthalene	30364-38-6
						C ₁₀ H ₁₄ N ₂ O ₂	Laccarin	175669-28-0
0.9	199037.8	25165	24.4	504.7985	501.7766	-	-	-
0.8	892675.6	25200	98.2	679.7948	2712.193	-	-	-
0.7	289011	25313	31.7	241.9995	240.9922	C ₈ H ₁₀ ClNO ₂ S	4-AMINO-3- (5-CHLOROTHIEN-2-YL)BUTANOIC ACID	-
24.3	382881.3	25382	30.9	345.2565	344.2497	C ₂₁ H ₃₂ N ₂ O ₂	4β-Hydroxystanozolol	125636-92-2
21.9	189583.8	25574	32.6	279.2319	278.2246	C ₁₈ H ₃₀ O ₂	10E,12E,14E-Hexadecatrienyl acetate	-

							3E,9Z,12Z-octadecatrienoic acid	-
0.9	147613.8	25691	25.7	136.922	135.9147	-	-	-
0.8	309544.4	25779	5.7	457.3834	456.3761	-	-	-
0.9	77572.52	26036	33.1	374.8458	373.8386	C ₁₂ H ₄ Cl ₆ O	2,2',3,3',6,6'-Hexachloro-4-biphenylol	74443-60-0
10.6	209509.6	26383	68.5	657.3665	636.5992	C ₃₅ H ₅₄ O ₁₀	Digitoxigenin bisdigitoxoside	16479-50-8
20.5	184389.8	26420	24.6	441.224	440.2167	C ₁₇ H ₂₈ N ₈ O ₆	Glu His Arg	-
							1α,25-dihydroxy-2β-(3-hydroxypropoxy)vitamin D3 - 1α,25-	-
						C ₃₀ H ₅₀ O ₅	dihydroxy-2β-(3-hydroxypropoxy)cholecalciferol	
0.8	1456044	26439	587.5	513.3571	514.3643		Alisol A	19885-10-0
							Acetoxolone	6277-14-1
						C ₃₂ H ₄₈ O ₅	Acetyl-11-keto-B-Boswellic Acid, 3-	67416-61-9
						C ₁₄ H ₂₆ O ₁₀	Isopropyl apiosylglucoside	147742-24-3
9.1	153214.1	26444	54.7	377.142	378.1493	C ₁₇ H ₂₀ N ₄ O ₆	His-Val-OH	-

							(Z)-3-(2,4,5-Trimethoxyphenyl)-2-propenal	99217-07-9
							Monoisobutyl phthalic acid	30833-53-5
8.7	169710.1	26469	15.5	223.0943	222.0871	C ₁₂ H ₁₄ O ₄		
							APIOLE	523-80-8
							Valeroyl Salicylate	64206-54-8
0.4	205322.6	26621	3.1	158.003	156.9957	C ₇ H ₅ NS	Benzothiazole	95-16-9
						C ₇ H ₇ NO ₂	Anthranilic acid	118-92-3
1.5	134153.9	26678	25.4	138.055	139.0623			
						C ₇ H ₇ NO ₂	3-Nitrotoluene	99—08-1
						C ₁₅ H ₁₈ N ₄	Ferimzone	89269-64-7
17.2	164694.5	26824	20.7	277.1433	276.1361	C ₁₄ H ₂₂ O ₄	C75	191282-48-1
						C ₁₆ H ₂₀ O ₄	Scorpioidin	76045-40-4
8.7	203733.6	26914	39.8	333.116	334.1232	C ₁₄ H ₂₀ O ₉	Leonuriside A	121748-12-7
0.9	62900.45	26936	51.3	316.8692	315.8619	-	-	-
1	172680.8	27039	9	142.9764	567.8769	C ₃ H ₄ O ₃ S	3-mercaptopyruvate	10255-67-1

19.9	168238.9	27193	25.3	441.2242	440.2169	C ₁₇ H ₂₈ N ₈ O ₆	Glu His Arg	-
9.6	164980.3	27444	20.8	212.1184	211.1111	C ₁₃ H ₁₃ N ₃	Trp-P-1	62450-06-0
10.3	202370.1	27614	62.8	182.1905	181.1833	C ₁₂ H ₂₃ N	Dicyclohexylamine	101-83-7
0.8	1781159	27884	309.8	820.7678	819.7606	-	-	-
20.2	217887.8	28344	21.7	282.2787	281.2714	-	-	-
1.6	154773.8	28415	13.2	104.031	102.0314	-	-	-
19	218664.3	28436	36.6	206.6221	411.2296	-	-	-
16.4	167921.3	28480	29.7	297.2426	296.2353	C ₁₈ H ₃₂ O ₃	(±)9-HODE	98524-19-7
0.8	544420.5	28550	41.5	484.8546	482.833	-	-	-
0.9	224385.6	28570	16.4	436.761	437.7683	-	-	-
10.6	526961.8	28859	24.9	229.1413	230.1486	C ₁₂ H ₂₀ O ₄	Traumatic acid	-
20.5	183753.3	29022	24.2	235.1691	234.1618	C ₁₅ H ₂₂ O ₂	Polygodial	6754-20-7
							Eremophilenolide	4871-90-3

							Alcyopterosins O	-
							Curmadione	-
							Macrophylllic acid A	-
							1,13-Dihydroxy-herbertene	-
						C ₈ H ₁₂ N ₄ O	1-(5-Hydroxy-2-pyrimidinyl)piperazine	55745-85-2
14	139053.3	29060	19	203.0915	202.0842		2-Amino-1,6-dimethylfuro[3,2-e]imidazo[4,5-b]pyridine	132898-08-9
						C ₁₀ H ₁₀ N ₄ O		
							Metamitron	41394-05-2
0.8	2999420	29269	65.4	730.7884	731.7957	-	-	-
0.6	490070.6	29310	3.4	158.0031	156.9958	C ₇ H ₅ NS	Benzothiazole	95-16-9
16	149020.6	29498	27.3	225.1961	224.1888	C ₁₃ H ₂₄ N ₂ O	Cuscohygrine	454-14-8
1.5	594521.6	29577	11	141.9587	140.9514	-	-	-
19	390546.1	29716	97.4	651.4784	652.4857	-	-	-
0.6	954144.4	29738	7.2	158.9616	157.9543	-	-	-

7.7	190524.1	29878	20.2	114.0915	113.0842	C ₆ H ₁₁ NO	2-Acetylpyrrolidine	60026-20-2
0.8	397160.3	29946	25.4	148.9757	146.9824	-	-	-
							6-Pentyl-2H-pyran-2-one	27593-23-3
							Oxocamphor	6004-71-3
10.8	218622.7	30016	31.4	167.1069	166.0996	C ₁₀ H ₁₄ O ₂	4-Butoxyphenol	122-94-1
							2E,6E,8E-decatrienoic acid	-
0.8	400163	30252	27.8	328.8977	329.9049	C ₆ H ₁₂ Br ₂ O ₄	Mitobronitol	488-41-5
0.9	62853.94	30515	21.7	322.8253	321.8181	-	-	-
10.6	175243.1	30857	63.6	652.4109	651.4036	-	-	-
							Benzoic acid	65-85-0
1.6	279445.3	31009	28.3	145.0251	144.0178	C ₇ H ₆ O ₂	Salicylaldehyde	90-02-8
0.9	50590.14	31040	689.8	362.9257	361.9184	-	-	-
0.9	146010.6	31073	33	376.8214	375.8141	-	-	-

1.6	128092.6	31267	347.4	113.0361	224.0577	-	-	-
0.9	266636.2	31372	34.3	382.837	381.83	-	-	-
0.8	3537821	31474	77.6	802.7382	803.7455	-	-	-
0.8	286987.7	31649	68.9	412.8651	411.8578	-	-	-
1	190927.3	31896	12.7	101.95	100.9427	-	-	-
8	140963.5	32124	39.4	289.0895	288.0823	C ₁₂ H ₁₆ O ₈	Glucosylisomaltol	85559-61-1
							p-Hydroxyphenethyl trans-ferulate	84873-15-4
17.9	206105.4	32267	44.5	315.12	314.1128	C ₁₈ H ₁₈ O ₅	6,3',4'-Trimethoxyflavanone	-
							4-Methoxyhomopterocarpin	-
						C ₁₄ H ₁₄ N ₆ O ₃	Dihydropteroic acid	2134-76-1
0.8	615353	32539	61.8	628.8068	627.7995	-	-	-
0.9	135550.3	32746	727.7	436.8097	435.8025	-	-	-
0.9	70009.59	32969	732.6	560.8695	559.8625	-	-	-

21.7	193132	33519	75.2	307.1382	612.2618	C ₁₄ H ₁₈ N ₄ O ₄	Trimethoprim 1-N-oxide	27653-68-5
1.6	221923.4	33572	64.4	349.0481	348.0412	-	-	-
0.9	351139.4	34139	33.6	518.755	517.7485	-	-	-
0.8	730954.8	34632	78.1	549.8354	548.8281	-	-	-
6.7	403205	35011	28.4	236.0116	237.0189	C ₅ H ₁₂ NO ₄ PS	Omethoate	1113-02-6
0.8	1279957	35409	107.5	634.8131	633.8059	-	-	-
6.6	214390.6	35424	51.2	231.0839	230.0766	C ₈ H ₁₆ O ₆	Dambonitol	523-94-4
10.4	320832.5	35432	71	613.34	614.3473	C ₃₀ H ₄₄ N ₈ O ₆	Phe Lys Tyr Arg	-
19	664624.4	35501	53.8	667.4438	666.4378	C ₃₇ H ₆₂ O ₁₀	Notoginsenoside	343962-54-9
1	288792.2	35602	34.8	127.0728	126.0655	C ₃ H ₆ N ₆	Melamine	108-78-1
							Butyric acid	107-92-6
1.6	160974.1	36674	64.5	89.0599	88.0526	C ₄ H ₈ O ₂	1-Hydroxy-2-butanone	5077-67-8
							1,4-Dioxane	123-91-1

							Ethyl acetate	141-78-6
3.6	12703288	36795	13.7	141.9587	140.9514	-	-	-
15.7	589153.3	36844	44.5	362.3265	361.3192	-	-	-
10.4	201497	36854	25.9	608.3849	607.3776	C ₃₃ H ₅₃ NO ₉	Malyngamide J	-
0.8	487948.5	36876	8.2	346.908	345.9007	-	-	-
0.8	823915.9	37034	66.3	558.8392	559.8465	-	-	-
0.8	1097586	37133	102.6	606.823	603.7849	-	-	-
							Amyl 2-furoate	4996-48-9
8.6	214234.3	37241	28.4	183.1019	182.0946	C ₁₀ H ₁₄ O ₃	2,4,5-Trimethoxytoluene	-
							MEPHENESIN	59-47-2
20.5	227085.7	37405	28.6	282.279	281.2717	C ₁₈ H ₃₅ NO	Elaidamide	4303-70-2
0.8	407736.6	37427	57.2	398.9066	397.8994	-	-	-
0.9	117695.5	37463	7.4	226.8909	225.8836	-	-	-

14.7	274636.6	37511	38.5	227.1254	228.1327	C ₁₀ H ₂₀ O ₄	3,7-Dimethyl-3-octene-1,2,6,7-tetrol	261949-44-4
8.5	225279.6	37571	60.1	319.1369	320.1442	C ₁₅ H ₁₈ N ₄ O ₄	AsparaginyI-Tryptophan	-
10.2	209993	38198	79	564.3592	563.352	-	-	-
0.8	422619.6	38364	426.3	327.4257	326.4184	-	-	-
0.9	109910.2	38719	27.4	356.909	355.9017	-	-	-
0.8	1432738	38783	89.4	752.7833	753.7906	-	-	-
10.2	376377.1	38799	85	569.3147	570.322	C ₂₆ H ₄₄ N ₆ O ₆ S	Lys Lys Met Tyr	-
8.8	192186.5	39414	28.2	344.2281	343.2208	-	-	-
0.9	291599.2	39966	56.8	158.9124	315.8096	-	-	-
							2,7-Oxepanedione	2035-75-8
0.8	440454.4	40517	8	151.0354	150.0281	C ₆ H ₈ O ₃	Osmundalactone	69308-39-0
							2-Oxo-4E-hexenoic acid	-
18.2	393901.3	40571	16	200.2007	199.1935	C ₁₂ H ₂₅ NO	dodecanamide	-

0.9	205447.3	42010	51.5	498.855	497.8477	-	-	-
0.9	106404.5	42346	75.2	368.822	367.8148	-	-	-
						C ₁₁ H ₁₂ N ₄	Heteropyrithiamine	-
							2E,4E,8E,10E-Dodecatetraenedioic acid	-
8.6	242346.7	42380	24.8	223.0945	222.0872	C ₁₂ H ₁₄ O ₄	APIOLE	523-80-8
							Valeroyl Salicylate	64206-54-8
0.9	305567	42702	108.4	222.9196	221.9126	-	-	-
0.9	292770	42738	58.9	213.9693	212.9621	C ₆ H ₆ ClNO ₂ S	p-Chlorobenzenesulfonylamide	98-64-6
10	368800.6	42822	67.9	525.288	526.2953	C ₂₄ H ₄₀ N ₆ O ₅ S	Cys Phe Lys Lys	-
10	233877.4	43004	146.6	520.3328	519.3255	-	-	-
						C ₂₂ H ₄₈ NO ₆ P	PC(O-12:0-O-2:0)	-
9.7	236075.1	43454	39.1	476.3064	475.2991	C ₂₁ H ₄₁ N ₅ O ₇	Netilmicin	-
17.3	666454.3	43530	80.8	302.3051	301.2979	C ₁₈ H ₃₉ NO ₂	Sphinganine	764-22-7

0.8	4258497	43809	105.1	566.8292	567.8365	-	-	-
15.5	260300.2	43971	37.6	207.0442	206.0369	C ₉ H ₁₂ O ₂ S	(+--)-3-[(2-methyl-3-furyl)thio]-2-butanone	61295-44-1
20.3	257975.3	44002	33.7	282.2788	281.2715	C ₁₈ H ₃₅ NO	Elaidamide	4303-70-2
9.7	480376.8	44393	83	481.2621	482.2694	C ₂₃ H ₃₆ N ₄ O ₇	Phe Ile Thr Thr	-
0.8	423628.2	44641	22.3	268.949	267.9418	-	-	-
0.9	499350.5	44807	23.2	394.8306	395.8379	-	-	-
1.6	157587.6	45090	82.1	237.0915	236.0842	C ₁₆ H ₁₂ O ₂	trans-4,5-Dihydroxy-4,5-dihydropyrene	56183-12-1
						C ₈ H ₁₆ N ₂ O ₄ S	Methionyl-Serine	-
1.5	280354.3	45471	39.8	152.0706	153.0779	C ₈ H ₉ NO ₂	N-(Acetyloxy)benzenamine	71825-04-2
							2-Phenylglycine	2835-06-5
11.2	426861	45553	39.3	107.0704	106.0631	C ₄ H ₁₀ O ₃	Diethylene glycol	111-46-6
0.8	798559.3	45813	80.2	428.8812	426.8581	-	-	-
9.2	226193.1	45925	18.4	388.2543	387.247	C ₁₇ H ₃₃ N ₅ O ₅	Ala Ala Lys Val	-

0.9	109936.2	45931	510.3	430.8534	429.8461	-	-	-
0.8	469538.1	46111	512.3	392.4047	782.7948	-	-	-
7.9	274802.8	46316	82.8	275.1104	276.1177	C ₁₀ H ₂₀ O ₇	2,3-Butanediol glucoside	146763-54-4
						C ₁₀ H ₁₆ N ₃ O ₆	Gamma-glutamyl-Glutamate	-
8	371987.6	46400	51.6	130.1591	129.1518	C ₈ H ₁₉ N	Octylamine	111-86-4
11.5	259210	46654	43.8	218.2115	217.2042	-	-	-
21.7	305222.8	47137	89.8	579.2925	578.2852	C ₂₅ H ₃₈ N ₈ O ₈	Glu Phe Gln Arg	-
0.9	322796.9	47171	45.2	398.8081	398.2768	-	-	-
9.5	233982.3	48967	25.6	432.2806	431.2733	C ₁₉ H ₃₇ N ₅ O ₆	Ala Lys Ile Thr	-
0.9	113371.9	49454	82.1	232.9086	231.9014	-	-	-
0.8	325454.9	49517	85.1	480.8538	479.8458	-	-	-
21.8	303382.1	49809	56.3	243.1356	242.1283	C ₁₄ H ₂₀ O ₂	2,6-di-tert-butylbenzoquinone	719-22-2
							Hexyl phenylacetate	5421-17-0

							13-Nor-6-eremophilene-8,11-dione	348119-85-7
						C ₁₁ H ₁₈ N ₂ O ₄	N-Hydroxypentobarbital	62298-51-5
							Bisphenol B	77-40-7
						C ₁₆ H ₁₈ O ₂		
							6E,8E,14Z-Hexadecatriene-10,12-dienoic acid	-
0.8	759679.9	50786	102.1	610.8081	609.8008	-	-	-
						C ₁₀ H ₁₆ O ₃	(1'R)-Nepetalic acid	21651-54-7
10.8	262983.4	51106	55.7	207.0993	206.092			
						C ₇ H ₁₄ N ₂ O ₅	Thr Ser	-
9.5	364802.8	51589	61.9	437.2358	438.2431	C ₂₁ H ₃₂ N ₄ O ₆	Ala Ala Tyr Ile	-
14.6	387991	52039	76.3	455.1884	456.1957	C ₁₈ H ₂₆ N ₆ O ₈	Asp His Pro Ser	-
0.9	415369.2	52611	85	278.8609	279.8682	-	-	-
0.8	472779.8	52636	86.2	102.9702	101.9629	-	-	-
						C ₁₉ H ₂₈ N ₄ O ₅	Ala Gly Phe Val	-
9.2	409450.9	53027	49	393.2096	371.1804			
						C ₂₅ H ₂₈ O ₄	4'-Geranyloxy-4,2'-dihydroxychalcone	-

							Kazinol B	-
0.9	374651.9	53819	58.8	177.9482	176.9409	-	-	-
23.3	21387362	54100	17.3	108.5175	215.0205	-	-	-
						C ₁₆ H ₂₂ O ₄	Diisobutyl phthalate	84-69-5
							alpha,alpha'-diethyl-3,4,3',4'-stilbenetetraol	-
21.8	846470.5	55179	64.4	301.1409	302.1481	C ₁₈ H ₂₀ O ₄	2'-Hydroxy-4',6'-dimethoxy-3'-methyldihydrochalcone	-
							4'-Hydroxy-5,7-dimethoxy-8-methylflavan	-
0.8	923124.2	55507	158.6	445.8755	444.8682	-	-	-
2.1	4291405	55749	41.4	129.0524	128.0452	C ₄ H ₁₀ O ₃	Diethylene glycol	111-46-6
0.8	654942.8	56117	1247	448.3783	447.371	C ₂₆ H ₅₁ NO ₃	C-8 Ceramide	74713-59-0
11.5	394462.7	56783	19.4	241.0683	240.061	C ₉ H ₁₄ O ₆	Triacetin	102-76-1
0.8	641474.5	58082	78.5	146.0299	145.0226	-	-	-
0.8	1665127	58544	83.2	684.8076	683.8017	-	-	-

21.7	446492.4	58897	151.1	658.2529	657.2457	C ₃₂ H ₃₇ N ₅ O ₉	Gln Tyr Tyr Tyr	-
0.8	188420.5	58942	56.6	282.9048	281.8975	-	-	-
0.9	464353.2	60002	46.1	294.8783	295.8855	-	-	-
23.3	30503164	60284	19.3	115.9639	114.9567	-	-	-
8.8	464408.3	60380	144.9	349.1836	350.1909	C ₁₆ H ₂₈ O ₈	(1S,2S,4R,5S,7S)-2,5,7-Fenchanetriol 2-O-b-D-glucoside	217960-85-5
						C ₁₂ H ₂₄ N ₆ O ₆	Ser Ser Arg	-
1.7	614123.9	61192	43.6	191.0229	190.0156	-	-	-
23.1	425824.1	61596	47.1	282.2787	281.2714	C ₁₈ H ₃₅ NO	Elaidamide	4303-70-2
17.2	385888	62290	53	317.1358	316.1285	C ₁₈ H ₂₀ O ₅	2'-Hydroxy-3',4',6'-trimethoxydihydrochalcone	-
							EPIAFZELECHIN TRIMETHYL ETHER	-
19	474973.3	62443	75.3	356.279	355.2717	-	-	-
0.9	308049.6	62962	65.8	304.8961	303.886	-	-	-
0.8	1735363	63970	121.4	616.8221	615.8145	-	-	-

0.9	188666.3	64599	57.8	113.1074	112.1001	C ₆ H ₁₂ N ₂	2-Imino-4-methylpiperidine	165383-72-2
0.8	620098.9	64865	40.2	130.9652	129.9579	C ₂ H ₄ Cl ₂ O ₂	2,2-Dichloro-1,1-ethanediol	16086-14-9
13.6	472925	66134	151.5	246.2428	245.2355	-	-	-
23.9	504080.3	67510	82.4	300.2893	299.282	C ₁₈ H ₃₇ NO ₂	2-amino-octadecanoic acid	-
23.3	524506.8	67517	51.7	282.2788	281.2715	C ₁₈ H ₃₅ NO	Palmitoyl Ethanolamide	544-31-0
0.9	505527.3	67603	153.1	262.8878	261.8809	-	-	-
0.9	211800.5	67737	188.1	424.8959	423.8886	-	-	-
0.8	861734.9	69356	79.4	167.0127	166.0054	-	-	-
0.9	164175.1	71511	17.4	158.964	157.9567	-	-	-
10.8	338637.2	73169	11.8	163.0392	162.0319	C ₉ H ₆ O ₃	3 Hydroxycoumarin	939-19-5
0.9	496220.9	73197	74.6	195.9588	194.9515	-	-	-
1.6	417049.9	73995	135.3	266.0451	265.0384	C ₁₀ H ₁₃ NO ₄ S	Mono-N-depropylprobenecid	10252-65-0

0.8	922215.9	74972	58.5	162.0073	160.0047	-	-	-
15.3	697650.7	75700	100.3	302.1363	303.1435	C ₁₂ H ₁₉ N ₃ O ₆	Pro Asp Ala	-
0.8	1548222	77731	148.9	501.8503	500.8431	-	-	-
0.7	868034.4	78934	16.5	99.5312	98.5239	-	-	-
1.6	483045.4	79090	125.6	297.0858	296.0785	C ₁₆ H ₁₂ N ₂ O ₄	5-Hydroxy-4-methoxy-3-methyl-2,6-canthinedione	129724-30-7
0.9	228040.2	81157	169.5	180.8944	179.8872	-	-	-
15.5	646943.2	81472	81.8	225.0548	224.0478	C ₁₄ H ₈ O ₃	Hydroxyanthraquinone	129-43-1
17.2	718866.8	82083	35.7	311.1852	310.1783	C ₁₅ H ₂₈ O ₅	6-Hydroxypentadecanedioic acid	38076-52-7
						C ₁₇ H ₂₆ O ₅	3-Hydroxy-6,8-dimethoxy-7(11)-eremophilen-12,8-olide	162613-65-2
0.8	251257.3	83000	119.4	300.9147	299.9074	-	-	-
0.8	1758027	87363	105.8	436.8704	871.7262	-	-	-
7.8	656876.2	89061	159.9	261.1311	262.1384	C ₁₂ H ₂₀ O ₆	Glycerol tripropanoate	139-45-7
8.4	696901.6	90274	97.8	305.1573	282.624	-	-	-

6.4	717319.1	90505	71.3	217.1049	218.1122	-	-	-
0.9	254903.8	92476	35.9	220.9344	219.9271	-	-	-
0.7	933063.5	93768	23	81.5205	161.0265	-	-	-
3.5	809069.5	95755	75.5	173.0786	174.0858	-	-	-
12.1	636528.4	98655	123.1	171.1491	170.1422	C ₉ H ₁₈ N ₂ O	3-Acrylamidopropyl trimethylammonium	45021-77-0
20.9	680959.5	99114	75.8	282.279	281.2717	C ₁₈ H ₃₅ NO	Elaidamide	4303-70-2
0.8	1124319	101304	63	239.9664	238.9592	-	-	-
0.8	529765.5	102760	98.2	486.8661	485.8588	-	-	-
21.8	779290.1	104258	77.2	205.0859	204.0787	C ₁₂ H ₁₂ O ₃	7-Ethoxy-4-methyl-2H-1-benzopyran-2-one	87-05-8
							Anofinic acid	34818-56-9
							3,4,5-Trimethoxycinnamic acid	-
10.8	851798.1	104328	113.4	239.0892	240.0965	C ₁₂ H ₁₄ O ₅	Trans-2, 3, 4-Trimethoxycinnamate	33130-03-9
							1-(2,4,5-Trimethoxyphenyl)-1,2-propanedione	2020-84-0

12.4	834831.8	105465	161.9	187.0394	186.0321	C ₁₁ H ₆ O ₃	Angelicin	-
15.1	847941.8	105540	116.1	684.3796	683.3728	-	-	-
19	763421.9	110589	115.3	297.2421	296.2356	C ₁₈ H ₃₂ O ₃	(±)9-HODE	98524-19-7
0.9	343291.7	115548	44.7	90.9767	89.9694	-	-	-
15.8	748382.9	116419	73.9	158.154	157.1467	-	-	-
0.8	3705898	117442	308.6	510.8542	509.847	-	-	-
0.8	345111.2	122784	101	350.8921	349.8848	-	-	-
0.8	1401479	128795	19.1	234.9611	233.9538	C ₇ H ₇ IO	2-Iodophenol methyl ether	-
							5-Nonyltetrahydro-2-oxo-3-furancarboxylic acid	-
21.7	1426756	130098	91.2	279.159	278.152	C ₁₄ H ₂₄ O ₄	Monomenthyl succinate	188709-97-9
23.2	45722172	130107	21.3	99.5123	197.01	-	-	-
21.7	729865.4	131180	97.1	205.0859	204.0786	C ₁₂ H ₁₂ O ₃	Anofinic acid	34818-56-9
19	904078.8	131638	168	279.2316	278.2244	C ₁₈ H ₃₀ O ₂	11Z,13E,15-Hexadecatrienyl acetate	-

							3E,9Z,12Z-octadecatrienoic acid	-
0.8	1508541	134689	7.2	198.9399	197.9326	-	-	-
0.9	271112.3	139722	113.3	150.1125	149.1052	C ₆ H ₁₅ NO ₃	Trolamine	102-71-6
0.8	1720602	149695	52.7	257.977	256.9698	-	-	-
0.8	2558751	165257	337	474.833	473.8257	-	-	-
21.7	980628.4	170772	107.9	149.0234	148.0161	-	-	-
0.8	1964178	173792	28.4	90.5259	89.5186	-	-	-
0.8	1874984	174657	83.6	216.9505	215.9432	-	-	-
0.8	1650639	182605	296.1	344.8752	343.8688	C ₈ HCl ₄ F ₃ N ₂	4,5,6,7-Tetrachloro-2-trifluoromethylbenzimidazole	2338-29-6
25	1629799	183388	222.7	256.2631	255.2558	C ₁₆ H ₃₃ NO	Palmitic amide	629-54-9
							PGF2α 1,15-lactone	55314-49-3
19	1545434	184768	169.2	337.2344	314.4907	C ₂₀ H ₃₂ O ₄	15-epi-PGA1	20897-92-1
0.8	2334545	202753	335.9	380.8964	379.8898	-	-	-

0.8	2859058	212974	140.7	492.8437	491.8364	-	-	-
0.9	1315072	214841	415.4	164.9205	165.9277	-	-	-
0.8	2557964	219835	447	362.8859	361.8786	C ₁₂ H ₈ Cl ₆	ALDRIN	309-00-2
15.6	2884980	236591	481.5	318.3003	317.293	C ₁₈ H ₃₉ NO ₃	Phytosphingosine	-
14	1683135	252895	259.5	299.11	300.1173	C ₁₃ H ₁₆ N ₄ O ₃	3'-Hydroxytrimethoprim	27653-69-6
24.2	1882222	284617	164.1	398.2321	397.2249	C ₁₇ H ₃₆ NO ₇ P	PE(12:0-0:0)	-
0.9	672119.2	292611	440.4	226.9515	225.9442	C ₆ H ₄ Cl ₂ O ₅	2,5-Dichloro-4-oxohex-2-enedioate	-
0.8	2970451	300787	259.4	255.944	253.9242	-	-	-
0.8	3256541	363568	534.4	273.9546	272.9473	-	-	-
1.6	1752365	398398	213.9	126.0441	250.0741	-	-	-
0.8	893244.5	417105	9269	288.9218	287.9145	-	-	-
0.8	4399411	418749	119.7	128.0193	127.012	-	-	-
11.2	7150336	503085	236.8	185.115	186.1223	C ₈ H ₁₈ O ₃	(3R,7R)-1,3,7-Octanetriol	217650-11-8

0.8	5333622	513653	371	110.0087	109.0014	-	-	-
0.8	4866920	534599	420.6	250.9387	249.9314	-	-	-
0.8	5495843	569056	194.7	143.9968	142.9895	-	-	-
1.6	6507270	637518	473.4	129.0524	130.0597	C ₄ H ₁₀ O ₃	Diethylene glycol	111-46-6
0.8	7830395	841702	352	232.9281	231.9208	C ₇ H ₅ Cl ₃ O	2,4,6-Trichloroanisole	87-40-1
15.4	8711714	853508	1120.3	274.2741	273.2669	C ₁₆ H ₃₅ NO ₂	C16 Sphinganine	-
0.8	9568139	1028954	168.9	214.9175	213.9103	-	-	-
0.8	14301652	1588981	434.4	125.9862	124.979	-	-	-
0.8	15600099	1669036	485	84.9596	83.9524	-	-	-

