

n°	Family	Metabolite	CF		D-CF		CC		D-CC		C-PEC	
			Intensity	Rel. %	Intensity	Rel. %	Intensity	Rel. %	Intensity	Rel. %	Intensity	Rel. %
1	Alkaloids and derivatives	Trans-zeatin	766838	0.02%	985560	0.02%	11862	0.00%	1906	0.00%	44	0.00%
2	Alkaloids and derivatives	Theophylline	21078565	0.47%	782316	0.02%	40704	0.01%	386	0.00%	46	0.00%
3	Alkaloids and derivatives	N6-methyl-lysine	494439	0.01%	16676	0.00%	13969	0.00%	1224	0.00%	113	0.00%
4	Alkaloids and derivatives	Thiamine	51095	0.00%	520493	0.01%	97169	0.02%	292365	0.15%	338	0.00%
5	Alkaloids and derivatives	Kynurenic acid	464145	0.01%	996037	0.02%	5484	0.00%	12860	0.01%	344	0.00%
6	Alkaloids and derivatives	Theobromine	2081219	0.05%	644292	0.01%	187191	0.04%	2295	0.00%	723	0.00%
7	Alkaloids and derivatives	Caffeine	59290567	1.31%	43309177	0.87%	19781	0.00%	50202	0.02%	1518	0.00%
8	Alkaloids and derivatives	1-cyclohexylpyrrolidin-2-one	4753706	0.11%	743859	0.01%	563	0.00%	9809	0.00%	4857	0.00%
9	Alkaloids and derivatives	4-(dimethylamino)phenylthiocyanate	56692	0.00%	1774226	0.04%	1530101	0.36%	371601	0.18%	5778	0.00%
10	Alkaloids and derivatives	Ecgonine	177760	0.00%	179893	0.00%	124360	0.03%	12887	0.01%	10451	0.00%
11	Alkaloids and derivatives	Pyridoxamine	271626	0.01%	235902	0.00%	547419	0.13%	16679	0.01%	13640	0.01%
12	Alkaloids and derivatives	4-hydroxyquinoline	11134515	0.25%	1818304	0.04%	285588	0.07%	15373	0.01%	16116	0.01%
13	Alkaloids and derivatives	Pyridoxal	260721	0.01%	406348	0.01%	65766	0.02%	51867	0.03%	17302	0.01%
14	Alkaloids and derivatives	Nicotinic acid	234954	0.01%	694722	0.01%	123228	0.03%	33082	0.02%	24712	0.01%
15	Alkaloids and derivatives	Pyridoxine	1564850	0.03%	489013	0.01%	224785	0.05%	26767	0.01%	28354	0.01%
16	Alkaloids and derivatives	1-methylnicotinamide	1093122	0.02%	723306	0.01%	28780	0.01%	32711	0.02%	32056	0.01%
17	Alkaloids and derivatives	4-imidazoleacetic acid	4884353	0.11%	904464	0.02%	177778	0.04%	62891	0.03%	39114	0.02%
18	Alkaloids and derivatives	Cytidine	2310945	0.05%	363727	0.01%	93809	0.02%	1715	0.00%	52335	0.02%
19	Alkaloids and derivatives	Ethyl-4-dimethylaminobenzoate	184595	0.00%	926776	0.02%	21786	0.01%	20068	0.01%	110400	0.05%
20	Alkaloids and derivatives	Nitritriethanol	698062	0.02%	23003290	0.46%	106270	0.02%	2150348	1.07%	137433	0.06%
21	Alkaloids and derivatives	Tetramethylpiperidone	184144	0.00%	16538176	0.33%	23843	0.01%	283116	0.14%	184503	0.08%
22	Alkaloids and derivatives	Niacinamide	33519383	0.74%	54668403	1.10%	3780900	0.88%	2685864	1.34%	193407	0.09%
23	Alkaloids and derivatives	Imidazole	78382	0.00%	2079360	0.04%	17753	0.00%	275426	0.14%	263320	0.12%
24	Alkaloids and derivatives	Choline	366567214	8.10%	3480096	0.07%	121340921	28.25%	544525	0.27%	361618	0.16%
25	Alkaloids and derivatives	Morpholine	356707	0.01%	29890113	0.60%	58306	0.01%	2290004	1.14%	960424	0.43%
26	Alkaloids and derivatives	Trigonelline	1963114831	43.39%	1626336984	32.71%	3595591	0.84%	632236	0.31%	3286120	1.46%
27	Amino acids and derivatives	N,n-dimethylarginine	2070583	0.05%	196459	0.00%	130671	0.03%	1379	0.00%	0	0.00%
28	Amino acids and derivatives	N-acetylhistidine	2181600	0.05%	52811	0.00%	635807	0.15%	2497	0.00%	338	0.00%
29	Amino acids and derivatives	N,n-Dimethyl-lysine	1433344	0.03%	15969	0.00%	74194	0.02%	677	0.00%	1059	0.00%
30	Amino acids and derivatives	Arginine	8771670	0.19%	26331	0.00%	35823	0.01%	4823	0.00%	1384	0.00%
31	Amino acids and derivatives	Diethanolamine	1171	0.00%	9852271	0.20%	401785	0.09%	56133	0.03%	2508	0.00%
32	Amino acids and derivatives	Acetyl-carnitine	12963	0.00%	972193	0.02%	175909	0.04%	484581	0.24%	3080	0.00%
33	Amino acids and derivatives	3,4-dihydroxy-L-phenylalanine	127676	0.00%	41195	0.00%	112398	0.03%	10145	0.01%	3611	0.00%
34	Amino acids and derivatives	L-histidine	904490	0.02%	196067	0.00%	217247	0.05%	29722	0.01%	4571	0.00%
35	Amino acids and derivatives	L-glutamine	2756649	0.06%	11693938	0.24%	3185068	0.74%	305754	0.15%	5349	0.00%
36	Amino acids and derivatives	Glutamic acid	7347389	0.16%	1895945	0.04%	1293283	0.30%	22296	0.01%	6982	0.00%
37	Amino acids and derivatives	Histidinol	645391	0.01%	122797	0.00%	658922	0.15%	28379	0.01%	7068	0.00%
38	Amino acids and derivatives	Dimethyl(tetradecyl)amine	5959	0.00%	5375291	0.11%	1464	0.00%	480223	0.24%	10075	0.00%
39	Amino acids and derivatives	Guanidinobutyric acid methyl ester	18794739	0.42%	3756388	0.08%	189	0.00%	40171	0.02%	12136	0.01%
40	Amino acids and derivatives	Nipecotamide	14696	0.00%	564175	0.01%	3799	0.00%	398076	0.20%	17868	0.01%
41	Amino acids and derivatives	Pyroglutamic acid	160082	0.00%	3979661	0.08%	8536459	1.99%	37481	0.02%	19862	0.01%
42	Amino acids and derivatives	Cyclo-prolylglycine	22920654	0.51%	3789185	0.08%	856664	0.20%	35779	0.02%	22245	0.01%
43	Amino acids and derivatives	Deoxycarnitine	3591828	0.08%	598847	0.01%	1070020	0.25%	44436	0.02%	24330	0.01%
44	Amino acids and derivatives	N,n-dimethyldodecylamine	91253	0.00%	23702705	0.48%	529	0.00%	493999	0.25%	25190	0.01%
45	Amino acids and derivatives	Dopamine	340009	0.01%	770438	0.02%	7305	0.00%	27110	0.01%	25550	0.01%
46	Amino acids and derivatives	Agmatine sulfate	681035	0.02%	54243	0.00%	19544	0.00%	2817	0.00%	29279	0.01%
47	Amino acids and derivatives	Methylimidazoleacetic acid	2151747	0.05%	2013510	0.04%	289854	0.07%	49778	0.02%	34226	0.02%
48	Amino acids and derivatives	Methioninesulfoxide	707100	0.02%	735544	0.01%	1255394	0.29%	14739	0.01%	43465	0.02%
49	Amino acids and derivatives	Ectoïne	937404	0.02%	1085525	0.02%	10467	0.00%	99371	0.05%	48923	0.02%

50	Amino acids and derivatives	L-tyrosine	32697020	0.72%	826776	0.02%	103663	0.02%	19180	0.01%	62245	0.03%
51	Amino acids and derivatives	Acetylcholine	831699	0.02%	736036	0.01%	10801	0.00%	49379	0.02%	67849	0.03%
52	Amino acids and derivatives	Myristamidopropyl betaine	133794	0.00%	42354273	0.85%	25678	0.01%	380184	0.19%	68614	0.03%
53	Amino acids and derivatives	4-hydroxy-L-proline	3086429	0.07%	1247369	0.03%	344638	0.08%	126353	0.06%	78551	0.03%
54	Amino acids and derivatives	2-hydroxyisocaproic acid	47936	0.00%	3479952	0.07%	8358	0.00%	207449	0.10%	78627	0.03%
55	Amino acids and derivatives	Aspartic acid	1463277	0.03%	135994	0.00%	439488	0.10%	4828	0.00%	81287	0.04%
56	Amino acids and derivatives	4-guanidinobutanoate	54465081	1.20%	9523139	0.19%	5278691	1.23%	84447	0.04%	84159	0.04%
57	Amino acids and derivatives	Glucosamine	1730372	0.04%	1201018	0.02%	356493	0.08%	120680	0.06%	94900	0.04%
58	Amino acids and derivatives	2-aminoadipic acid	10025186	0.22%	1315145	0.03%	1415946	0.33%	142127	0.07%	96980	0.04%
59	Amino acids and derivatives	Myristamine oxide	54180	0.00%	4634874	0.09%	35346	0.01%	160442	0.08%	100135	0.04%
60	Amino acids and derivatives	N,n-dimethylglycine	66588	0.00%	3233542	0.07%	124377	0.03%	132962	0.07%	107924	0.05%
61	Amino acids and derivatives	L-beta-Homoproline	462011	0.01%	1152958	0.02%	5091	0.00%	141496	0.07%	112663	0.05%
62	Amino acids and derivatives	L-carnitine	24523897	0.54%	10761000	0.22%	792852	0.18%	2042698	1.02%	161149	0.07%
63	Amino acids and derivatives	N-acetyl putrescine	1025975	0.02%	2218428	0.04%	2111	0.00%	164074	0.08%	162377	0.07%
64	Amino acids and derivatives	Ketoleucine	427562	0.01%	8406888	0.17%	3473602	0.81%	9100957	4.52%	199521	0.09%
65	Amino acids and derivatives	Dibenzylamine	80591	0.00%	1571161	0.03%	117541	0.03%	177265	0.09%	217588	0.10%
66	Amino acids and derivatives	Lauramidopropyl betaine	398561	0.01%	211367823	4.25%	9005	0.00%	1687668	0.84%	250383	0.11%
67	Amino acids and derivatives	Asparagine	4634504	0.10%	440808	0.01%	680924	0.16%	9259	0.00%	279002	0.12%
68	Amino acids and derivatives	N8-acetylspermidine	1315607	0.03%	947525	0.02%	687	0.00%	106230	0.05%	287637	0.13%
69	Amino acids and derivatives	Butylamine	3038200	0.07%	112307292	2.26%	3393	0.00%	1546762	0.77%	306358	0.14%
70	Amino acids and derivatives	b-alanine	6352545	0.14%	5088862	0.10%	2325428	0.54%	360373	0.18%	371575	0.16%
71	Amino acids and derivatives	Creatinine	145101	0.00%	101430940	2.04%	11186	0.00%	4460969	2.22%	422898	0.19%
72	Amino acids and derivatives	g-aminobutyric acid	20349257	0.45%	2509807	0.05%	1374225	0.32%	241485	0.12%	432482	0.19%
73	Amino acids and derivatives	5-oxo-L-proline	3198595	0.07%	20558639	0.41%	956057	0.22%	910890	0.45%	574691	0.25%
74	Amino acids and derivatives	Pipecolic acid ethyl ester	319211	0.01%	784421	0.02%	4338725	1.01%	47713	0.02%	792318	0.35%
75	Amino acids and derivatives	Piperidine	2531069	0.06%	10947115	0.22%	959562	0.22%	899279	0.45%	881260	0.39%
76	Amino acids and derivatives	L-(-)-phenylalanine	65835	0.00%	705094	0.01%	26942	0.01%	60787	0.03%	1124647	0.50%
77	Amino acids and derivatives	Lauryldimethylamine oxide	887958	0.02%	13242550	0.27%	59670	0.01%	1481032	0.74%	1140980	0.51%
78	Amino acids and derivatives	Isoleucine	1501573	0.03%	17441736	0.35%	16903	0.00%	1363970	0.68%	1388054	0.61%
79	Amino acids and derivatives	L-norvaline	754017	0.02%	20286957	0.41%	351475	0.08%	1812962	0.90%	1827368	0.81%
80	Amino acids and derivatives	L-valine	3142042	0.07%	20497120	0.41%	133368	0.03%	1795791	0.89%	1838221	0.81%
81	Amino acids and derivatives	Pipecolic acid	1463583	0.03%	5839812	0.12%	194742	0.05%	1013774	0.50%	2642643	1.17%
82	Amino acids and derivatives	Lauryldiethanolamine	1917267	0.04%	34857615	0.70%	352181	0.08%	3067734	1.52%	3558648	1.58%
83	Amino acids and derivatives	Proline	18197036	0.40%	4823436	0.10%	22099	0.01%	415127	0.21%	6608934	2.93%
84	Amino acids and derivatives	Betaine	105855737	2.34%	260908042	5.25%	13498	0.00%	27957460	13.90%	26605624	11.79%
85	Aromatic compounds (non-phenolic)	1-naphthalenesulfonate	23990	0.00%	1386397	0.03%	1250765	0.29%	78344	0.04%	1702	0.00%
86	Aromatic compounds (non-phenolic)	4-methyl-5-thiazoleethanol	74743	0.00%	723154	0.01%	86300	0.02%	20044	0.01%	2138	0.00%
87	Aromatic compounds (non-phenolic)	2-hydroxybenzothiazole	6145	0.00%	10248943	0.21%	1676638	0.39%	557841	0.28%	2656	0.00%
88	Aromatic compounds (non-phenolic)	Maltol	435796	0.01%	460991	0.01%	82833	0.02%	136477	0.07%	22767	0.01%
89	Aromatic compounds (non-phenolic)	m-Toluic acid	185625	0.00%	5079212	0.10%	15917	0.00%	372351	0.19%	29503	0.01%
90	Aromatic compounds (non-phenolic)	Phenylacetaldehyde	43222459	0.96%	13717041	0.28%	142044	0.03%	316614	0.16%	44634	0.02%
91	Aromatic compounds (non-phenolic)	Diphenylamine	143751	0.00%	2128294	0.04%	99	0.00%	183428	0.09%	194276	0.09%
92	Aromatic compounds (non-phenolic)	Diphenylphosphate	29141	0.00%	1236623	0.02%	34128	0.01%	512351	0.25%	358341	0.16%
93	Aromatic compounds (non-phenolic)	N-(2,4-dimethylphenyl)formamide	44707	0.00%	320344	0.01%	81	0.00%	14785	0.01%	649071	0.29%
94	Aromatic compounds (non-phenolic)	2-pyridinol	299559	0.01%	2738395	0.06%	333086	0.08%	178862	0.09%	822081	0.36%
95	Aromatic compounds (non-phenolic)	4-nitrophenol	521498	0.01%	1055677	0.02%	51302	0.01%	423480	0.21%	2032378	0.90%
96	Aromatic compounds (non-phenolic)	4-dimethylaminobenzaldehyde	0	0.00%	132707	0.00%	23355	0.01%	10776	0.01%	5651660	2.50%
97	Aromatic compounds (non-phenolic)	3-pyridinol	32693809	0.72%	93039741	1.87%	180593	0.04%	2052752	1.02%	75014683	33.23%
98	Carboxylic acids, lactones and derivatives	Pantothenic acid	577739	0.01%	45537	0.00%	3897716	0.91%	6898	0.00%	628	0.00%
99	Carboxylic acids, lactones and derivatives	Haematommic acid	337454	0.01%	37857360	0.76%	60285	0.01%	333146	0.17%	1140	0.00%
100	Carboxylic acids, lactones and derivatives	1-hydroxy-2-naphthoic acid	54554	0.00%	5439036	0.11%	6172	0.00%	13354	0.01%	1701	0.00%
101	Carboxylic acids, lactones and derivatives	Perfluorobutyric acid	2194	0.00%	1202154	0.02%	173	0.00%	2988	0.00%	3481	0.00%
102	Carboxylic acids, lactones and derivatives	Meso-tartaric acid	2926146	0.06%	3417304	0.07%	11127777	2.59%	583210	0.29%	4827	0.00%

103	Carboxylic acids, lactones and derivatives	8-oxo-cyclopentenyl-octanoic acid	268781	0.01%	1537655	0.03%	698908	0.16%	192655	0.10%	13900	0.01%
104	Carboxylic acids, lactones and derivatives	1,4-cyclohexanedicarboxylic acid	4484	0.00%	14393095	0.29%	240	0.00%	779233	0.39%	25103	0.01%
105	Carboxylic acids, lactones and derivatives	3-methylsalicylic acid	8463792	0.19%	3881547	0.08%	223255	0.05%	146861	0.07%	35395	0.02%
106	Carboxylic acids, lactones and derivatives	Isonicotinic acid	2148608	0.05%	904338	0.02%	371452	0.09%	64610	0.03%	56619	0.03%
107	Carboxylic acids, lactones and derivatives	4-chlorobenzoic acid	4133721	0.09%	11682834	0.23%	739226	0.17%	682184	0.34%	68327	0.03%
108	Carboxylic acids, lactones and derivatives	Cis-aconitic acid	6315952	0.14%	16859818	0.34%	399406	0.09%	851397	0.42%	69208	0.03%
109	Carboxylic acids, lactones and derivatives	9-hydroxy-octadecadienoic acid	26872	0.00%	4261250	0.09%	1001	0.00%	84254	0.04%	73243	0.03%
110	Carboxylic acids, lactones and derivatives	2-chlorobenzoate	4932574	0.11%	4918693	0.10%	1496	0.00%	271957	0.14%	73527	0.03%
111	Carboxylic acids, lactones and derivatives	2-hydroxyhexanedioic acid	4258183	0.09%	2592073	0.05%	1510267	0.35%	134158	0.07%	75591	0.03%
112	Carboxylic acids, lactones and derivatives	13-hydroxy-octadecatrienoic acid	81160	0.00%	7541888	0.15%	7237	0.00%	141898	0.07%	92886	0.04%
113	Carboxylic acids, lactones and derivatives	DL-2-hydroxyvaleric acid	414679	0.01%	21008240	0.42%	22536	0.01%	317082	0.16%	96393	0.04%
114	Carboxylic acids, lactones and derivatives	Dihydroxy-valerate	1573384	0.03%	1371422	0.03%	235522	0.05%	105120	0.05%	98962	0.04%
115	Carboxylic acids, lactones and derivatives	2,6-dihydropyridine	22791069	0.50%	743113	0.01%	1682	0.00%	59368	0.03%	152538	0.07%
116	Carboxylic acids, lactones and derivatives	Fumaric acid	11994783	0.27%	90311170	1.82%	1138292	0.26%	1006649	0.50%	202441	0.09%
117	Carboxylic acids, lactones and derivatives	6-hydroxynicotinic acid	960016	0.02%	970140	0.02%	73331	0.02%	163915	0.08%	236587	0.10%
118	Carboxylic acids, lactones and derivatives	Pyruvic acid	2426321	0.05%	5844091	0.12%	653053	0.15%	603013	0.30%	242248	0.11%
119	Carboxylic acids, lactones and derivatives	D-(+)-malic acid	20389480	0.45%	44435453	0.89%	31069918	7.23%	2365831	1.18%	252432	0.11%
120	Carboxylic acids, lactones and derivatives	Citramalic acid	60914257	1.35%	229658767	4.62%	8238722	1.92%	14584994	7.25%	261355	0.12%
121	Carboxylic acids, lactones and derivatives	Pantothenol	805281	0.02%	11894437	0.24%	18426	0.00%	1404133	0.70%	305476	0.14%
122	Carboxylic acids, lactones and derivatives	3-hydroxyglutaric acid	4868554	0.11%	6870248	0.14%	1834775	0.43%	985972	0.49%	318027	0.14%
123	Carboxylic acids, lactones and derivatives	Urocanic acid	1775246	0.04%	9006879	0.18%	56248	0.01%	620961	0.31%	351546	0.16%
124	Carboxylic acids, lactones and derivatives	Pyroole-2-carboxylic acid	7697012	0.17%	1356581	0.03%	237027	0.06%	76246	0.04%	389624	0.17%
125	Carboxylic acids, lactones and derivatives	Quinic acid	303124	0.01%	9516115	0.19%	1840	0.00%	88215	0.04%	393682	0.17%
126	Carboxylic acids, lactones and derivatives	Isobutyric acid	440823	0.01%	22334388	0.45%	37999	0.01%	2298053	1.14%	423871	0.19%
127	Carboxylic acids, lactones and derivatives	Hydroxymethylglutaric acid	21623	0.00%	29135152	0.59%	58898	0.01%	1835202	0.91%	452157	0.20%
128	Carboxylic acids, lactones and derivatives	Threonic acid	2235819	0.05%	97112238	1.95%	541177	0.13%	5284156	2.63%	493548	0.22%
129	Carboxylic acids, lactones and derivatives	Glycolic acid	936654	0.02%	17757075	0.36%	250421	0.06%	847278	0.42%	499762	0.22%
130	Carboxylic acids, lactones and derivatives	Citraconic acid	4481121	0.10%	19962154	0.40%	238885	0.06%	1445635	0.72%	526770	0.23%
131	Carboxylic acids, lactones and derivatives	S-citramalic acid	7945026	0.18%	9103310	0.18%	8754382	2.04%	1279833	0.64%	542068	0.24%
132	Carboxylic acids, lactones and derivatives	Glyceric acid	3209411	0.07%	41965158	0.84%	1252270	0.29%	2737683	1.36%	678501	0.30%
133	Carboxylic acids, lactones and derivatives	a-ketoglutaric acid	348899	0.01%	14429996	0.29%	50073	0.01%	2785183	1.38%	835673	0.37%
134	Carboxylic acids, lactones and derivatives	3-hydroxypropanoic acid	1742480	0.04%	38794330	0.78%	1310463	0.31%	1559363	0.78%	1158486	0.51%
135	Carboxylic acids, lactones and derivatives	Maleic acid	2737848	0.06%	33846181	0.68%	256712	0.06%	6779952	3.37%	1293222	0.57%
136	Carboxylic acids, lactones and derivatives	Isethionic acid	234873	0.01%	2834621	0.06%	85173	0.02%	548407	0.27%	1420158	0.63%
137	Carboxylic acids, lactones and derivatives	Succinic acid	414600	0.01%	34457479	0.69%	2575739	0.60%	6759979	3.36%	1896463	0.84%
138	Carboxylic acids, lactones and derivatives	Malonic acid	1390638	0.03%	78862649	1.59%	1641325	0.38%	8195594	4.07%	6143285	2.72%
139	Fatty acids and steroids	Nandrolone	186395	0.00%	1221256	0.02%	80135	0.02%	54460	0.03%	5428	0.00%
140	Fatty acids and steroids	Lignoceric acid	101231	0.00%	2808707	0.06%	9528	0.00%	285847	0.14%	9753	0.00%
141	Fatty acids and steroids	g-linolenic acid	195585	0.00%	10930262	0.22%	49588	0.01%	193799	0.10%	13763	0.01%
142	Fatty acids and steroids	Dehydrophytosphingosine	466995	0.01%	3699069	0.07%	1945	0.00%	119304	0.06%	48909	0.02%
143	Fatty acids and steroids	Sphinganine	732720	0.02%	21434908	0.43%	9718	0.00%	134409	0.07%	50932	0.02%
144	Fatty acids and steroids	Linoleic acid	321315	0.01%	16461529	0.33%	13937	0.00%	759258	0.38%	111509	0.05%
145	Fatty acids and steroids	SN-glycero-3-phosphocholine	89603338	1.98%	52492933	1.06%	2744475	0.64%	125533	0.06%	134127	0.06%
146	Fatty acids and steroids	Oleic acid	260071	0.01%	23064038	0.46%	7445	0.00%	2779629	1.38%	265290	0.12%
147	Fatty acids and steroids	D-ribo-phytosphingosine	173641	0.00%	8170492	0.16%	85496	0.02%	690395	0.34%	1041645	0.46%
148	Fatty acids and steroids	Stearic acid	612405	0.01%	116395742	2.34%	0	0.00%	9233443	4.59%	1151188	0.51%
149	Fatty acids and steroids	Palmitic acid	1215114	0.03%	92853325	1.87%	32779	0.01%	13731697	6.83%	2431231	1.08%
150	Fatty acids and steroids	Canrenone	3981717	0.09%	266363617	5.36%	471728	0.11%	14290975	7.10%	4377613	1.94%
151	Nucleic acids and derivatives	5-methylcytosine	84457	0.00%	245463	0.00%	213278	0.05%	25114	0.01%	61550	0.03%
152	Nucleic acids and derivatives	Adenosine	1371791	0.03%	8364090	0.17%	145092	0.03%	249812	0.12%	69036	0.03%
153	Nucleic acids and derivatives	Purine	673569	0.01%	3344289	0.07%	386880	0.09%	192301	0.10%	117296	0.05%

154	Nucleic acids and derivates	3-methyladenine	1512168	0.03%	1006787	0.02%	375799	0.09%	14464	0.01%	123048	0.05%
155	Nucleic acids and derivates	Cytosine	14343396	0.32%	1950572	0.04%	561139	0.13%	39349	0.02%	198316	0.09%
156	Nucleic acids and derivates	O6-methylguanine	100589	0.00%	1934317	0.04%	26508	0.01%	173344	0.09%	233455	0.10%
157	Nucleic acids and derivates	Guanine	27865982	0.62%	3126425	0.06%	3089136	0.72%	148822	0.07%	815531	0.36%
158	Nucleic acids and derivates	Adenine	293438466	6.49%	52104611	1.05%	64143203	14.93%	2528486	1.26%	6177424	2.74%
159	Others	3,6,9,12-tetraoxatetracosan-1-ol	109365	0.00%	8392224	0.17%	12873	0.00%	113966	0.06%	36179	0.02%
160	Others	4-hydroxy-TEMPO	357605	0.01%	195331048	3.93%	52355	0.01%	408267	0.20%	70405	0.03%
161	Others	4-hydroxy-6-methyl-2-pyrone	116372	0.00%	256465	0.01%	11718	0.00%	32134	0.02%	7026706	3.11%
162	Phenolics and derivates	Fisetin	1447360	0.03%	0	0.00%	190	0.00%	0	0.00%	0	0.00%
163	Phenolics and derivates	Vanillylmandelic acid	0	0.00%	3279	0.00%	230085	0.05%	3293	0.00%	53	0.00%
164	Phenolics and derivates	Fraxetin	566101	0.01%	61081	0.00%	12177	0.00%	593	0.00%	194	0.00%
165	Phenolics and derivates	Propyl gallate	349162	0.01%	7926374	0.16%	92580	0.02%	16056	0.01%	2012	0.00%
166	Phenolics and derivates	Ethylvanillin	0	0.00%	8419500	0.17%	13708	0.00%	47858	0.02%	4968	0.00%
167	Phenolics and derivates	4-hydroxymandelonitrile	426954	0.01%	155015	0.00%	72078	0.02%	17441	0.01%	8038	0.00%
168	Phenolics and derivates	4-hydroxyphenyl acetic acid	3607171	0.08%	10083161	0.20%	628364	0.15%	435898	0.22%	12939	0.01%
169	Phenolics and derivates	Vanillic acid	338623	0.01%	426788	0.01%	190787	0.04%	35356	0.02%	19124	0.01%
170	Phenolics and derivates	g-valerolactone	475653	0.01%	290266	0.01%	109244	0.03%	26241	0.01%	23695	0.01%
171	Phenolics and derivates	Gentisic acid	846042	0.02%	2654299	0.05%	227308	0.05%	121639	0.06%	28410	0.01%
172	Phenolics and derivates	Paeonol	156808	0.00%	677644	0.01%	19234	0.00%	52902	0.03%	29645	0.01%
173	Phenolics and derivates	Methylgallate	249295	0.01%	19569479	0.39%	86439	0.02%	182638	0.09%	39538	0.02%
174	Phenolics and derivates	4-hydroxybenzoic acid	1893280	0.04%	2400378	0.05%	12893	0.00%	94026	0.05%	44928	0.02%
175	Phenolics and derivates	3-hydroxybenzoic acid	618690	0.01%	1946287	0.04%	219564	0.05%	76986	0.04%	46241	0.02%
176	Phenolics and derivates	Catechol	1270021	0.03%	6366210	0.13%	3223	0.00%	89064	0.04%	50140	0.02%
177	Phenolics and derivates	Pyrogallol	611157	0.01%	320909	0.01%	9529	0.00%	64948	0.03%	53803	0.02%
178	Phenolics and derivates	Lolilide	174613	0.00%	638058	0.01%	75089	0.02%	63760	0.03%	56961	0.03%
179	Phenolics and derivates	Protocatechuic acid	8154291	0.18%	2438712	0.05%	63683	0.01%	172801	0.09%	74730	0.03%
180	Phenolics and derivates	Salicylic acid	1068876	0.02%	1304140	0.03%	367293	0.09%	101824	0.05%	94952	0.04%
181	Phenolics and derivates	3-amino-4-hydroxybenzoic acid	18223557	0.40%	1503333	0.03%	54066	0.01%	72135	0.04%	99278	0.04%
182	Phenolics and derivates	D(-)-gulono-g-lactone	4190466	0.09%	1515809	0.03%	388265	0.09%	194471	0.10%	144461	0.06%
183	Phenolics and derivates	Gulonic acid g-lactone	1869013	0.04%	905020	0.02%	124853	0.03%	101051	0.05%	172330	0.08%
184	Phenolics and derivates	Ascorbic acid	774320838	17.12%	3673707	0.07%	59601075	13.87%	1385132	0.69%	176846	0.08%
185	Phenolics and derivates	Dehydroascorbic acid	62997866	1.39%	34242196	0.69%	6067973	1.41%	386387	0.19%	192293	0.09%
186	Phenolics and derivates	Glucono-1,5-lactone	11073585	0.24%	2948718	0.06%	62545	0.01%	118430	0.06%	269925	0.12%
187	Phenolics and derivates	2-aminophenol	630768	0.01%	4552012	0.09%	114863	0.03%	235113	0.12%	369006	0.16%
188	Phenolics and derivates	Hesperetin	575	0.00%	3993	0.00%	3367	0.00%	0	0.00%	2171613	0.96%
189	Phenolics and derivates	Nobiletin	12268	0.00%	0	0.00%	17	0.00%	267	0.00%	2819955	1.25%
190	Phenolics and derivates	Tangeretin	7986	0.00%	0	0.00%	145	0.00%	0	0.00%	4895969	2.17%
191	Phenolics and derivates	4-aminophenol	5102006	0.11%	12046042	0.24%	387187	0.09%	298813	0.15%	5611285	2.49%
192	Phenolics and derivates	3-amino-5-hydroxybenzoic acid	3284496	0.07%	2959164	0.06%	944976	0.22%	1298115	0.65%	6627259	2.94%
193	Sugars and derivates	D-mannitol	1242483	0.03%	68483	0.00%	35587	0.01%	10040	0.00%	182	0.00%
194	Sugars and derivates	Lactulose	45340	0.00%	11344	0.00%	743714	0.17%	0	0.00%	922	0.00%
195	Sugars and derivates	L-iditol	3587916	0.08%	187637	0.00%	379905	0.09%	22735	0.01%	1961	0.00%
196	Sugars and derivates	D-mannosamine	568248	0.01%	249825	0.01%	23204280	5.40%	15740	0.01%	13665	0.01%
197	Sugars and derivates	Inositol	255941	0.01%	356526	0.01%	851674	0.20%	71316	0.04%	69975	0.03%
198	Sugars and derivates	L-sorbose	607153	0.01%	1425162	0.03%	208465	0.05%	150494	0.07%	84969	0.04%
199	Sugars and derivates	Mannose	462645	0.01%	490752	0.01%	1261611	0.29%	82975	0.04%	100292	0.04%
200	Sugars and derivates	Ribose	3449100	0.08%	888040	0.02%	384724	0.09%	44056	0.02%	441975	0.20%
201	Sugars and derivates	Sucrose	0	0.00%	0	0.00%	0	0.00%	281	0.00%	459786	0.20%
202	Sugars and derivates	Levoglucozan	45263	0.00%	55460	0.00%	71864	0.02%	11680	0.01%	702437	0.31%
203	Sugars and derivates	Turanose	8250	0.00%	0	0.00%	63839	0.01%	0	0.00%	2991001	1.33%
204	Sugars and derivates	Melibiose	7861	0.00%	212018	0.00%	4052	0.00%	5175	0.00%	3542951	1.57%
205	Sugars and derivates	Trehalose	0	0.00%	0	0.00%	2803	0.00%	128	0.00%	4293652	1.90%
			4523995305	100.00%	4972120426	100.00%	429582263	100.00%	201186906	100.00%	225724142	100.00%