

Supplementary Table 3: Table providing the loading values derived from Partial Least Squares Discriminant Analysis (PLS-DA), representing the contribution of each identified feature/compound to the observed clustering and separation among the analyzed samples. Variables with higher absolute loading values are considered more influential in distinguishing between sample groups.

Name	Comp 1	Comp 2	Comp 3	Comp 4	Comp 5	Comp 6	Comp 7	Comp 8
9-HpODE	0.022644	0.048738	-0.02813	0.023839	-0.01022	0.009372	-0.00277	-0.00131
Malic acid	0.13711	0.11535	0.081724	-0.05928	0.012797	-0.01405	0.022895	0.030958
(15Z)-9,12,13-Trihydroxy-15-octadecenoic acid	0.031255	0.010852	0.1152	-0.04849	0.22282	-0.01269	0.2335	0.027036
(1S)-1,5-Anhydro-2-O-(6-deoxy- α -L-mannopyranosyl)-1-[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-6-yl]-D-glucitol	0.036471	-0.12289	0.030614	-0.01824	0.025309	-0.00667	0.010078	-0.01299
(1 ξ)-1,5-Anhydro-1-[(2R,3R)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro-2H-chromen-6-yl]-D-glucitol	-0.09812	-0.00147	-0.07354	0.054704	-0.0129	0.004424	-0.00916	-0.01598
1-(4-Amino-4-carboxybutanoyl)-2-piperidinecarboxylic acid	0.042669	0.000205	-0.37289	-0.04751	0.50213	-0.51022	-0.28222	0.58644
1-(5,8-Dimethoxy-2,2-dimethyl-2H-chromen-6-yl)ethanone	0.19446	0.12214	0.27561	-0.21883	0.069518	-0.0034	0.03467	0.005219
1,3,6-Trigalloyl glucose	0.063649	-0.03932	-0.1042	0.099806	-0.02192	0.010249	-0.00134	0.004985
1,6-Bis-O-(3,4,5-trihydroxybenzoyl)hexopyranose	0.057847	-0.07603	-0.05576	0.053886	-0.00071	0.001867	0.004532	0.01085
1-[(3-Carboxypropyl)amino]-1-deoxy-beta-D-fructofuranose	0.086963	-0.16656	0.075359	-0.04967	0.023871	-0.00208	-0.00084	-0.02806
13(S)-HpOTrE	0.021607	0.008125	-0.11579	0.10147	-0.03792	0.013018	-0.01062	0.000711
13-HOTrE	0.036399	0.079983	0.053625	-0.0396	0.016098	0.005761	0.010667	0.001633
1-Oxo-1,2,4-butanetricarboxylic acid	-0.03579	0.059185	-0.05252	0.047604	-0.01912	0.021064	0.000903	0.020462
1-Vinyl-2-pyrrolidone	-0.07437	-0.07747	-0.09129	0.071781	-0.02582	0.0005	-0.01191	-0.00189
2-(2-phenylethoxy)-6-[[[(3,4,5-trihydroxyoxan-2-yl)oxy]methyl]oxane-3,4,5-triol	-0.0685	0.015342	-0.05807	0.04017	-0.02068	0.006826	-0.00997	-0.00417
2-(acetylamino)-3-(1H-indol-3-yl)propanoic acid	-0.03121	0.12495	0.097581	-0.09346	-0.0024	-0.00057	0.003697	-0.00899
2,4-Dihydroxybenzoic acid	0.00246	-0.02758	-0.12035	0.10482	-0.03618	0.005454	-0.00605	0.017363
2,5-Furandicarboxylic acid	0.018241	0.045349	-0.08503	0.064673	-0.02211	0.010543	0.026869	0.041382
2,6-Diamino-4-hexenoic acid	-0.08498	-0.06525	-0.10153	0.010841	0.045083	-0.04914	0.082495	0.12891
2-[1-(2H-1,3-benzodioxol-5-yl)propan-2-yl]-6-methoxy-4-(prop-2-en-1-yl)phenol	0.17429	0.10944	0.21037	-0.14339	0.064762	-0.01742	0.067168	0.03291
2-Coumaroylquinic acid	-0.07505	0.027693	0.047286	-0.04763	0.008934	-0.00216	0.007701	0.002106
2'-deoxymugineic acid	-0.02377	-0.08805	-0.20918	0.19485	-0.1002	0.016163	0.078677	-0.02186
2-Deoxypentose	-0.02674	0.035667	-0.06607	0.048132	-0.01648	0.009943	-0.00393	-0.007
2-monolinolenin	0.04359	0.006561	0.23903	-0.20581	0.069377	-0.00454	0.006594	0.014504
3-(Sulfooxy)butanoic acid	-0.0167	0.1067	-0.04685	0.033564	-0.03359	0.016334	0.000305	0.011556
3,4,5-trihydroxycyclohex-1-ene-1-carboxylic acid	-0.0305	0.026815	-0.06702	0.054283	-0.01705	0.002254	-0.01334	0.005439
3,4-Dihydroxybenzaldehyde	0.097326	-0.06903	0.07324	-0.08768	0.019069	0.043938	-0.06638	0.023292
3,5-Dihydroxy-4-(sulfooxy)benzoic acid	-0.04614	0.037055	0.10342	-0.09307	0.03546	0.002014	0.004502	-0.01519
3,6-Dideoxy-6-sulfohex-2-ulosonic acid	0.0017	0.1259	-0.03277	0.015402	-0.019	0.025927	-0.02287	-0.0267
3-Amino-2-azepanone	-0.07643	-0.02463	-0.01406	0.006284	-0.00487	-0.00172	-0.01263	0.007737
3-Coumaric acid	-0.02617	0.10461	0.044154	-0.04029	-0.00997	-0.00752	0.018636	0.007844
3-Hydroxy-4-methoxy-5-(sulfooxy)benzoic acid	0.093927	0.022277	0.099917	-0.07585	0.037009	-0.00217	0.014992	0.00797
3-Hydroxy-N-(2-oxotetrahydro-3-furanyl)butanamide	-0.05947	-0.01096	0.069801	-0.06584	0.010363	-0.00747	3.7062e-05	-0.00147
3-Isopropylmalic acid	-0.06811	0.14141	0.019036	-0.0305	-0.01041	0.004725	0.006933	-0.01182
3-Methylxanthine	-0.03611	-0.04969	0.070131	-0.05899	0.014704	-0.00663	0.003278	-0.00216
3-sulfolactic acid	0.048251	-0.01872	-0.01176	0.016483	-0.00052	0.015495	-0.00194	-0.01111
3-sulfopropanediol	-0.02576	0.031504	-0.11005	0.091735	-0.0223	0.017629	-0.00068	-0.00084
4,5-Dihydroxy-3-oxo-1-	-0.00566	0.012983	-0.17509	0.14988	-0.05117	0.014584	-0.0286	0.013405

cyclohexene-1-carboxylic acid								
4-acetamidobutyrate	-0.02933	-0.10555	0.064974	-0.05362	0.027642	-0.0127	-0.00126	-0.01831
4-Coumaric acid	-0.06002	-0.06617	0.022892	-0.02403	0.015297	-0.00115	0.004578	-0.00864
4-Hydroxy-8-(beta-D-talopyranosyloxy)-2-quinolinecarboxylic acid	0.073647	-0.00384	-0.11673	0.11127	-0.02628	0.015786	-0.00054	-0.00233
4-Hydroxybenzaldehyde	-0.07011	0.033127	0.079768	-0.07672	0.011775	-0.00132	0.002384	-0.00361
4-Hydroxybenzoic acid	-0.00159	0.013319	-0.09917	0.087116	-0.03194	0.001427	0.002552	0.00779
4-Methyleneglutamic acid	0.099275	0.082801	-0.00448	0.006435	-0.02317	-0.00603	-0.02562	0.025092
4-METHYLBELLIFERYL- α -D-GLUCOSE	-0.06326	0.037435	0.015981	-0.02034	-0.00363	-0.00531	0.001757	0.015362
4-Oxoproline	-0.01698	-0.07543	0.039841	-0.03584	0.014996	-0.00944	0.001898	-0.00694
4-p-Coumaroylquinic acid	-0.06676	0.073305	0.087708	0.036171	0.12202	0.021479	-0.24391	0.060981
5-(2-Carboxyethyl)-2-hydroxyphenyl beta-D-glucopyranosiduronic acid	0.11069	-0.00733	-0.08515	0.081249	-0.0128	0.008918	-0.00042	-0.01081
5,7-Dihydroxy-2-(4-hydroxyphenyl)-6,8-bis[3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl]-4H-chromen-4-one	0.036792	0.063608	0.022198	-0.01039	-0.00044	0.016529	-0.0162	-0.01649
5-[5-(methoxycarbonyl)-5,8a-dimethyl-2-methylidene-decahydronaphthalen-1-yl]-3-methylpentanoic acid	0.076423	0.064689	-0.1068	0.097419	-0.02796	0.010044	0.00705	-0.00366
5-Hydroxy-2-furoic acid	0.017259	0.048308	-0.07795	0.063831	-0.01855	0.008209	0.017834	0.031495
5-hydroxy-4-methoxy-5,6-dihydro-2H-pyran-2-one	-0.01836	-0.16773	-0.04177	0.043111	-0.00333	-0.08404	0.02939	-0.04065
7-Hydroxycoumarine	0.04603	-0.08237	0.062994	-0.04646	0.026663	-0.01324	0.005859	0.003225
8-hydroxy-deoxyguanosine	-0.0235	-0.05239	-0.00038	0.000281	-0.01142	-0.01198	-0.00089	-0.00405
Acetophenone	-0.0712	0.076487	0.069762	-0.07387	0.009712	-0.0108	0.015276	0.034698
Adenine	0.037221	-0.01833	-0.13334	0.017242	-0.09417	-0.11233	-0.06389	0.090451
Adenosine	-0.02014	-0.07321	0.21703	-0.17999	0.062432	-0.03435	0.02373	-0.01143
Adenosine 3'5'-cyclic monophosphate	-0.05255	-0.13795	0.002242	-0.00644	0.013806	-0.0057	-0.02003	-0.03375
Adenosine 5'-monophosphate	-0.00492	-0.00565	0.12909	-0.11242	0.029088	-0.01408	0.006644	-0.00573
Azefelin	0.048739	0.1768	0.04803	-0.04405	-0.03781	-0.02834	0.033717	0.018823
alpha-D-Xylopyranosyl-(1->6)-beta-D-glucopyranosyl-(1->4)-beta-D-glucopyranose	0.13133	-0.05517	-0.07393	0.078252	-0.0013	0.010337	-0.00087	-0.00149
alpha-Ketoglutaric acid	0.020445	0.039292	-0.08415	0.067694	-0.03454	-0.01294	0.031873	0.03541
Asparagine	-0.03939	0.093526	-0.51474	-0.02995	0.84821	-0.01226	0.000839	-0.34806
Astragalin	0.080433	0.037512	0.020845	-0.00085	0.027191	-0.02573	0.031387	-0.01701
Astringin	0.033512	-0.02011	-0.1826	0.15152	-0.04231	0.006512	-0.02214	0.010788
Benzoic acid	0.094113	-0.07728	0.058331	-0.03999	0.033721	-0.00032	0.011336	0.010661
Betaine	-0.02755	-0.0433	0.002601	0.006224	0.003585	-0.01529	-0.00461	-0.02912
Caffeine	-0.04266	0.020379	-0.00461	-0.01079	0.01142	-0.02772	-0.01533	0.017835
Catechin	0.10654	-0.05715	0.16173	-0.12338	0.067637	-0.01665	0.017034	0.009493
Catechin Gallate	0.076638	-0.03641	0.12676	-0.04767	0.002793	-0.05087	-0.02982	-0.28166
Chlorogenic acid	0.056102	-0.06806	0.096798	-0.07366	0.025625	-0.01526	0.010989	0.001065
Choline	0.031552	-0.03459	0.050352	-0.03353	0.030159	-0.00034	0.010607	-0.00114
Citric acid	0.008597	0.049649	-0.06458	0.058216	-0.02044	0.008039	0.001826	-0.00959
L-coprine	0.003574	0.063658	-0.04313	0.022873	-0.01146	0.0298	-0.00106	0.089411
Corchorifatty acid F	0.046719	0.061384	-0.05759	0.057272	-0.02592	-0.00899	-0.02969	0.044481
corilagin	0.10468	-0.01964	0.023654	-0.00997	0.008852	-0.00254	0.012348	0.008105
Corymboside	0.11501	0.033772	-0.02407	0.02924	-0.00765	0.00961	-0.00144	0.008983
Coumarin	-0.05641	0.047623	0.024162	-0.03	0.000755	-0.00068	0.004318	-0.01054
Cyanidin	-0.01785	-0.00371	0.052538	-0.06266	0.054034	-0.02705	-0.02366	0.012765
Cytosine	-0.05614	-0.01025	0.065981	-0.06719	0.028277	0.008304	0.01006	-0.01828
D-(-)-Quinic acid	0.042355	-0.01611	0.003403	-0.00053	0.003518	-0.00648	0.006706	-0.01895
D-(-)-Glutamine	-0.05453	0.046044	-0.06751	0.051282	-0.01538	-0.00123	-0.00402	0.006605
dihomomethionine	-0.11408	-0.04059	-0.14252	0.11031	-0.04378	0.004296	-0.01602	-0.0036
DL-2,6-Diaminopimelic acid	-0.05184	-0.06331	-0.07841	0.062258	-0.0216	-0.0062	-0.00928	0.007332
DL-Arginine	-0.09915	-0.00939	0.033482	-0.03237	0.020868	-0.00755	-0.00831	0.002405
D-PANTOTHENIC ACID	0.008091	0.034987	-0.10414	0.087822	-0.02918	0.010904	-0.01193	0.016535
D-(+)-Pyroglutamic Acid	-0.05034	0.029562	-0.08565	0.073409	-0.02785	0.006181	-0.01708	-0.0357
D-Sucrose	0.10454	-0.06513	-0.0825	0.081572	0.003288	0.018987	-0.00258	0.015309
Ellagic acid	-0.06692	0.052644	0.12268	-0.11406	0.023133	-0.00764	0.012692	-0.00015
Epicatechin	0.10997	-0.06598	0.16232	-0.12139	0.041379	-0.00256	0.015837	-0.01678
EPIGALLOCATECHIN 3-O-(3-O-METHYL)GALLATE	0.19149	-0.03766	-0.05225	0.006075	0.14235	-0.18413	-0.15429	-0.09119
Epigallocatechin gallate	0.079404	-0.09762	0.079792	-0.04495	0.039729	-0.02562	0.033169	-0.00555

Esculetin	0.04716	0.055909	0.14175	-0.11552	0.040734	-0.0116	0.008539	0.001602
Frovatriptan	0.12874	0.074574	-0.17321	0.15818	-0.04972	0.021159	-0.01279	0.006729
Fructoselysine	0.035163	-0.09807	0.08195	-0.06434	0.036081	-0.01153	0.000977	-0.00872
Fukiic acid	0.045379	-0.05482	0.003351	-0.00335	0.033583	-0.01111	-0.01161	0.027769
Fumaric acid	0.080626	-0.07966	-0.14128	-0.08546	-0.43109	0.74118	-0.65017	0.19033
Galactonic acid	0.071389	-0.05826	-0.04864	0.054524	-0.00838	0.006047	-0.00517	0.004675
Gallic acid	-8.50E-06	-0.04876	0.14501	-0.11842	0.045133	-0.01593	0.014788	-0.01161
Gallocatechin	0.11302	-0.05949	0.14577	-0.119	0.050591	-0.02661	-0.00043	-0.0167
gamma-Aminobutyric acid	0.010322	-0.10914	0.038383	-0.02981	0.033565	-0.00945	0.002464	0.023665
gamma-glutamyltyramine	-0.11512	0.053749	0.092156	-0.09256	0.017134	-0.00818	0.005379	0.007981
Glucogallin	-0.03303	0.028461	-0.03878	0.036144	-0.02337	0.005589	-0.01054	0.006191
Glu-Glu	-0.05755	-0.05402	0.080341	-0.06625	0.023018	-0.02037	0.005692	-0.01446
L-Glutamic acid	-0.04223	0.027002	-0.08915	0.073469	-0.02553	0.000954	-0.00015	-0.00759
Guanine	-0.02345	-0.05113	0.009149	-0.00192	-0.01176	-0.01176	0.002026	5.0953e-05
Guanosine monophosphate (GMP)	-0.01235	-0.09085	0.047622	-0.03774	0.028295	-0.00831	-0.00932	-0.01059
Heptylbenzene	0.095798	0.024942	-0.11657	0.11117	-0.03156	0.022507	0.002225	-0.00617
Hex-2-ulose	0.02965	-0.00806	0.16018	0.079387	-0.09709	-0.01903	0.31307	-0.40468
Hexaric acid	0.051108	-0.01271	-0.10297	0.095133	-0.02761	0.016513	-0.01073	0.013218
DL-Histidine	-0.08949	0.06936	-0.02463	0.004802	-0.01186	-0.0018	-0.00603	0.002685
Isocitric acid	0.001262	0.029759	-0.1542	0.13025	-0.04675	0.017563	-0.02131	0.001151
Isoleucine	-0.09086	0.051641	0.00057	-0.00986	-0.01488	-0.00019	-0.00187	-0.00421
isopropylmalic acid	0.013856	-0.07148	-0.12272	0.10926	-0.02495	0.009447	-0.01675	-3.73E-05
Juglalin	0.10557	0.019441	-0.07237	0.085952	-0.01627	0.028387	0.033581	0.062791
Kaempferol	0.066472	0.036041	-0.0278	0.027366	-0.00685	0.004454	-0.00338	0.01563
Kaempferol-3-O-(6'''-trans-P-coumaroyl-2''-glucosyl)rhamnoside	-0.00086	-0.02983	-0.14283	0.12354	-0.03069	0.012097	-0.01605	-0.02357
Kynurenic acid	0.019816	0.039801	-0.06466	0.048833	-0.02735	0.009449	-0.01379	0.004098
Lamiide	0.084129	0.015363	-0.12906	0.1175	-0.02049	0.023778	0.000442	-0.0073
Leucine	-0.08944	0.044809	-0.00516	-0.00677	-0.01083	-0.00571	-0.0052	-0.00584
Leucylproline	-0.00595	-0.10516	-0.0389	0.028224	0.014381	-0.0098	-0.00214	0.000591
DL-Glutamine	0.097417	0.026708	-0.08021	0.071574	-0.01636	0.009174	0.006218	0.017347
L-Pyroglutamic acid	-0.01596	-0.07186	0.033525	-0.02872	0.01483	-0.00998	9.2481e-05	0.004646
Luteolin	-0.01635	0.006412	0.10725	-0.08731	0.066071	-0.02496	0.022522	-0.01809
DL-Lysine	-0.05276	0.072057	0.011348	0.08624	0.20365	-0.56866	0.3046	-0.21168
Maleamic acid	-0.14489	0.048652	0.052465	-0.03493	0.039936	0.039184	-0.00369	-0.03496
Metharbital	0.044387	-0.19902	0.002213	0.022736	0.041685	-0.01915	0.004571	-0.03297
Methyl cinnamate	-0.08605	-0.01154	-0.01317	0.001588	-0.01554	-0.00574	0.006475	-0.0051
Methyl gallate	0.14774	-0.00796	-0.06721	0.057091	-0.00443	-0.01871	-0.02773	-0.01871
MFC00135810	0.10154	-0.11437	0.022518	0.000894	0.033122	-0.01035	0.009187	-0.01301
Miglitol	0.088278	-0.15359	-0.07519	0.032595	0.07478	-0.06048	-0.0311	0.0779
muramic acid	0.08096	-0.11779	0.061802	-0.01731	0.035473	-0.0105	-0.00153	0.023495
Myricetin	0.1381	-0.03545	-0.00299	0.018465	0.010102	0.007173	0.006164	0.006222
myricetin 3-O-beta-D-galactopyranoside	0.13846	-0.03685	-0.00724	0.020344	0.009162	0.005355	0.005411	0.005614
N-(3-Carboxypropanoyl)-5-hydroxynorvaline	0.089237	-0.1206	0.03911	-0.01266	-0.02097	-0.11567	-0.00754	-0.13465
N-acetyl-L-2-amino adipic acid	0.00294	0.017985	0.044088	-0.05434	-0.02154	-0.02259	-0.01935	-0.04721
N-Acetylneuraminic acid	0.061939	-0.12913	-0.03275	0.037863	0.006155	-0.00313	-0.01511	-0.00589
N-Acetylorithine	-0.04813	0.050292	-0.01491	0.006148	-0.00179	0.003751	0.0112	0.002949
Naringenin	0.080753	-0.04025	0.056396	-0.04953	-0.09039	0.018022	0.038072	0.067817
N-Benzylformamide	-0.07021	0.033019	0.084952	-0.07542	0.013277	-0.00549	0.00572	0.004877
Neochlorogenic acid	0.038316	-0.08781	0.053394	-0.03631	0.009138	0.01205	0.020371	-0.00553
N-Glycosyl-L-asparagine	-0.05689	-0.05403	0.07749	-0.07021	0.019006	-0.01444	-0.00119	-0.00737
Niacin	-0.0276	-0.05813	-0.05371	0.051071	-0.02058	-0.00495	-0.00403	0.02374
nicotianamine	-0.07454	-0.00418	-0.05362	0.038947	-0.01924	0.005317	-0.00231	0.00774
Nicotinamide	0.031276	-0.02369	0.076633	-0.05952	0.006158	-0.00552	0.000851	-0.02775
Nicotinic acid	-0.03769	0.004305	-0.08363	0.069245	-0.01281	0.010597	-0.01704	0.00175
Nipecotinic acid	-0.09181	0.044669	0.007812	-0.0185	-0.01007	0.000612	-0.00782	-0.01592
Nor Leucine	-0.0414	0.053628	0.087262	-0.07789	0.01613	-0.00441	-0.00635	-0.01186
NP-000358	0.11967	-0.0554	0.16278	-0.12399	0.055568	-0.01144	0.017243	0.007209
NP-000587	-0.06603	-0.06938	0.007808	-0.01077	0.005948	-0.00523	0.00146	-0.00911
NP-001346	-0.09343	-0.06804	-0.00469	-0.00117	0.00199	-0.00546	-0.00427	-0.00549
NP-003191	0.051614	0.048448	-0.0545	0.054527	-0.0235	0.001464	-0.0072	0.022925
NP-020139	0.025246	0.001767	-0.16252	0.13997	-0.03759	0.022561	-0.00524	-0.01317
NP-020760	0.038139	0.044234	-0.14512	0.12667	-0.03082	0.022594	-0.02026	0.004348
N-Succinyl-L-diaminopimelic	-0.01281	-0.08822	-0.05872	0.04785	-0.00811	0.000764	-0.02183	-0.00891

acid								
N-Vinyl-2-pyrrolidone	-0.04909	-0.11382	-0.19395	0.16686	-0.03502	0.01653	-0.01759	-0.02208
Oxypinnatanine	-0.04038	-0.01034	0.056848	-0.05373	0.013079	-0.00221	0.009885	-0.00526
Patuletin	-0.11582	-0.04313	0.31382	0.097841	0.10527	-0.01934	-0.09775	0.18912
L-Phenylalanine	-0.07494	0.04789	0.030936	-0.03658	-0.00299	-0.00102	-0.0002	-0.01193
Phloionolic acid	0.068372	0.033233	0.12157	-0.10438	0.02922	0.001608	0.024731	-0.00526
Pipecolic acid	-0.0707	-0.0778	-0.08689	0.066846	-0.02088	0.006038	-0.01532	0.002175
Pirbuterol	-0.11899	-0.2382	0.10335	-0.10115	0.067691	0.048027	0.011192	0.07491
Procyanidin A2	-0.03038	0.055517	-0.0762	0.084356	-0.11042	0.057306	0.11545	0.19791
Procyanidin B2	0.091215	-0.05174	0.070266	-0.05039	0.040786	-0.0167	-0.00458	-0.01032
Prodelphinidin B1	0.041534	-0.09816	0.090317	-0.07266	0.042611	-0.00897	-0.00217	-0.00612
Proline	0.024085	0.086865	0.041923	-0.03202	-0.00083	0.00339	0.001616	-0.00109
Quercetin	0.052004	-0.11134	0.025425	0.000862	0.039787	-0.02869	0.030815	-0.00488
QUERCETIN 3,7-DIGLUCOSIDE	0.087983	0.036846	-0.00263	0.008005	0.016198	0.019461	0.00101	0.001591
Quercetin 3-O-caffeyl-glucoside	0.075262	0.053083	-0.25013	0.072655	-0.03003	-0.03071	0.021875	0.026123
Quercetin-3-O-β-pentoside	0.092106	0.058678	-0.05961	0.063697	-0.02462	0.011168	0.002707	0.009321
Quercetin-3β-D-glucoside	0.060581	0.043629	-0.0106	0.013902	-0.00405	-0.00055	-0.00115	0.025613
Robinin	-0.01041	-0.09215	-0.15675	0.13472	-0.03675	0.003707	-0.01579	-0.00086
Rutin	0.066655	0.07091	-0.02404	0.028105	-0.01346	0.010374	-0.00016	0.009231
saccharopine	0.072867	-0.12097	0.001841	0.01303	0.025018	-0.00732	0.01493	-0.00377
D-Serine	-0.01571	0.020487	-0.11202	0.092533	-0.04199	0.010037	-0.00106	0.013481
Spermidine	0.027844	-0.06921	-0.09736	0.081758	-0.01534	0.016674	-0.00933	0.011856
Spermine	-0.11927	-0.0547	0.030142	-0.04561	0.019687	0.005898	-0.00944	-0.03042
DL-Stachydrine	-0.06975	-0.07213	-0.08687	0.06859	-0.02028	0.001566	-0.01092	-0.00234
Suberic acid	-0.08665	0.077052	0.005063	-0.01833	0.001621	0.012059	-0.00262	-0.00965
Succinic acid	0.056566	-0.00367	0.003191	-0.00274	0.010896	-0.00606	0.002347	0.008094
Syringetin	0.10161	-0.05304	0.077216	-0.05495	0.032556	-0.00808	0.00908	-0.02065
Theaflavin-3-gallate	-0.01673	0.083123	0.059488	-0.03664	0.10999	0.23677	-0.38991	0.025739
Theobromine	-0.06654	-0.01629	0.076689	-0.06743	0.016145	-0.01597	0.011972	0.008353
Theogallin	0.048146	-0.06627	0.0592	-0.04116	0.026518	-0.00924	0.003371	-0.00762
Theophylline	0.038116	-0.01076	-0.15981	-0.04846	-0.04504	-0.11716	0.17379	0.03522
Threonine	-0.05766	0.04562	0.001844	-0.00716	-0.00807	0.000562	-0.00687	-0.01271
Tiliroside	0.069665	0.10132	-0.01753	0.036434	-0.00387	-0.0568	0.025469	-0.09592
trans-3-Indoleacrylic acid	-0.07395	0.064047	-0.01126	-0.0034	-0.01312	0.002025	-0.00199	0.00391
Traumatic Acid	0.087576	-0.02499	0.051493	-0.0358	0.027205	-0.0095	0.009744	0.003703
Tricin	-0.03655	0.060203	0.38813	0.049859	0.18897	-0.05388	-0.68963	0.43657
Trifolin	0.072112	0.043671	-0.02403	0.026274	-0.00756	0.005134	0.000244	0.015076
Tryptophan	-0.09391	0.0616	-0.00897	-0.00306	-0.00702	-0.0035	-0.00953	-0.00484
Tyrosine	-0.06897	0.03389	0.075883	-0.06812	0.009687	-0.00447	0.002978	0.008992
tyr-thr	0.014379	-0.20547	0.046304	-0.01198	0.12592	-0.03837	0.038375	0.050663
Uracil	0.032703	-0.06476	0.037122	-0.02723	0.03881	-0.01167	0.020782	0.033379
Uridine 5'-diphosphogalactose	-0.03829	-0.02794	-0.18084	0.14555	-0.03857	0.012501	-0.0163	0.000832
Uridine monophosphate (UMP)	0.033028	-0.0137	0.10987	-0.10554	0.039466	-0.00345	0.0098	-0.03421
Valine	0.008038	-0.06503	0.039927	-0.06795	0.08026	-0.05086	-0.01153	0.063321
Vanillyl mandelic acid	-0.01957	-0.01101	-0.13367	0.11795	-0.04115	0.010747	0.00402	-0.01673
Vitexin	-0.01169	0.061157	0.082433	-0.07628	0.009734	-0.00052	0.006033	0.005673
Xanthine	-0.07982	0.033931	0.077133	-0.0776	0.011728	-0.00074	0.002658	-0.00784
Xanthosine	-0.08443	0.024058	0.083862	-0.07757	0.012745	-0.00904	0.011486	-0.00809
ZINGEROL	0.034778	0.059999	-0.09335	0.081798	-0.0299	0.008037	-0.00076	0.002769
α,α-Trehalose	0.12066	-0.03023	-0.07826	0.0869	-0.02943	0.022113	-0.0152	0.013574