

Table S1 Standard information

CAS	Compounds	Brand
63-91-2	L-phenylalanine	TRC
327-97-9	Chlorogenic acid	zzstandard®
480-41-1	Naringenin	zzstandard®
529-55-5	Prunin	ES
552-58-9	Eriodictyol	zzstandard®
520-18-3	Kaempferol	zzstandard®
154-23-4	C	ES
490-46-0	EC	zzstandard®
3371-27-5	GC	zzstandard®
970-74-1	EGC	zzstandard®
1257-08-5	ECG	zzstandard®
989-51-5	EGCG	zzstandard®
149-91-7	GA	zzstandard®
38953-85-4	Isovitexin	zzstandard®
5373-11-5	Cynaroside	zzstandard®
520-32-1	Tricin	zzstandard®
482-39-3	Kaempferin	zzstandard®
18609-17-1	Baimaside	zzstandard®
572-30-5	Avicularin	zzstandard®
23567-23-9	Procyanidin B3	zzstandard®
N/A	Procyanidin B4	zzstandard®
21293-29-8	Abscisic acid	zzstandard®
69-89-6	Xanthine	TRC
552-62-5	7-Methylxanthine	TRC

58-08-2	Caffeine	TRC
58-55-9	Theophylline	zzstandard®
56-86-0	L-Glutamic Acid	TRC
56-41-7	L-Alanine	TRC
3081-61-6	L-Theanine	zzstandard®
73-24-5	Adenine	TRC
73-40-5	Guanine	TRC
65-71-4	Thymine	TRC
147-85-3	L-Proline	TRC
56-45-1	L-Serine	TRC
56-84-8	L-Aspartic acid	TRC
56-87-1	L-Lysine	TRC
74-79-3	L-Arginine	TRC
672-15-1	L-Homoserine	TRC
60-18-4	L-Tyrosine	TRC
73-32-5	L-Isoleucine	TRC
73-22-3	L-Tryptophan	TRC
17365-11-6	Theogallin	zzstandard®
87-99-0	Xylitol	zzstandard®
60-82-2	Phloretin	zzstandard®
906-33-2	Neochlorogenic acid	zzstandard®
501-52-0	Hydrocinnamic acid	zzstandard®
107-43-7	Betaine	zzstandard®
57-48-7	D-Fructose	zzstandard®
99-20-7	D-Trehalose	zzstandard®
526-95-4	D-Gluconic Acid (50% in Water)	TRC

6556-12-3	D(+)-Glucuronic Acid	WAKO
599-54-2	Vitamin B (Pantothenic acid calcium salt hydrate)	IsoReag®
531-75-9	Esculin	zzstandard®
110-15-6	Succinic acid	zzstandard®
617-48-1	Malic Acid	IsoReag®
77-92-9	Anhydrous citric acid	zzstandard®

Table S2 Primers for qRT-PCR

Gene name	Forward primer(5'-3')	Reverse primer(5'-3')
TEA034012	CCCGCAAAAAGATGACGTTG	GGCTGCGGACATGTAGTTT
TEA022960	TGCATTAATGACATGATAAAACCAG	CTTCGGCAAACCTCCAAGCA
TEA009266	GGCAATCCAAGGAGTGCTTA	ACTCGACATCTGACCAGTGA
TEA015769	TGGCTAACAATGCTTGTGGT	GAGGAGCTCTTCTTTGCCTC
TEA032730	CACCAAGCCTAATCACTGCT	CTATCCCCTTAAACTCGGGC
TEA023790	TTTCTACCCGAAATGCCAC	TGGAGTTCACTACTGCCTGA
TEA006847	ACTCTCTCTCCCTCGAATGG	GGACCATACGCAACCCTAAG
TEA006643	AACAGCAAGGCTATCGAAGG	CACCGTGATCTGTGATGAGG
novel.5740	GAGCTTCTCTCAGAGGGACTA	CCAAACTTGAAGACCGGGAA

Table S3 Genes of flavonoid

Name	Number	Sp01_FPKM	Su01_FPKM	Au01_FPKM
4CL	TEA034012	160.20	244.13	255.01
	TEA033429	5.17	9.88	9.27
	TEA005753	2.76	3.90	0.80
	novel.7909	0.42	0.89	1.38
ANR	TEA022960	660.96	719.29	452.11
	TEA009266	314.66	177.89	230.90
ANS	TEA015769	9.83	14.35	3.66
	TEA015762	1.22	5.69	2.97
C4H	TEA014864	186.09	353.83	316.85
	TEA034001	164.06	205.71	196.08
CHI	TEA033031	471.94	666.91	598.33
CHS	TEA023340	1053.62	1633.95	1589.13
	TEA023333	411.79	474.55	393.70
	TEA023331	55.69	69.67	67.75
	TEA018665	4.89	7.16	7.86
DFR	TEA032730	251.88	201.67	184.16
F3'5'H	TEA013315	550.94	561.09	619.06
F3H	TEA023790	652.43	666.37	627.57
	novel.10606	4.68	7.58	6.91
	TEA021203	1.11	1.33	1.39
F3'H	TEA006847	170.09	330.95	260.69
FLS	TEA006643	1007.35	1192.29	1021.64
	novel.5740	11.33	11.31	10.93
LAR	TEA027582	1098.74	1187.17	1077.69

PAL	TEA023243	270.91	398.71	430.77
	TEA024587	135.20	147.51	153.01
	TEA034008	56.71	68.31	60.27
	TEA014056	22.12	68.55	62.13

Table S4 Levels of catechins

Name	GC	EGC	C	EC	EGCG	GCG	ECG	CQI
Sp01a	0.06%	2.28%	0.46%	0.83%	8.97%	0.08%	1.82%	474
Sp01b	0.06%	2.06%	0.51%	0.70%	9.23%	0.08%	1.88%	558
Sp01c	0.06%	1.94%	0.48%	0.63%	8.93%	0.08%	1.86%	572
Sp02a	0.06%	1.81%	0.47%	0.54%	9.02%	0.08%	1.91%	612
Sp02b	0.08%	1.64%	0.66%	0.55%	8.25%	0.08%	1.94%	656
Sp02c	0.15%	1.33%	0.91%	0.56%	7.82%	0.09%	2.03%	789
Sp03a	0.22%	1.02%	1.14%	0.56%	7.08%	0.08%	2.07%	898
Sp03b	0.20%	0.90%	0.95%	0.45%	6.76%	0.07%	1.86%	969
Sp03c	0.13%	0.80%	0.76%	0.32%	6.48%	0.07%	1.67%	1041
Sp04a	0.06%	0.71%	0.61%	0.19%	6.53%	0.06%	1.54%	1137
Sp04b	0.10%	1.07%	0.61%	0.38%	7.58%	0.09%	2.06%	1008
Sp04c	0.10%	1.53%	0.62%	0.59%	8.69%	0.11%	2.55%	829
Sp05a	0.18%	1.99%	0.57%	0.82%	9.53%	0.14%	2.97%	630
Sp05b	0.14%	1.93%	0.51%	0.80%	9.96%	0.12%	2.64%	662
Sp05c	0.14%	1.77%	0.43%	0.74%	10.36%	0.10%	2.27%	726
Sp06a	0.06%	1.56%	0.39%	0.64%	10.75%	0.07%	1.97%	818
Sp06b	0.06%	1.67%	0.64%	0.66%	11.04%	0.07%	2.14%	798
Sp06c	0.06%	1.52%	0.87%	0.62%	10.64%	0.13%	2.32%	884
Sp07a	0.08%	1.59%	1.08%	0.65%	10.82%	0.14%	2.38%	860
Sp07b	0.08%	1.50%	1.30%	0.47%	9.94%	0.28%	2.18%	836
Sp07c	0.10%	1.62%	1.45%	0.38%	9.35%	0.33%	1.95%	696
Sp08a	1.38%	1.56%	1.58%	0.21%	8.13%	0.45%	1.73%	629
Sp08b	1.38%	1.40%	1.28%	0.23%	8.01%	0.46%	1.58%	697
Sp08c	3.98%	1.33%	1.12%	0.27%	8.50%	0.54%	1.58%	774

Sp09a	2.71%	1.18%	0.95%	0.29%	8.92%	0.61%	1.58%	892
Sp09b	2.84%	1.18%	0.95%	0.38%	9.96%	0.46%	2.24%	1038
Sp09c	0.29%	1.16%	0.93%	0.45%	11.03%	0.27%	2.90%	1195
Sp10a	0.35%	1.15%	0.93%	0.52%	11.82%	0.38%	3.44%	1330
Sp10b	0.22%	1.83%	0.70%	0.37%	11.39%	0.39%	3.02%	1030
Sp10c	0.15%	2.56%	0.44%	0.24%	10.56%	0.41%	2.51%	704
Su01a	0.06%	3.18%	0.20%	0.12%	10.25%	0.16%	2.15%	391
Su01b	0.06%	2.78%	0.24%	0.11%	10.07%	0.14%	2.07%	458
Su01c	0.06%	2.38%	0.25%	0.11%	10.94%	0.15%	2.23%	570
Su02a	0.06%	2.07%	0.32%	0.12%	11.16%	0.14%	2.27%	649
Su02b	0.06%	1.92%	0.32%	0.12%	11.44%	0.12%	2.59%	743
Su02c	0.06%	1.74%	0.36%	0.10%	10.90%	0.17%	2.78%	795
Su03a	0.06%	1.66%	0.32%	0.08%	10.58%	0.22%	2.85%	814
Su03b	0.06%	1.70%	0.29%	0.06%	10.94%	0.22%	2.67%	800
Su03c	0.06%	1.61%	0.27%	0.06%	11.12%	0.14%	2.47%	856
Su04a	0.06%	1.58%	0.27%	0.04%	11.76%	0.17%	2.41%	903
Su04b	0.06%	2.07%	0.31%	0.09%	11.68%	0.17%	2.76%	783
Su04c	0.06%	2.61%	0.36%	0.13%	11.80%	0.16%	3.16%	618
Su05a	0.06%	3.29%	0.40%	0.70%	11.49%	0.06%	3.45%	460
Su05b	0.06%	2.80%	0.35%	0.89%	11.09%	0.10%	3.18%	558
Su05c	0.06%	2.42%	0.29%	0.97%	10.65%	0.12%	2.76%	619
Su06a	0.06%	1.84%	0.25%	0.41%	10.41%	0.11%	2.48%	703
Su06b	0.06%	1.73%	0.65%	0.35%	9.92%	0.10%	2.29%	716
Su06c	0.06%	1.64%	1.06%	0.43%	9.09%	0.08%	2.11%	693
Su07a	0.06%	1.54%	1.50%	0.42%	8.53%	0.09%	2.00%	689
Su07b	0.06%	1.77%	1.38%	0.41%	8.61%	0.12%	1.97%	602

Su07c	0.06%	1.87%	1.15%	0.34%	9.14%	0.17%	1.96%	595
Su08a	0.06%	2.03%	0.85%	0.51%	9.23%	0.34%	1.84%	550
Su08b	2.09%	2.01%	0.91%	0.51%	9.59%	0.63%	1.81%	569
Su08c	4.16%	2.14%	1.00%	0.54%	9.75%	0.85%	1.72%	539
Su09a	6.05%	2.09%	1.10%	0.52%	9.91%	0.96%	1.67%	554
Su09b	6.42%	2.23%	0.94%	0.79%	11.16%	0.61%	2.48%	605
Su09c	6.69%	2.38%	0.83%	1.03%	12.43%	0.34%	3.30%	653
Su10a	6.65%	2.59%	0.69%	1.27%	13.73%	0.06%	3.95%	685
Su10b	4.25%	2.89%	0.46%	1.13%	11.52%	0.06%	2.92%	519
Su10c	1.92%	3.24%	0.27%	1.02%	9.48%	0.06%	1.94%	376
Au01a	0.06%	3.48%	0.10%	0.92%	7.27%	0.06%	1.13%	242
Au01b	0.06%	3.25%	0.10%	0.84%	8.03%	0.07%	1.27%	299
Au01c	0.06%	2.82%	0.10%	0.72%	8.52%	0.12%	1.42%	366
Au02a	0.06%	2.64%	0.11%	0.66%	9.73%	0.12%	1.69%	433
Au02b	0.06%	2.44%	0.13%	0.67%	9.55%	0.13%	1.79%	470
Au02c	0.06%	2.27%	0.14%	0.67%	9.42%	0.08%	1.90%	508
Au03a	0.06%	1.96%	0.14%	0.63%	8.62%	0.09%	1.83%	533
Au03b	0.06%	2.02%	0.12%	0.44%	8.59%	0.08%	1.64%	508
Au03c	0.06%	2.21%	0.11%	0.27%	9.30%	0.09%	1.62%	493
Au04a	0.06%	2.39%	0.10%	0.10%	9.91%	0.08%	1.61%	481
Au04b	0.06%	2.77%	0.12%	0.19%	10.37%	0.07%	2.19%	459
Au04c	0.06%	3.15%	0.20%	0.28%	10.13%	0.06%	2.51%	409
Au05a	0.06%	3.50%	0.22%	0.37%	10.36%	0.05%	2.90%	380
Au05b	0.06%	3.14%	0.20%	0.28%	9.82%	0.05%	2.39%	397
Au05c	0.06%	2.70%	0.12%	0.20%	9.68%	0.06%	1.95%	438
Au06a	0.06%	2.33%	0.12%	0.14%	9.51%	0.06%	1.69%	481

Au06b	0.06%	2.20%	0.40%	0.14%	9.60%	0.06%	1.64%	512
Au06c	0.06%	2.25%	0.74%	0.16%	9.24%	0.06%	1.71%	492
Au07a	0.06%	2.09%	0.90%	0.16%	9.23%	0.09%	1.53%	526
Au07b	0.06%	2.18%	0.69%	0.15%	8.81%	0.10%	1.50%	482
Au07c	0.06%	2.15%	0.45%	0.09%	8.55%	0.10%	1.37%	472
Au08a	0.06%	2.30%	0.34%	0.08%	7.98%	0.08%	1.33%	406
Au08b	0.06%	2.34%	0.47%	0.11%	8.12%	0.07%	1.32%	404
Au08c	0.06%	2.41%	0.52%	0.13%	8.10%	0.21%	1.20%	388
Au09a	1.70%	2.39%	0.56%	0.25%	7.65%	0.20%	1.04%	364
Au09b	1.70%	2.72%	0.45%	0.56%	8.84%	0.21%	1.54%	374
Au09c	1.70%	2.75%	0.40%	0.63%	10.04%	0.10%	2.29%	442
Au10a	0.06%	2.74%	0.35%	0.70%	11.46%	0.12%	2.89%	535
Au10b	0.04%	1.63%	0.23%	0.33%	7.47%	0.08%	1.97%	582
Au10c	0.02%	0.74%	0.09%	0.22%	3.66%	0.04%	0.88%	619

Table S5 Spring vs autumn

Name	t.stat	p-value	-Lg(p)	FDR
4-Hydroxybenzoic acid	26.00	1.18E-33	32.929	1.18E-31
Kaempferol	21.41	3.24E-29	28.49	1.62E-27
Adenine	20.12	7.84E-28	27.106	2.61E-26
Adenosine diphosphate	-19.21	7.96E-27	26.099	1.99E-25
Phloretin	18.76	2.67E-26	25.574	5.33E-25
Ellagic acid	-17.65	5.42E-25	24.266	9.04E-24
Gallic acid	16.80	6.04E-24	23.219	8.63E-23
Guanine	15.44	3.36E-22	21.474	4.20E-21
Digallic acid	-15.33	4.66E-22	21.331	4.93E-21
Eriodictyol	15.31	4.93E-22	21.307	4.93E-21
Trehalose	-15.07	1.03E-21	20.987	9.37E-21
D-Gluconic Acid	14.71	3.18E-21	20.498	2.65E-20
2-Aminoadipic acid	13.03	7.03E-19	18.153	5.41E-18
Naringenin	12.54	3.75E-18	17.426	2.68E-17
Glutathione	-11.96	2.73E-17	16.564	1.82E-16
Guanosine monophosphate	11.07	6.20E-16	15.208	3.88E-15
L-Glutamic acid	-10.97	9.06E-16	15.043	5.33E-15
S-Adenosyl-L-homocysteine	-10.45	5.86E-15	14.232	3.25E-14
L-Pyroglutamic acid	-10.01	3.02E-14	13.52	1.59E-13
Theasinensin B	9.87	5.02E-14	13.299	2.51E-13
L-Histidine	-9.55	1.67E-13	12.776	7.97E-13
Glutamine	-9.33	3.80E-13	12.42	1.73E-12
Gallocatechin-4alpha-8-epigallocatechin	9.31	4.05E-13	12.392	1.76E-12
L-Serine	-9.01	1.29E-12	11.89	5.37E-12

Tricetin	8.89	2.03E-12	11.692	8.13E-12
Epigallocatechin	8.85	2.34E-12	11.63	9.02E-12
L-Theanine	-8.76	3.31E-12	11.48	1.23E-11
Epigallocatechin-4beta-8-epicatechin-3-O-gallate ester	8.55	7.46E-12	11.127	2.67E-11
L-Aspartic acid	-8.34	1.62E-11	10.789	5.44E-11
Xylitol	8.34	1.63E-11	10.787	5.44E-11
Tyrosine	8.01	5.82E-11	10.235	1.88E-10
Betaine	7.70	1.97E-10	9.7054	6.16E-10
Glucuronic Acid	7.44	5.29E-10	9.2768	1.60E-09
L-Isoleucine	6.59	1.40E-08	7.8534	4.12E-08
L-Arginine	-6.56	1.63E-08	7.7875	4.66E-08
3-Hydroxy-3-methylglutaric acid	6.54	1.73E-08	7.7609	4.82E-08
Glutathione oxidized	-6.49	2.13E-08	7.6726	5.74E-08
Lysine	6.15	7.60E-08	7.1195	2.00E-07
Quercetin 3-O-sophoroside	6.03	1.22E-07	6.9124	3.14E-07
Beta-Alanine	-5.93	1.75E-07	6.7564	4.38E-07
Prunin	-5.57	6.98E-07	6.1564	1.70E-06
Epigallocatechin 3-O-3-O-methyl gallate	5.39	1.35E-06	5.871	3.20E-06
Alpha-ketoglutaric acid	4.97	6.37E-06	5.1957	1.48E-05
2,4-Dihydroxybenzoic acid	4.61	2.28E-05	4.6418	5.18E-05
Schaftoside	4.56	2.68E-05	4.5718	5.96E-05
Theogallin	-4.46	3.85E-05	4.4148	8.36E-05
Epicatechin gallate	-4.37	5.13E-05	4.2896	0.00010921
2-hydroxy cinnamic acid	-4.11	0.00012495	3.9033	0.00026031
Citric acid	4.10	0.00013228	3.8785	0.00026814
Isovitexin	4.09	0.00013407	3.8727	0.00026814

Myricetin	4.08	0.00013936	3.8559	0.00027325
Naringenin chalcone	-4.05	0.00015327	3.8145	0.00029475
Shikimic acid	-3.95	0.00021096	3.6758	0.00039804
3'-Adenosine monophosphate	3.77	0.00037865	3.4218	0.00070121
gamma-Aminobutyric acid	-3.73	0.00043173	3.3648	0.00078495
Gallocatechin	3.73	0.00044143	3.3551	0.00078827
4-Oxoproline	-3.62	0.00062421	3.2047	0.0010951
Procyanidin B4	-3.59	0.00067097	3.1733	0.0011425
Theobromine	-3.59	0.00067407	3.1713	0.0011425
Theophylline	-3.56	0.0007398	3.1309	0.001233
Glycyl-L-leucine	3.42	0.0011557	2.9372	0.0018946
Esculin	-3.26	0.0018851	2.7247	0.0030405
Succinic acid	3.23	0.0020391	2.6906	0.0032366
Cynaroside	-3.09	0.0031163	2.5064	0.0048693
Xanthine	-3.07	0.0032228	2.4918	0.0049581
4-Hydroxybenzaldehyde	-2.82	0.0065805	2.1817	0.0099705
L-Proline	2.58	0.012563	1.9009	0.01875
7-Methylxanthine	-2.50	0.015332	1.8144	0.022547
Malonic acid	2.30	0.025159	1.5993	0.036462
Caffeine	2.17	0.034414	1.4633	0.049163

Table S6 Spring vs summer

Name	t.stat	<i>p</i> -value	-Lg(p)	FDR
4-Hydroxybenzoic acid	-25.49	3.41E-33	32.4680	3.41E-31
L-Glutamic acid	15.19	7.13E-22	21.1470	3.57E-20
L-Aspartic acid	14.28	1.22E-20	19.9120	4.08E-19
beta-Alanine	12.52	3.95E-18	17.4030	9.88E-17
Glutamine	11.89	3.42E-17	16.4660	6.40E-16
L-Pyroglutamic acid	11.86	3.84E-17	16.4160	6.40E-16
Xylitol	-11.69	7.04E-17	16.1520	1.01E-15
L-Theanine	11.25	3.35E-16	15.4750	4.19E-15
L-Serine	11.17	4.33E-16	15.3630	4.82E-15
L-Histidine	10.69	2.45E-15	14.6110	2.45E-14
L-Isoleucine	9.82	6.02E-14	13.2200	5.48E-13
Tricetin	-9.54	1.72E-13	12.7640	1.44E-12
L-Arginine	9.05	1.08E-12	11.9650	8.13E-12
gamma-Aminobutyric acid	9.04	1.14E-12	11.9440	8.13E-12
Gallocatechin-4alpha-8-epigallocatechin	-8.90	1.94E-12	11.7130	1.29E-11
Ellagic acid	8.80	2.85E-12	11.5450	1.78E-11
2-Aminoadipic acid	-8.76	3.32E-12	11.4790	1.95E-11
Glutathione oxidized	8.54	7.62E-12	11.1180	4.23E-11
Glutathione	7.85	1.09E-10	9.9640	5.72E-10
D-Fructose	7.56	3.37E-10	9.4720	1.69E-09
Adenosine diphosphate	7.36	7.15E-10	9.1460	3.40E-09
Quercetin 3-O-sophoroside	-7.17	1.53E-09	8.8152	6.96E-09
Epigallocatechin-4beta-8-epicatechin-3-O-gallate ester	-7.00	2.89E-09	8.5397	1.25E-08
Caffeine	-6.91	4.10E-09	8.3873	1.71E-08

Theasinensin B	-6.87	4.86E-09	8.3136	1.94E-08
L-Homoserine	6.81	6.01E-09	8.2210	2.31E-08
Uridine monophosphate	6.76	7.36E-09	8.1333	2.72E-08
Myricetin	-6.69	9.57E-09	8.0190	3.42E-08
Guanosine monophosphate	6.66	1.08E-08	7.9656	3.73E-08
Epigallocatechin EGC	-6.44	2.57E-08	7.5906	8.56E-08
Catechin	-6.12	8.61E-08	7.0650	2.78E-07
D-Gluconic Acid	-5.67	4.66E-07	6.3314	1.46E-06
3-Hydroxy-3-methylglutaric acid	-5.43	1.14E-06	5.9427	3.40E-06
Epigallocatechin 3-O-3-O-methyl gallate	-5.43	1.15E-06	5.9377	3.40E-06
Trehalose	5.33	1.71E-06	5.7667	4.89E-06
Glucuronic Acid	-5.31	1.79E-06	5.7464	4.98E-06
Malic Acid	5.28	2.04E-06	5.6898	5.52E-06
Eriodictyol	-5.26	2.15E-06	5.6675	5.66E-06
Gallocatechin	-5.21	2.57E-06	5.5898	6.59E-06
S-Adenosyl-L-homocysteine	5.16	3.15E-06	5.5014	7.88E-06
Alpha-ketoglutaric acid	-5.15	3.31E-06	5.4805	8.07E-06
Esculin	-5.11	3.78E-06	5.4230	8.99E-06
Schaftoside	-5.04	4.82E-06	5.3170	1.12E-05
kaempferol	-4.97	6.35E-06	5.1970	1.44E-05
Theogallin	4.78	1.23E-05	4.9094	2.74E-05
Glycyl-L-leucine	4.67	1.81E-05	4.7420	3.94E-05
Isovitexin	-4.43	4.20E-05	4.3764	8.94E-05
3'-Adenosine monophosphate	4.36	5.44E-05	4.2643	0.00011336
L-Proline	4.34	5.79E-05	4.2374	0.00011813
4-Oxoproline	4.20	9.47E-05	4.0238	0.00018936

2,4-Dihydroxybenzoic acid	-4.12	0.00012006	3.9206	0.00023541
Betaine	-4.12	0.00012287	3.9106	0.00023629
Procyanidin B3	-3.97	0.00019915	3.7008	0.00037576
Citric acid	-3.95	0.00021716	3.6632	0.00040215
Quercetin	-3.67	0.00053557	3.2712	0.00097377
Quercetin-3beta-D-glucoside	-3.53	0.00082822	3.0819	0.001479
2-hydroxy cinnamic acid	3.44	0.0010918	2.9618	0.0018924
Guanine	3.44	0.0010976	2.9596	0.0018924
Delphinidin-3-O-rutinoside chloride	-3.30	0.0016496	2.7826	0.002796
Cynaroside	3.14	0.0026446	2.5776	0.0044076
Epicatechin	-3.06	0.0033482	2.4752	0.0054889
Epigallocatechin 3-O-gallate	-2.76	0.0078288	2.1063	0.012627
Adenine	2.71	0.0088653	2.0523	0.014072
Fumaric acid	2.59	0.011971	1.9219	0.018705

Table S7 Summer vs autumn

Name	t.stat	p-value	-Lg(p)	FDR
Phloretin	26.493	4.30E-34	33.367	3.09E-32
Adenine	26.314	6.18E-34	33.209	3.09E-32
Guanine	18.708	3.03E-26	25.519	1.01E-24
Gallic acid	15.824	1.04E-22	21.983	2.60E-21
Kaempferol	15.51	2.67E-22	21.573	5.34E-21
Guanosine monophosphate	14.424	7.68E-21	20.115	1.28E-19
Trehalose	-12.548	3.59E-18	17.444	5.14E-17
Eriodictyol	11.345	2.36E-16	15.628	2.68E-15
L-Isoleucine	11.338	2.41E-16	15.617	2.68E-15
Naringenin	10.956	9.43E-16	15.025	9.43E-15
Digallic acid	-10.04	2.67E-14	13.573	2.43E-13
Lysine	9.6901	9.84E-14	13.007	8.20E-13
Adenosine diphosphate	-9.2967	4.31E-13	12.365	3.32E-12
D-Gluconic Acid	9.1699	6.96E-13	12.157	4.97E-12
Glycyl-L-leucine	7.7746	1.46E-10	9.8347	9.75E-10
Esculin	-7.5063	4.13E-10	9.3839	2.58E-09
Ellagic acid	-7.4388	5.36E-10	9.2705	3.16E-09
3'-Adenosine monophosphate	6.6028	1.36E-08	7.8672	7.54E-08
L-Proline	6.2048	6.25E-08	7.2043	3.20E-07
D-Fructose	6.1984	6.40E-08	7.1936	3.20E-07
Uridine monophosphate	5.6091	5.95E-07	6.2253	2.83E-06
Tyrosine	5.4146	1.23E-06	5.9105	5.59E-06
Caffeine	-5.3842	1.38E-06	5.8616	5.98E-06
gamma-Aminobutyric acid	5.1624	3.11E-06	5.507	1.30E-05

Prunin	-4.9558	6.59E-06	5.181	2.64E-05
Beta-Alanine	4.8847	8.51E-06	5.0699	3.27E-05
Succinic acid	4.7487	1.38E-05	4.8587	5.13E-05
Epicatechin gallate	-4.6963	1.67E-05	4.778	5.95E-05
L-Aspartic acid	4.66	1.90E-05	4.7223	6.54E-05
S-Adenosyl-L-homocysteine	-4.5651	2.65E-05	4.5772	8.82E-05
Catechin	-4.5532	2.76E-05	4.5591	8.90E-05
2-Aminoadipic acid	4.4849	3.50E-05	4.4557	0.00010943
L-Glutamic acid	4.3822	5.00E-05	4.3013	0.00015143
4-Hydroxybenzaldehyde	-4.3735	5.15E-05	4.2883	0.00015143
Naringenin chalcone	-4.2153	8.84E-05	4.0537	0.00025249
Theasinensin B	4.1283	0.0001185	3.9263	0.00032916
Fumaric acid	3.956	0.00021012	3.6775	0.00056789
Procyanidin B4	-3.8662	0.00028186	3.55	0.00074174
Epigallocatechin gallate	-3.6555	0.00055422	3.2563	0.0014211
Glutathione oxidized	3.5952	0.00067011	3.1739	0.0016753
Epigallocatechin	3.5601	0.00074792	3.1261	0.0018242
Procyanidin B3	-3.4651	0.0010038	2.9983	0.0023901
L-Homoserine	3.4168	0.0011638	2.9341	0.0027065
Epigallocatechin-3'-glucuronide	-3.3523	0.0014157	2.849	0.0032176
L-Phenylalanine	3.3157	0.0015807	2.8012	0.0035126
Abscisic acid	3.3009	0.0016525	2.7819	0.0035923
Malic Acid	3.1908	0.0022905	2.6401	0.0048734
Shikimic acid	-3.0579	0.0033697	2.4724	0.0070203
Theophylline	-2.9875	0.004117	2.3854	0.008402
Xylitol	-2.862	0.0058468	2.2331	0.011694

Betaine	2.7566	0.0077939	2.1082	0.015282
Pantothenic acid	-2.7432	0.0080817	2.0925	0.015542
L-Tryptophan	-2.6562	0.010188	1.9919	0.019223
Xanthine	-2.5177	0.014597	1.8357	0.027032
Epigallocatechin-4beta-8-epicatechin-3-O-gallate ester	2.4649	0.01669	1.7776	0.030345
Delphinidin-3-O-rutinoside chloride	-2.327	0.023477	1.6294	0.041732
Glutamine	2.3216	0.023787	1.6237	0.041732
Gallocatechin-4alpha-8-epigallocatechin	2.2436	0.028691	1.5423	0.049467
Theobromine	-3.59	0.00067407	3.1713	0.0011425
Theophylline	-3.56	0.0007398	3.1309	0.001233
Glycyl-L-leucine	3.42	0.0011557	2.9372	0.0018946
Esculin	-3.26	0.0018851	2.7247	0.0030405
Succinic acid	3.23	0.0020391	2.6906	0.0032366
Cynaroside	-3.09	0.0031163	2.5064	0.0048693
Xanthine	-3.07	0.0032228	2.4918	0.0049581
4-Hydroxybenzaldehyde	-2.82	0.0065805	2.1817	0.0099705
L-Proline	2.58	0.012563	1.9009	0.01875
7-Methylxanthine	-2.50	0.015332	1.8144	0.022547
Malonic acid	2.30	0.025159	1.5993	0.036462
Caffeine	2.17	0.034414	1.4633	0.049163

Table S8-1 Corrected PCC

PCC	Epigallocatechin.gallate	Catechin	Epicatechin	Gallocatechin	Methylxanthine	Abscisic.acid	Adenine	Avicularin	Quercetin.3.O.sophoroside	Betaine
Epigallocatechin.gallate	1.00	0.19	0.56	-0.09	0.10	-0.03	-0.32	0.04	0.26	0.09
Catechin	0.19	1.00	0.15	0.86	0.21	-0.30	-0.21	-0.26	0.36	0.14
Epicatechin	0.56	0.15	1.00	-0.19	-0.21	0.01	-0.19	0.22	0.27	0.29
Gallocatechin	-0.09	0.86	-0.19	1.00	0.20	-0.22	0.04	-0.37	0.35	0.14
Methylxanthine	0.10	0.21	-0.21	0.20	1.00	-0.37	-0.11	-0.54	-0.02	-0.38
Abscisic.acid	-0.03	-0.30	0.01	-0.22	-0.37	1.00	0.27	0.18	0.04	0.08
Adenine	-0.32	-0.21	-0.19	0.04	-0.11	0.27	1.00	-0.01	0.23	0.31
Avicularin	0.04	-0.26	0.22	-0.37	-0.54	0.18	-0.01	1.00	0.23	0.28
Quercetin.3.O.sophoroside	0.26	0.36	0.27	0.35	-0.02	0.04	0.23	0.23	1.00	0.41
Betaine	0.09	0.14	0.29	0.14	-0.38	0.08	0.31	0.28	0.41	1.00
Caffeine	0.44	0.47	0.18	0.42	0.20	-0.09	0.00	-0.25	0.45	0.01
Epicatechin.gallate	0.59	0.22	0.52	-0.23	0.28	-0.31	-0.55	0.02	-0.07	-0.07
Chlorogenic.acid	-0.17	0.17	-0.60	0.29	0.31	-0.17	-0.06	-0.04	-0.12	-0.21
Cynaroside	-0.28	-0.25	-0.19	-0.17	-0.10	0.41	-0.13	0.27	-0.18	-0.22
Glucuronic.Acid	-0.01	0.17	-0.05	0.30	0.11	0.07	0.50	0.01	0.55	0.28
D.Fructose	-0.40	-0.41	-0.28	-0.14	0.05	0.07	0.49	-0.04	-0.07	0.02
D.Gluconic.Acid	-0.01	-0.08	0.20	0.02	-0.26	0.21	0.74	0.01	0.25	0.46
Lysine	-0.36	-0.13	-0.21	0.13	0.19	-0.01	0.82	-0.19	0.18	0.16
Tyrosine	-0.17	-0.22	-0.10	0.02	-0.25	0.27	0.75	0.26	0.36	0.32
Trehalose	0.03	-0.03	0.04	-0.21	0.10	-0.18	-0.75	0.03	-0.36	-0.51
Epigallocatechin	0.30	0.09	0.66	0.08	-0.33	0.19	0.40	0.14	0.47	0.51
Esculin	0.20	0.19	0.38	-0.07	-0.18	-0.02	-0.37	0.51	0.24	-0.15
Gallic.acid	-0.28	-0.14	-0.23	0.13	-0.05	0.24	0.92	-0.10	0.21	0.37
gamma.Aminobutyric.acid	-0.31	-0.26	-0.51	-0.10	0.38	-0.14	0.02	-0.21	-0.37	-0.39

Glutathione	-0.07	-0.37	-0.12	-0.36	0.09	0.01	-0.43	-0.17	-0.63	-0.47
Guanine	-0.33	-0.19	-0.21	0.08	-0.03	0.17	0.97	-0.06	0.23	0.24
Isovitexin	0.39	0.25	0.65	0.02	-0.24	-0.02	-0.04	0.22	0.36	0.43
Kaempferin	0.06	-0.19	0.49	-0.34	-0.34	-0.01	-0.10	0.39	-0.17	0.21
kaempferol	-0.02	-0.23	0.04	-0.13	-0.28	0.29	0.64	0.33	0.26	0.53
L.Serine	-0.19	-0.23	-0.31	-0.14	0.47	-0.13	-0.19	-0.43	-0.52	-0.53
L.Arginine	-0.29	-0.16	-0.33	-0.09	0.44	-0.30	-0.14	-0.32	-0.39	-0.40
L.Aspartic.acid	-0.16	-0.44	-0.24	-0.37	0.37	-0.01	-0.12	-0.35	-0.52	-0.44
L.Glutamic.acid	-0.28	-0.40	-0.35	-0.31	0.32	0.00	-0.13	-0.33	-0.61	-0.51
L.Homoserine	-0.29	0.05	-0.37	0.26	0.56	-0.02	0.22	-0.60	-0.15	-0.21
L.Isoleucine	-0.36	-0.25	-0.24	0.05	0.07	0.12	0.89	-0.17	0.16	0.13
L.Phenylalanine	-0.28	-0.35	-0.11	-0.13	-0.16	0.10	0.58	0.11	0.11	0.02
L.Proline	-0.39	-0.30	-0.36	-0.03	0.21	0.15	0.56	-0.11	-0.09	-0.12
L.Theanine	-0.19	-0.29	-0.28	-0.23	0.35	-0.10	-0.23	-0.51	-0.53	-0.61
L.Tryptophan	0.33	-0.06	0.46	-0.14	-0.22	0.17	-0.25	0.15	-0.09	-0.03
Malic.Acid	0.00	-0.17	0.22	-0.23	-0.07	0.20	-0.05	-0.11	-0.25	0.06
Naringenin	-0.18	-0.15	-0.03	0.02	-0.28	0.27	0.71	0.12	0.07	0.46
Neochlorogenic.acid	0.09	-0.19	-0.30	-0.10	-0.27	-0.08	0.02	0.29	0.10	0.30
Pantothenic.acid	0.10	0.25	-0.03	0.32	0.30	-0.15	-0.18	-0.23	-0.06	-0.24
Phloretin	-0.29	-0.22	-0.11	0.02	-0.23	0.44	0.92	0.06	0.21	0.38
Procyanidin.B4	0.58	0.07	0.70	-0.34	0.07	-0.13	-0.52	0.23	0.09	-0.02
Procyanidin.B3	0.64	0.43	0.71	0.05	-0.06	-0.20	-0.37	0.26	0.30	0.33
Prunin	0.01	-0.14	-0.15	-0.20	-0.31	0.02	-0.47	0.43	-0.40	-0.20
Theogallin	0.08	-0.16	-0.44	-0.14	0.17	-0.02	-0.18	-0.25	-0.34	-0.12
Theophylline	-0.19	0.15	-0.41	0.22	0.42	-0.22	-0.12	-0.30	-0.31	-0.42
Thymine	-0.26	0.28	-0.25	0.50	0.45	-0.27	0.26	-0.23	0.26	-0.09

Tricetin	0.39	0.20	0.64	0.05	-0.26	0.04	0.15	0.24	0.55	0.55
Xanthine	-0.03	0.09	-0.25	0.12	0.46	-0.20	-0.12	-0.19	-0.17	-0.33
Xylitol	0.11	0.22	0.22	0.24	-0.15	-0.04	0.15	0.38	0.74	0.19
Beta.Alanine	-0.45	-0.48	-0.46	-0.29	0.26	0.09	0.10	-0.33	-0.50	-0.49
hydroxy.cinnamic.acid	0.16	-0.10	0.09	-0.13	0.13	0.45	-0.24	-0.14	-0.19	-0.35
Citric.acid	-0.03	-0.26	-0.11	-0.18	-0.35	0.22	0.40	0.42	0.36	0.26
Succinic.acid	-0.26	-0.44	-0.27	-0.27	-0.36	0.42	0.41	0.30	-0.20	-0.01
Alpha.ketoglutaric.acid	0.05	-0.21	0.00	-0.18	-0.41	0.13	0.30	0.50	0.40	0.29
Hydroxycoumarine	-0.20	0.15	-0.64	0.26	0.33	-0.20	-0.09	-0.06	-0.16	-0.24
Coumarin	0.14	-0.26	0.38	-0.29	-0.33	0.63	-0.04	0.18	0.06	-0.06
Glutamine	-0.20	-0.25	-0.32	-0.17	0.44	-0.13	-0.21	-0.41	-0.55	-0.53
Delphinidin.3.O.rutinoside.chloride	-0.08	0.65	-0.22	0.77	0.30	-0.05	0.02	-0.32	0.53	0.01
Eriodictyol	-0.16	-0.20	-0.17	-0.01	-0.33	0.32	0.68	0.34	0.18	0.41
Glycyl.L.leucine	-0.30	-0.11	-0.37	0.18	0.38	-0.01	0.72	-0.43	0.05	-0.05
Guanosine.monophosphate	-0.33	-0.18	-0.24	0.08	0.04	0.04	0.91	-0.17	0.15	0.12
Glutathione.oxidized	-0.10	-0.23	-0.36	-0.13	0.50	0.12	-0.09	-0.28	-0.34	-0.53
L.Histidine	-0.16	-0.10	-0.34	-0.03	0.44	-0.21	-0.18	-0.27	-0.38	-0.42
L.Pyroglutamic.acid	-0.20	-0.24	-0.32	-0.16	0.44	-0.13	-0.24	-0.41	-0.56	-0.54
Myricetin	0.12	0.08	0.47	-0.06	-0.46	0.39	0.07	0.64	0.51	0.34
Naringenin.chalcone	0.57	0.24	0.57	-0.22	0.20	-0.32	-0.54	0.04	-0.08	-0.01
Quercetin	-0.12	0.32	-0.22	0.37	-0.38	0.02	0.09	0.20	0.17	0.21
Quercetin.3beta.D.glucoside	-0.14	-0.18	0.09	-0.24	-0.54	0.35	0.03	0.89	0.29	0.18
Schaftoside	0.20	0.12	0.40	0.04	-0.53	0.11	0.00	0.48	0.12	0.40
Uridine.monophosphate	-0.43	-0.26	-0.56	-0.03	0.36	0.09	0.42	-0.26	-0.27	-0.34
Digallic.acid	0.04	0.22	-0.27	0.13	0.10	-0.19	-0.40	-0.07	-0.15	-0.23
dihomomethionine	-0.09	-0.46	-0.08	-0.27	-0.27	0.58	0.22	0.21	0.02	0.11

Epigallocatechin.3.O..3.O.methyl.gallate	-0.16	0.64	-0.20	0.72	0.09	-0.20	0.24	-0.28	0.24	0.09
Epigallocatechin..4beta..8..epicatechin.3.O.gallate.ester	0.21	0.31	0.42	0.37	-0.01	-0.11	0.31	-0.05	0.41	0.51
Epigallocatechin.3..glucuronide	0.31	-0.15	0.18	-0.23	-0.54	0.09	-0.31	0.64	0.08	0.23
Galocatechin..4alpha..8..epigallocatechin	0.25	0.02	0.38	-0.13	-0.20	0.03	0.22	0.37	0.09	0.50
S.Adenosyl.L.homocysteine	-0.10	0.07	-0.44	0.14	0.60	-0.17	-0.37	-0.44	-0.41	-0.68
Theasinensin.B	0.22	0.02	0.40	0.11	-0.03	-0.01	0.44	0.03	0.38	0.43
Malonic.acid	0.13	0.17	0.27	-0.10	-0.03	0.02	0.15	0.26	0.10	0.09
4.Dihydroxybenzoic.acid	0.33	0.04	0.43	-0.05	-0.43	0.07	0.04	0.38	0.31	0.46
Aminoadipic.acid	-0.03	0.30	0.05	0.38	-0.10	0.00	0.43	0.10	0.36	0.63
.Adenosine.monophosphate	-0.28	-0.25	-0.24	-0.02	0.14	0.06	0.70	-0.07	0.23	0.09
Hydroxy.3.methylglutaric.acid	0.17	-0.10	0.17	-0.06	-0.30	0.18	0.28	0.08	-0.02	0.17
Hydroxybenzoic.acid	-0.04	0.64	-0.14	0.76	0.37	-0.11	0.05	-0.64	0.26	-0.01
Hydroxybenzaldehyde	0.64	0.30	0.61	-0.16	0.19	-0.30	-0.49	0.07	0.05	0.05
Hydroxybenzoic.acid	0.35	0.25	0.26	0.18	-0.26	-0.13	0.15	0.42	0.64	0.51
Oxoproline	-0.17	-0.02	-0.27	0.08	0.33	-0.18	-0.09	-0.45	-0.36	-0.36
Adenosine.diphosphate	0.01	-0.13	-0.16	-0.20	0.29	-0.15	-0.65	-0.17	-0.52	-0.60
Ellagic.acid	-0.13	-0.28	-0.29	-0.34	0.12	-0.01	-0.51	-0.03	-0.56	-0.51
Ethylmalonic.acid	0.04	-0.22	0.06	-0.20	-0.38	0.59	0.19	0.25	-0.06	0.24
Fumaric.acid	-0.37	0.05	-0.56	0.32	0.38	-0.02	0.35	-0.35	0.01	-0.07
Cyanidin.3.O.galactoside	-0.09	0.24	-0.23	0.37	-0.26	0.23	0.00	-0.01	0.05	0.32
Quinic.acid	-0.18	0.17	-0.20	0.28	0.19	0.09	0.14	0.16	0.09	-0.20
Theobromine	0.27	0.11	0.00	-0.05	0.87	-0.40	-0.27	-0.39	-0.07	-0.27
trans.p.Coumaric.acid	0.19	-0.09	0.26	-0.11	-0.02	0.47	-0.11	-0.11	-0.08	-0.22
Shikimic.acid	0.14	0.05	0.04	0.02	0.23	0.34	-0.28	-0.22	-0.13	-0.47

Table S8-2 Corrected PCC

PCC	Caffeine	Epicatechin.gallate	Chlorogenic.acid	Cynaroside	Glucuronic.Acid	D.Fructose	D.Gluconic.Acid	Lysine	Tyrosine	Trehalose
Epigallocatechin.gallate	0.44	0.59	-0.17	-0.28	-0.01	-0.40	-0.01	-0.36	-0.17	0.03
Catechin	0.47	0.22	0.17	-0.25	0.17	-0.41	-0.08	-0.13	-0.22	-0.03
Epicatechin	0.18	0.52	-0.60	-0.19	-0.05	-0.28	0.20	-0.21	-0.10	0.04
Gallocatechin	0.42	-0.23	0.29	-0.17	0.30	-0.14	0.02	0.13	0.02	-0.21
Methylxanthine	0.20	0.28	0.31	-0.10	0.11	0.05	-0.26	0.19	-0.25	0.10
Abscisic.acid	-0.09	-0.31	-0.17	0.41	0.07	0.07	0.21	-0.01	0.27	-0.18
Adenine	0.00	-0.55	-0.06	-0.13	0.50	0.49	0.74	0.82	0.75	-0.75
Avicularin	-0.25	0.02	-0.04	0.27	0.01	-0.04	0.01	-0.19	0.26	0.03
Quercetin.3.O.sophoroside	0.45	-0.07	-0.12	-0.18	0.55	-0.07	0.25	0.18	0.36	-0.36
Betaine	0.01	-0.07	-0.21	-0.22	0.28	0.02	0.46	0.16	0.32	-0.51
Caffeine	1.00	0.14	-0.07	-0.31	0.34	-0.27	0.12	-0.01	0.05	-0.23
Epicatechin.gallate	0.14	1.00	-0.17	-0.16	-0.25	-0.50	-0.32	-0.49	-0.58	0.39
Chlorogenic.acid	-0.07	-0.17	1.00	0.17	-0.07	0.09	-0.31	-0.06	-0.10	0.12
Cynaroside	-0.31	-0.16	0.17	1.00	-0.04	0.15	-0.41	-0.16	-0.06	0.41
Glucuronic.Acid	0.34	-0.25	-0.07	-0.04	1.00	0.10	0.51	0.50	0.49	-0.61
D.Fructose	-0.27	-0.50	0.09	0.15	0.10	1.00	0.17	0.56	0.43	-0.14
D.Gluconic.Acid	0.12	-0.32	-0.31	-0.41	0.51	0.17	1.00	0.58	0.63	-0.78
Lysine	-0.01	-0.49	-0.06	-0.16	0.50	0.56	0.58	1.00	0.66	-0.62
Tyrosine	0.05	-0.58	-0.10	-0.06	0.49	0.43	0.63	0.66	1.00	-0.66
Trehalose	-0.23	0.39	0.12	0.41	-0.61	-0.14	-0.78	-0.62	-0.66	1.00
Epigallocatechin	0.30	-0.14	-0.51	-0.32	0.41	-0.01	0.73	0.29	0.47	-0.58
Esculin	0.20	0.29	0.01	0.24	-0.04	-0.40	-0.26	-0.40	-0.21	0.34
Gallic.acid	0.03	-0.53	-0.01	-0.22	0.48	0.47	0.77	0.78	0.67	-0.78
gamma.Aminobutyric.acid	-0.44	-0.21	0.44	0.13	-0.24	0.49	-0.20	0.22	0.00	0.23

Glutathione	-0.35	0.15	-0.03	0.47	-0.52	0.22	-0.57	-0.32	-0.39	0.65
Guanine	0.02	-0.55	-0.06	-0.12	0.50	0.54	0.68	0.88	0.76	-0.70
Isovitexin	0.09	0.24	-0.29	-0.30	0.02	-0.27	0.40	-0.01	0.04	-0.15
Kaempferin	-0.34	0.25	-0.21	0.13	-0.21	-0.04	-0.06	-0.23	-0.11	0.17
kaempferol	-0.20	-0.32	-0.07	-0.12	0.32	0.26	0.63	0.41	0.57	-0.61
L.Serine	-0.29	0.02	0.21	0.32	-0.31	0.38	-0.42	0.09	-0.23	0.42
L.Arginine	-0.36	0.03	0.29	0.13	-0.18	0.39	-0.33	0.17	-0.18	0.28
L.Aspartic.acid	-0.29	0.07	-0.01	0.29	-0.24	0.46	-0.32	0.07	-0.17	0.32
L.Glutamic.acid	-0.41	-0.02	0.13	0.38	-0.36	0.46	-0.37	0.07	-0.20	0.44
L.Homoserine	0.00	-0.23	0.21	0.24	0.14	0.45	-0.05	0.45	0.03	-0.02
L.Isoleucine	0.02	-0.57	-0.07	-0.07	0.44	0.64	0.56	0.88	0.73	-0.57
L.Phenylalanine	0.01	-0.47	-0.14	0.05	0.26	0.55	0.38	0.62	0.74	-0.29
L.Proline	-0.19	-0.53	0.16	0.24	0.27	0.57	0.22	0.61	0.49	-0.25
L.Theanine	-0.15	0.04	0.05	0.10	-0.38	0.30	-0.37	-0.03	-0.35	0.42
L.Tryptophan	0.12	0.12	-0.38	0.20	-0.08	-0.09	-0.05	-0.16	0.12	0.13
Malic.Acid	-0.26	0.18	-0.14	0.06	-0.27	0.14	-0.01	-0.10	-0.30	0.13
Naringenin	-0.10	-0.31	-0.10	-0.09	0.27	0.15	0.59	0.41	0.42	-0.62
Neochlorogenic.acid	-0.06	-0.14	0.14	-0.21	-0.02	0.12	0.05	-0.06	0.23	-0.13
Pantothenic.acid	0.11	-0.04	0.28	0.07	-0.09	0.21	-0.26	-0.02	-0.08	0.20
Phloretin	-0.04	-0.55	-0.14	-0.10	0.46	0.47	0.79	0.68	0.72	-0.74
Procyanidin.B4	0.06	0.76	-0.27	0.11	-0.30	-0.27	-0.33	-0.45	-0.39	0.52
Procyanidin.B3	0.22	0.65	-0.18	-0.16	-0.10	-0.45	-0.04	-0.33	-0.17	0.14
Prunin	-0.18	0.12	0.13	0.30	-0.42	-0.33	-0.45	-0.52	-0.22	0.45
Theogallin	-0.07	0.21	0.25	-0.02	-0.33	-0.05	-0.34	-0.29	-0.32	0.18
Theophylline	-0.09	-0.07	0.59	-0.15	-0.27	0.11	-0.27	0.00	-0.20	0.17
Thymine	0.12	-0.35	0.20	0.08	0.46	0.39	0.01	0.57	0.35	-0.18

Tricetin	0.26	0.10	-0.33	-0.35	0.34	-0.30	0.57	0.06	0.24	-0.43
Xanthine	-0.14	-0.01	0.56	0.12	-0.18	0.23	-0.31	0.03	-0.16	0.21
Xylitol	0.42	-0.19	-0.07	-0.14	0.45	-0.05	0.26	0.13	0.43	-0.26
Beta.Alanine	-0.39	-0.26	0.11	0.37	-0.20	0.59	-0.18	0.26	0.01	0.29
hydroxy.cinnamic.acid	-0.07	0.10	-0.10	0.46	-0.33	0.07	-0.44	-0.27	-0.27	0.40
Citric.acid	0.19	-0.29	0.06	0.14	0.47	0.14	0.35	0.14	0.47	-0.38
Succinic.acid	-0.23	-0.43	0.15	0.24	0.06	0.19	0.36	0.16	0.40	-0.18
Alpha.ketoglutaric.acid	0.16	-0.20	-0.03	0.07	0.48	-0.03	0.35	0.05	0.41	-0.37
Hydroxycoumarine	-0.11	-0.14	0.99	0.19	-0.09	0.08	-0.36	-0.06	-0.14	0.16
Coumarin	-0.06	-0.06	-0.41	0.46	-0.04	0.01	-0.08	-0.18	0.04	0.11
Glutamine	-0.32	0.03	0.22	0.31	-0.35	0.37	-0.43	0.07	-0.25	0.43
Delphinidin.3.O.rutinoside.chloride	0.37	-0.17	0.16	0.07	0.40	-0.08	-0.14	0.11	0.00	-0.07
Eriodictyol	-0.12	-0.41	0.03	-0.03	0.31	0.30	0.49	0.38	0.60	-0.59
Glycyl.L.leucine	0.04	-0.42	0.14	-0.05	0.39	0.55	0.41	0.76	0.48	-0.49
Guanosine.monophosphate	0.05	-0.52	-0.06	-0.21	0.41	0.52	0.62	0.84	0.67	-0.61
Glutathione.oxidized	-0.16	0.00	0.32	0.35	-0.15	0.35	-0.33	-0.04	-0.20	0.31
L.Histidine	-0.26	0.00	0.46	0.22	-0.28	0.31	-0.39	0.04	-0.19	0.32
L.Pyroglutamic.acid	-0.31	0.03	0.23	0.32	-0.36	0.36	-0.46	0.05	-0.27	0.45
Myricetin	0.07	-0.01	-0.24	0.26	0.28	-0.22	0.23	-0.10	0.24	-0.18
Naringenin.chalcone	0.13	0.96	-0.19	-0.20	-0.31	-0.50	-0.29	-0.47	-0.58	0.40
Quercetin	0.23	-0.20	0.08	-0.22	0.06	-0.13	0.07	-0.13	0.08	-0.19
Quercetin.3beta.D.glucoside	-0.19	-0.13	-0.03	0.50	0.10	-0.04	-0.04	-0.16	0.24	0.09
Schaftoside	0.01	0.01	-0.15	0.09	0.14	-0.31	0.27	-0.13	0.18	-0.18
Uridine.monophosphate	-0.21	-0.38	0.35	-0.01	0.04	0.53	0.15	0.46	0.25	-0.15
Digallic.acid	0.13	0.16	0.22	-0.22	-0.27	-0.26	-0.34	-0.36	-0.30	0.24
dihomomethionine	-0.15	-0.37	-0.08	0.55	0.04	0.29	0.04	0.06	0.32	-0.09

Epigallocatechin.3.O.3.O.methyl.gallate	0.37	-0.22	0.19	-0.48	0.18	-0.14	0.27	0.23	0.13	-0.35
Epigallocatechin.4beta.8.epicatechin.3.O.gallate.ester	0.16	-0.14	-0.23	-0.33	0.34	-0.04	0.50	0.34	0.31	-0.51
Epigallocatechin.3.glucuronide	0.06	0.11	-0.11	0.08	-0.12	-0.30	-0.15	-0.45	0.08	0.07
Galocatechin.4alpha.8.epigallocatechin	-0.22	0.16	-0.11	-0.18	0.10	-0.22	0.37	0.03	0.20	-0.36
S.Adenosyl.L.homocysteine	0.06	0.06	0.43	0.14	-0.27	0.07	-0.57	-0.17	-0.39	0.42
Theasinensin.B	0.12	-0.20	-0.32	-0.27	0.43	0.05	0.58	0.45	0.48	-0.57
Malonic.acid	-0.02	0.29	0.03	-0.16	0.08	-0.18	0.23	0.09	0.02	-0.12
4.Dihydroxybenzoic.acid	0.15	-0.03	-0.28	-0.30	0.17	-0.12	0.43	0.01	0.36	-0.35
Aminoadipic.acid	0.09	-0.18	0.04	-0.10	0.46	-0.08	0.46	0.33	0.31	-0.59
.Adenosine.monophosphate	-0.01	-0.46	0.04	-0.02	0.37	0.57	0.43	0.67	0.60	-0.43
Hydroxy.3.methylglutaric.acid	0.20	-0.14	-0.10	-0.07	0.25	-0.18	0.44	0.11	0.29	-0.38
Hydroxybenzoic.acid	0.48	-0.11	0.12	-0.05	0.29	-0.02	-0.02	0.20	-0.03	-0.11
Hydroxybenzaldehyde	0.24	0.96	-0.21	-0.26	-0.20	-0.54	-0.21	-0.45	-0.50	0.30
Hydroxybenzoic.acid	0.39	-0.03	-0.11	-0.38	0.33	-0.10	0.38	0.08	0.41	-0.36
Oxoproline	-0.06	-0.10	0.22	0.21	-0.19	0.27	-0.29	0.14	-0.17	0.26
Adenosine.diphosphate	-0.15	0.29	0.20	0.33	-0.52	0.03	-0.73	-0.49	-0.61	0.76
Ellagic.acid	-0.42	0.24	0.22	0.37	-0.61	0.07	-0.67	-0.40	-0.47	0.76
Ethylmalonic.acid	-0.03	-0.14	-0.12	0.28	0.17	0.14	0.23	0.02	0.25	-0.19
Fumaric.acid	-0.03	-0.44	0.49	0.03	0.19	0.43	0.02	0.48	0.21	-0.30
Cyanidin.3.O.galactoside	0.10	-0.15	0.20	0.27	0.02	-0.21	-0.11	-0.20	-0.09	-0.10
Quinic.acid	0.01	-0.28	0.48	0.47	0.32	0.11	-0.12	0.18	0.18	-0.04
Theobromine	0.13	0.54	0.16	-0.01	0.07	-0.06	-0.28	0.03	-0.35	0.20
trans.p.Coumaric.acid	0.05	0.07	-0.30	0.41	-0.17	0.04	-0.25	-0.19	-0.15	0.27
Shikimic.acid	0.16	0.08	-0.01	0.38	-0.26	-0.03	-0.50	-0.30	-0.33	0.39

Table S8-3 Corrected PCC

PCC	Epigallocatechin	Esculin	Gallic.acid	gamma.Aminobutyric.acid	Glutathione	Guanine	Isovitexin	Kaempferin	kaempferol	L.Serine
Epigallocatechin.gallate	0.30	0.20	-0.28	-0.31	-0.07	-0.33	0.39	0.06	-0.02	-0.19
Catechin	0.09	0.19	-0.14	-0.26	-0.37	-0.19	0.25	-0.19	-0.23	-0.23
Epicatechin	0.66	0.38	-0.23	-0.51	-0.12	-0.21	0.65	0.49	0.04	-0.31
Gallocatechin	0.08	-0.07	0.13	-0.10	-0.36	0.08	0.02	-0.34	-0.13	-0.14
Methylxanthine	-0.33	-0.18	-0.05	0.38	0.09	-0.03	-0.24	-0.34	-0.28	0.47
Abscisic.acid	0.19	-0.02	0.24	-0.14	0.01	0.17	-0.02	-0.01	0.29	-0.13
Adenine	0.40	-0.37	0.92	0.02	-0.43	0.97	-0.04	-0.10	0.64	-0.19
Avicularin	0.14	0.51	-0.10	-0.21	-0.17	-0.06	0.22	0.39	0.33	-0.43
Quercetin.3.O.sophoroside	0.47	0.24	0.21	-0.37	-0.63	0.23	0.36	-0.17	0.26	-0.52
Betaine	0.51	-0.15	0.37	-0.39	-0.47	0.24	0.43	0.21	0.53	-0.53
Caffeine	0.30	0.20	0.03	-0.44	-0.35	0.02	0.09	-0.34	-0.20	-0.29
Epicatechin.gallate	-0.14	0.29	-0.53	-0.21	0.15	-0.55	0.24	0.25	-0.32	0.02
Chlorogenic.acid	-0.51	0.01	-0.01	0.44	-0.03	-0.06	-0.29	-0.21	-0.07	0.21
Cynaroside	-0.32	0.24	-0.22	0.13	0.47	-0.12	-0.30	0.13	-0.12	0.32
Glucuronic.Acid	0.41	-0.04	0.48	-0.24	-0.52	0.50	0.02	-0.21	0.32	-0.31
D.Fructose	-0.01	-0.40	0.47	0.49	0.22	0.54	-0.27	-0.04	0.26	0.38
D.Gluconic.Acid	0.73	-0.26	0.77	-0.20	-0.57	0.68	0.40	-0.06	0.63	-0.42
Lysine	0.29	-0.40	0.78	0.22	-0.32	0.88	-0.01	-0.23	0.41	0.09
Tyrosine	0.47	-0.21	0.67	0.00	-0.39	0.76	0.04	-0.11	0.57	-0.23
Trehalose	-0.58	0.34	-0.78	0.23	0.65	-0.70	-0.15	0.17	-0.61	0.42
Epigallocatechin	1.00	0.04	0.41	-0.51	-0.50	0.36	0.58	0.24	0.52	-0.51
Esculin	0.04	1.00	-0.46	-0.35	-0.16	-0.37	0.28	0.09	-0.27	-0.25
Gallic.acid	0.41	-0.46	1.00	0.08	-0.46	0.87	0.05	-0.23	0.67	-0.21
gamma.Aminobutyric.acid	-0.51	-0.35	0.08	1.00	0.34	0.06	-0.31	-0.27	-0.08	0.66

Glutathione	-0.50	-0.16	-0.46	0.34	1.00	-0.38	-0.44	0.13	-0.41	0.73
Guanine	0.36	-0.37	0.87	0.06	-0.38	1.00	-0.08	-0.14	0.55	-0.12
Isovitexin	0.58	0.28	0.05	-0.31	-0.44	-0.08	1.00	0.10	0.25	-0.38
Kaempferin	0.24	0.09	-0.23	-0.27	0.13	-0.14	0.10	1.00	0.16	-0.18
kaempferol	0.52	-0.27	0.67	-0.08	-0.41	0.55	0.25	0.16	1.00	-0.36
L.Serine	-0.51	-0.25	-0.21	0.66	0.73	-0.12	-0.38	-0.18	-0.36	1.00
L.Arginine	-0.50	-0.23	-0.16	0.70	0.44	-0.06	-0.34	-0.13	-0.31	0.81
L.Aspartic.acid	-0.44	-0.32	-0.14	0.52	0.79	-0.06	-0.41	-0.12	-0.27	0.89
L.Glutamic.acid	-0.55	-0.28	-0.15	0.65	0.80	-0.08	-0.39	-0.15	-0.28	0.94
L.Homoserine	-0.22	-0.39	0.30	0.46	0.28	0.29	-0.28	-0.39	-0.13	0.65
L.Isoleucine	0.27	-0.38	0.77	0.17	-0.20	0.94	-0.21	-0.19	0.37	0.07
L.Phenylalanine	0.20	-0.12	0.42	0.11	-0.01	0.65	-0.14	-0.13	0.18	0.12
L.Proline	0.04	-0.26	0.47	0.33	0.04	0.60	-0.31	-0.08	0.36	0.32
L.Theanine	-0.53	-0.20	-0.25	0.49	0.67	-0.17	-0.43	-0.21	-0.47	0.75
L.Tryptophan	0.30	0.27	-0.35	-0.25	0.27	-0.21	0.14	0.21	-0.21	0.13
Malic.Acid	-0.02	-0.08	-0.05	-0.04	0.32	-0.11	0.07	0.24	0.07	0.20
Naringenin	0.41	-0.33	0.73	-0.20	-0.37	0.63	0.06	0.14	0.67	-0.40
Neochlorogenic.acid	-0.07	-0.24	0.18	0.10	-0.07	-0.01	-0.01	-0.14	0.41	-0.19
Pantothenic.acid	-0.08	-0.13	-0.23	0.35	0.23	-0.11	-0.24	0.06	-0.23	0.40
Phloretin	0.47	-0.38	0.92	0.03	-0.42	0.86	0.03	-0.10	0.68	-0.27
Procyanidin.B4	0.06	0.43	-0.56	-0.20	0.27	-0.50	0.39	0.33	-0.26	0.10
Procyanidin.B3	0.32	0.40	-0.35	-0.36	-0.16	-0.38	0.63	0.25	-0.01	-0.21
Prunin	-0.41	0.35	-0.54	-0.08	0.30	-0.46	-0.21	0.19	-0.30	-0.05
Theogallin	-0.59	-0.38	-0.10	0.16	0.39	-0.21	-0.43	-0.21	-0.13	0.23
Theophylline	-0.47	-0.10	-0.09	0.55	0.10	-0.09	-0.30	-0.26	-0.27	0.40
Thymine	0.04	-0.11	0.22	0.24	-0.12	0.40	-0.24	-0.20	-0.05	0.26

Tricetin	0.81	0.23	0.20	-0.51	-0.63	0.08	0.77	0.16	0.48	-0.60
Xanthine	-0.35	-0.11	-0.12	0.64	0.21	-0.09	-0.20	-0.16	-0.18	0.56
Xylitol	0.45	0.39	0.08	-0.28	-0.55	0.16	0.30	-0.07	0.14	-0.46
Beta.Alanine	-0.46	-0.34	0.06	0.67	0.65	0.16	-0.45	-0.20	-0.13	0.81
hydroxy.cinnamic.acid	-0.20	0.03	-0.30	0.11	0.54	-0.23	-0.34	0.02	-0.25	0.38
Citric.acid	0.22	0.11	0.29	-0.23	-0.32	0.36	-0.01	-0.01	0.41	-0.39
Succinic.acid	0.06	-0.07	0.39	0.19	-0.10	0.35	-0.11	0.10	0.41	-0.21
Alpha.ketoglutaric.acid	0.29	0.18	0.20	-0.34	-0.37	0.25	0.11	0.08	0.43	-0.50
Hydroxycoumarine	-0.58	-0.01	-0.05	0.47	0.02	-0.09	-0.33	-0.22	-0.10	0.26
Coumarin	0.28	0.26	-0.17	-0.26	0.27	-0.08	-0.05	0.23	0.03	0.03
Glutamine	-0.53	-0.25	-0.22	0.66	0.75	-0.14	-0.36	-0.18	-0.35	1.00
Delphinidin.3.O.rutinoside.chloride	-0.06	0.01	0.03	-0.09	-0.25	0.08	-0.16	-0.41	-0.20	-0.09
Eriodictyol	0.32	-0.26	0.68	-0.07	-0.34	0.61	-0.02	0.10	0.83	-0.33
Glycyl.L.leucine	0.07	-0.47	0.67	0.34	-0.09	0.78	-0.28	-0.35	0.26	0.30
Guanosine.monophosphate	0.28	-0.37	0.81	0.09	-0.31	0.96	-0.16	-0.20	0.40	-0.06
Glutathione.oxidized	-0.50	-0.19	-0.08	0.61	0.58	-0.08	-0.49	-0.25	-0.20	0.68
L.Histidine	-0.49	-0.19	-0.20	0.71	0.47	-0.12	-0.31	-0.17	-0.28	0.80
L.Pyroglutamic.acid	-0.55	-0.24	-0.25	0.66	0.76	-0.16	-0.38	-0.17	-0.38	0.99
Myricetin	0.46	0.61	-0.04	-0.46	-0.41	0.00	0.50	0.17	0.24	-0.50
Naringenin.chalcone	-0.08	0.31	-0.52	-0.23	0.11	-0.54	0.33	0.30	-0.31	-0.02
Quercetin	-0.04	0.03	0.14	-0.28	-0.28	0.05	-0.14	-0.13	0.04	-0.50
Quercetin.3beta.D.glucoside	0.05	0.58	-0.08	-0.22	-0.17	-0.01	0.14	0.20	0.22	-0.40
Schaftoside	0.50	0.40	-0.06	-0.50	-0.28	-0.04	0.50	0.37	0.31	-0.43
Uridine.monophosphate	-0.34	-0.34	0.41	0.61	0.06	0.46	-0.43	-0.35	0.04	0.38
Digallic.acid	-0.48	0.11	-0.36	0.06	0.04	-0.38	-0.20	-0.28	-0.40	-0.01
dihomomethionine	0.12	-0.09	0.13	0.04	0.22	0.17	-0.16	0.12	0.30	0.14

Epigallocatechin.3.O..3.O.methyl..gallate	0.08	-0.05	0.32	-0.10	-0.51	0.25	0.10	-0.45	-0.01	-0.30
Epigallocatechin..4beta..8..epicatechin.3.O. gallate.ester	0.76	-0.16	0.38	-0.33	-0.48	0.30	0.45	0.19	0.48	-0.37
Epigallocatechin.3..glucuronide	0.07	0.31	-0.37	-0.38	-0.01	-0.33	0.05	0.27	0.01	-0.40
Gallocatechin..4alpha..8..epigallocatechin	0.46	0.01	0.19	-0.32	-0.37	0.13	0.33	0.45	0.57	-0.43
S.Adenosyl.L.homocysteine	-0.66	-0.07	-0.38	0.49	0.50	-0.30	-0.57	-0.32	-0.56	0.66
Theasinensin.B	0.80	-0.15	0.43	-0.32	-0.47	0.45	0.38	0.21	0.55	-0.37
Malonic.acid	0.14	0.31	0.13	-0.12	-0.36	0.10	0.43	0.04	0.18	-0.23
4.Dihydroxybenzoic.acid	0.60	0.08	0.09	-0.32	-0.40	0.01	0.62	0.12	0.41	-0.48
Aminoadipic.acid	0.46	-0.16	0.53	-0.30	-0.58	0.37	0.31	0.09	0.55	-0.47
.Adenosine.monophosphate	0.16	-0.23	0.58	0.20	-0.20	0.75	-0.18	-0.18	0.38	0.06
Hydroxy.3.methylglutaric.acid	0.49	0.06	0.18	-0.40	-0.29	0.24	0.18	0.17	0.32	-0.31
Hydroxybenzoic.acid	0.00	-0.08	0.09	-0.06	-0.11	0.11	-0.03	-0.52	-0.29	0.18
Hydroxybenzaldehyde	0.02	0.34	-0.46	-0.32	-0.01	-0.50	0.38	0.26	-0.25	-0.13
Hydroxybenzoic.acid	0.51	0.16	0.21	-0.34	-0.60	0.14	0.51	-0.09	0.45	-0.60
Oxoproline	-0.29	-0.21	-0.10	0.45	0.48	-0.03	-0.24	-0.20	-0.25	0.79
Adenosine.diphosphate	-0.66	0.09	-0.66	0.37	0.72	-0.60	-0.43	0.07	-0.64	0.59
Ellagic.acid	-0.79	0.05	-0.51	0.47	0.68	-0.46	-0.43	0.02	-0.52	0.52
Ethylmalonic.acid	0.20	-0.02	0.18	-0.13	-0.01	0.12	-0.03	0.15	0.26	-0.17
Fumaric.acid	-0.21	-0.34	0.37	0.45	-0.03	0.36	-0.30	-0.39	0.13	0.44
Cyanidin.3.O.galactoside	-0.12	-0.05	0.04	-0.30	-0.06	-0.06	-0.13	-0.01	0.03	-0.27
Quinic.acid	-0.03	0.28	0.00	0.12	-0.09	0.17	-0.24	0.07	0.03	0.16
Theobromine	-0.28	-0.10	-0.20	0.26	0.21	-0.20	-0.05	-0.16	-0.24	0.48
trans.p.Coumaric.acid	0.05	0.04	-0.22	-0.11	0.41	-0.11	-0.29	0.20	-0.18	0.19
Shikimic.acid	-0.21	0.16	-0.35	0.05	0.43	-0.27	-0.41	-0.06	-0.39	0.33

Table S8-4 Corrected PCC

PCC	L.Arginine	L.Aspartic.acid	L.Glutamic.acid	L.Homoserine	L.Isoleucine	L.Phenylalanine	L.Proline	L.Theanine	L.Tryptophan	Malic.Acid
Epigallocatechin.gallate	-0.29	-0.16	-0.28	-0.29	-0.36	-0.28	-0.39	-0.19	0.33	0.00
Catechin	-0.16	-0.44	-0.40	0.05	-0.25	-0.35	-0.30	-0.29	-0.06	-0.17
Epicatechin	-0.33	-0.24	-0.35	-0.37	-0.24	-0.11	-0.36	-0.28	0.46	0.22
Gallocatechin	-0.09	-0.37	-0.31	0.26	0.05	-0.13	-0.03	-0.23	-0.14	-0.23
Methylxanthine	0.44	0.37	0.32	0.56	0.07	-0.16	0.21	0.35	-0.22	-0.07
Abscisic.acid	-0.30	-0.01	0.00	-0.02	0.12	0.10	0.15	-0.10	0.17	0.20
Adenine	-0.14	-0.12	-0.13	0.22	0.89	0.58	0.56	-0.23	-0.25	-0.05
Avicularin	-0.32	-0.35	-0.33	-0.60	-0.17	0.11	-0.11	-0.51	0.15	-0.11
Quercetin.3.O.sophoroside	-0.39	-0.52	-0.61	-0.15	0.16	0.11	-0.09	-0.53	-0.09	-0.25
Betaine	-0.40	-0.44	-0.51	-0.21	0.13	0.02	-0.12	-0.61	-0.03	0.06
Caffeine	-0.36	-0.29	-0.41	0.00	0.02	0.01	-0.19	-0.15	0.12	-0.26
Epicatechin.gallate	0.03	0.07	-0.02	-0.23	-0.57	-0.47	-0.53	0.04	0.12	0.18
Chlorogenic.acid	0.29	-0.01	0.13	0.21	-0.07	-0.14	0.16	0.05	-0.38	-0.14
Cynaroside	0.13	0.29	0.38	0.24	-0.07	0.05	0.24	0.10	0.20	0.06
Glucuronic.Acid	-0.18	-0.24	-0.36	0.14	0.44	0.26	0.27	-0.38	-0.08	-0.27
D.Fructose	0.39	0.46	0.46	0.45	0.64	0.55	0.57	0.30	-0.09	0.14
D.Gluconic.Acid	-0.33	-0.32	-0.37	-0.05	0.56	0.38	0.22	-0.37	-0.05	-0.01
Lysine	0.17	0.07	0.07	0.45	0.88	0.62	0.61	-0.03	-0.16	-0.10
Tyrosine	-0.18	-0.17	-0.20	0.03	0.73	0.74	0.49	-0.35	0.12	-0.30
Trehalose	0.28	0.32	0.44	-0.02	-0.57	-0.29	-0.25	0.42	0.13	0.13
Epigallocatechin	-0.50	-0.44	-0.55	-0.22	0.27	0.20	0.04	-0.53	0.30	-0.02
Esculin	-0.23	-0.32	-0.28	-0.39	-0.38	-0.12	-0.26	-0.20	0.27	-0.08
Gallic.acid	-0.16	-0.14	-0.15	0.30	0.77	0.42	0.47	-0.25	-0.35	-0.05
gamma.Aminobutyric.acid	0.70	0.52	0.65	0.46	0.17	0.11	0.33	0.49	-0.25	-0.04

Glutathione	0.44	0.79	0.80	0.28	-0.20	-0.01	0.04	0.67	0.27	0.32
Guanine	-0.06	-0.06	-0.08	0.29	0.94	0.65	0.60	-0.17	-0.21	-0.11
Isovitexin	-0.34	-0.41	-0.39	-0.28	-0.21	-0.14	-0.31	-0.43	0.14	0.07
Kaempferin	-0.13	-0.12	-0.15	-0.39	-0.19	-0.13	-0.08	-0.21	0.21	0.24
kaempferol	-0.31	-0.27	-0.28	-0.13	0.37	0.18	0.36	-0.47	-0.21	0.07
L.Serine	0.81	0.89	0.94	0.65	0.07	0.12	0.32	0.75	0.13	0.20
L.Arginine	1.00	0.71	0.74	0.50	0.07	0.09	0.22	0.62	-0.04	0.10
L.Aspartic.acid	0.71	1.00	0.93	0.55	0.12	0.17	0.28	0.78	0.13	0.34
L.Glutamic.acid	0.74	0.93	1.00	0.59	0.09	0.17	0.33	0.80	0.10	0.32
L.Homoserine	0.50	0.55	0.59	1.00	0.40	0.20	0.52	0.45	-0.13	0.12
L.Isoleucine	0.07	0.12	0.09	0.40	1.00	0.74	0.66	0.01	-0.11	-0.08
L.Phenylalanine	0.09	0.17	0.17	0.20	0.74	1.00	0.50	0.09	0.26	-0.08
L.Proline	0.22	0.28	0.33	0.52	0.66	0.50	1.00	0.12	-0.09	-0.03
L.Theanine	0.62	0.78	0.80	0.45	0.01	0.09	0.12	1.00	0.03	0.42
L.Tryptophan	-0.04	0.13	0.10	-0.13	-0.11	0.26	-0.09	0.03	1.00	-0.02
Malic.Acid	0.10	0.34	0.32	0.12	-0.08	-0.08	-0.03	0.42	-0.02	1.00
Naringenin	-0.35	-0.29	-0.31	-0.02	0.45	0.17	0.26	-0.40	-0.29	0.06
Neochlorogenic.acid	-0.15	-0.11	-0.11	-0.26	-0.07	-0.02	-0.14	-0.20	-0.27	-0.17
Pantothenic.acid	0.44	0.22	0.23	0.24	0.00	0.05	0.15	0.19	0.26	-0.07
Phloretin	-0.20	-0.15	-0.17	0.15	0.75	0.46	0.45	-0.28	-0.23	-0.01
Procyanidin.B4	-0.02	0.13	0.06	-0.19	-0.48	-0.24	-0.41	0.03	0.33	0.23
Procyanidin.B3	-0.20	-0.28	-0.31	-0.30	-0.45	-0.29	-0.46	-0.37	0.31	0.02
Prunin	-0.13	-0.10	0.02	-0.43	-0.45	-0.12	-0.20	-0.01	0.30	-0.11
Theogallin	0.14	0.35	0.31	0.13	-0.19	-0.21	-0.18	0.40	-0.34	0.31
Theophylline	0.47	0.20	0.31	0.21	-0.02	-0.04	0.20	0.32	-0.17	-0.08
Thymine	0.30	0.08	0.11	0.56	0.51	0.37	0.54	-0.01	0.06	-0.33

Tricetin	-0.49	-0.57	-0.65	-0.36	-0.08	-0.08	-0.21	-0.61	0.14	-0.05
Xanthine	0.64	0.38	0.40	0.34	-0.02	-0.05	0.19	0.25	-0.09	-0.11
Xylitol	-0.32	-0.50	-0.52	-0.23	0.11	0.24	-0.06	-0.46	0.14	-0.43
Beta.Alanine	0.62	0.81	0.90	0.61	0.32	0.32	0.53	0.75	-0.03	0.27
hydroxy.cinnamic.acid	0.11	0.39	0.38	0.22	-0.12	-0.10	0.02	0.33	0.30	0.27
Citric.acid	-0.29	-0.22	-0.31	-0.28	0.25	0.34	0.12	-0.28	-0.08	-0.12
Succinic.acid	-0.23	-0.17	-0.04	-0.12	0.26	0.26	0.37	-0.13	-0.11	-0.07
Alpha.ketoglutaric.acid	-0.37	-0.33	-0.43	-0.41	0.11	0.23	0.00	-0.39	-0.07	-0.18
Hydroxycoumarine	0.34	0.04	0.18	0.23	-0.09	-0.16	0.16	0.11	-0.41	-0.12
Coumarin	-0.13	0.13	0.07	-0.07	-0.03	0.09	0.03	0.02	0.53	0.23
Glutamine	0.82	0.90	0.95	0.63	0.04	0.09	0.29	0.76	0.11	0.22
Delphinidin.3.O.rutinoside.chloride	-0.06	-0.22	-0.21	0.31	0.11	-0.10	0.00	-0.11	-0.19	-0.19
Eriodictyol	-0.27	-0.23	-0.24	-0.12	0.44	0.27	0.36	-0.41	-0.26	-0.05
Glycyl.L.leucine	0.30	0.31	0.28	0.61	0.83	0.52	0.65	0.22	-0.23	0.01
Guanosine.monophosphate	-0.01	-0.01	-0.03	0.30	0.94	0.65	0.55	-0.06	-0.21	-0.15
Glutathione.oxidized	0.50	0.70	0.71	0.54	0.04	0.02	0.30	0.63	-0.11	0.31
L.Histidine	0.86	0.65	0.68	0.44	-0.01	0.02	0.22	0.49	0.00	-0.01
L.Pyroglutamic.acid	0.81	0.90	0.95	0.61	0.02	0.09	0.28	0.77	0.13	0.22
Myricetin	-0.41	-0.44	-0.47	-0.43	-0.12	0.07	-0.14	-0.52	0.30	0.00
Naringenin.chalcone	-0.02	-0.01	-0.06	-0.25	-0.58	-0.47	-0.54	0.01	0.13	0.17
Quercetin	-0.40	-0.44	-0.45	-0.39	-0.03	-0.02	-0.24	-0.29	-0.30	-0.10
Quercetin.3beta.D.glucoside	-0.33	-0.34	-0.29	-0.44	-0.12	0.14	-0.03	-0.42	0.10	-0.12
Schaftoside	-0.39	-0.42	-0.43	-0.42	-0.17	-0.03	-0.13	-0.50	0.40	0.01
Uridine.monophosphate	0.42	0.35	0.44	0.43	0.53	0.36	0.54	0.41	-0.23	0.04
Digallic.acid	0.01	-0.05	0.02	-0.16	-0.33	-0.16	-0.17	0.18	-0.09	-0.04
dihomomethionine	0.00	0.24	0.21	0.16	0.20	0.23	0.31	0.01	0.25	0.15

Epigallocatechin.3.O.3.O.methyl..gallate	-0.22	-0.45	-0.37	0.02	0.18	0.01	0.00	-0.20	-0.31	-0.21
Epigallocatechin..4beta..8..epicatechin.3.O .gallate.ester	-0.31	-0.44	-0.49	0.03	0.20	0.03	0.12	-0.52	0.11	-0.08
Epigallocatechin.3..glucuronide	-0.35	-0.31	-0.37	-0.69	-0.37	-0.02	-0.38	-0.37	0.41	-0.22
Galocatechin..4alpha..8..epigallocatechin	-0.35	-0.42	-0.45	-0.33	-0.03	-0.11	0.00	-0.60	0.03	0.00
S.Adenosyl.L.homocysteine	0.55	0.53	0.58	0.39	-0.14	-0.07	0.14	0.66	0.03	0.07
Theasinensin.B	-0.32	-0.37	-0.44	-0.02	0.38	0.23	0.29	-0.48	0.19	-0.13
Malonic.acid	-0.11	-0.24	-0.20	-0.18	-0.05	-0.06	-0.04	-0.25	-0.12	0.01
4.Dihydroxybenzoic.acid	-0.37	-0.42	-0.46	-0.52	-0.10	0.12	-0.19	-0.49	0.37	-0.19
Aminoadipic.acid	-0.37	-0.51	-0.52	0.13	0.18	-0.08	0.14	-0.64	-0.24	-0.13
.Adenosine.monophosphate	0.08	0.09	0.10	0.35	0.79	0.60	0.65	0.03	-0.14	-0.07
Hydroxy.3.methylglutaric.acid	-0.32	-0.30	-0.32	-0.22	0.14	0.15	0.17	-0.31	0.25	-0.16
Hydroxybenzoic.acid	0.08	0.03	0.03	0.51	0.19	0.03	0.06	0.12	-0.03	-0.03
Hydroxybenzaldehyde	-0.12	-0.11	-0.18	-0.29	-0.55	-0.46	-0.56	-0.11	0.13	0.10
Hydroxybenzoic.acid	-0.49	-0.60	-0.63	-0.45	0.01	0.10	-0.18	-0.64	0.02	-0.39
Oxoproline	0.62	0.62	0.68	0.65	0.08	0.09	0.31	0.56	0.08	0.09
Adenosine.diphosphate	0.51	0.55	0.60	0.20	-0.45	-0.22	-0.15	0.67	0.14	0.20
Ellagic.acid	0.45	0.48	0.61	0.13	-0.33	-0.11	-0.09	0.59	0.04	0.21
Ethylmalonic.acid	-0.21	-0.04	-0.06	-0.08	0.07	0.14	0.16	-0.15	0.23	0.18
Fumaric.acid	0.43	0.31	0.36	0.62	0.41	0.21	0.49	0.29	-0.27	0.09
Cyanidin.3.O.galactoside	-0.29	-0.23	-0.25	-0.04	-0.12	-0.23	-0.18	-0.18	-0.19	0.22
Quinic.acid	0.20	-0.04	0.02	0.24	0.16	0.11	0.41	-0.13	0.15	-0.28
Theobromine	0.42	0.45	0.36	0.43	-0.14	-0.28	0.03	0.31	-0.10	0.03
trans.p.Coumaric.acid	-0.05	0.22	0.19	0.11	-0.02	0.00	0.02	0.19	0.43	0.26
Shikimic.acid	0.12	0.30	0.28	0.21	-0.15	-0.14	0.02	0.34	0.27	0.14

Table S8-5 Corrected PCC

PCC	Naringenin	Neochlorogenic.acid	Pantothenic.acid	Phloretin	Procyanidin.B4	Procyanidin.B3	Prunin	Theogallin	Theophylline	Thymine
Epigallocatechin.gallate	-0.18	0.09	0.10	-0.29	0.58	0.64	0.01	0.08	-0.19	-0.26
Catechin	-0.15	-0.19	0.25	-0.22	0.07	0.43	-0.14	-0.16	0.15	0.28
Epicatechin	-0.03	-0.30	-0.03	-0.11	0.70	0.71	-0.15	-0.44	-0.41	-0.25
Gallocatechin	0.02	-0.10	0.32	0.02	-0.34	0.05	-0.20	-0.14	0.22	0.50
Methylxanthine	-0.28	-0.27	0.30	-0.23	0.07	-0.06	-0.31	0.17	0.42	0.45
Abscisic.acid	0.27	-0.08	-0.15	0.44	-0.13	-0.20	0.02	-0.02	-0.22	-0.27
Adenine	0.71	0.02	-0.18	0.92	-0.52	-0.37	-0.47	-0.18	-0.12	0.26
Avicularin	0.12	0.29	-0.23	0.06	0.23	0.26	0.43	-0.25	-0.30	-0.23
Quercetin.3.O.sophoroside	0.07	0.10	-0.06	0.21	0.09	0.30	-0.40	-0.34	-0.31	0.26
Betaine	0.46	0.30	-0.24	0.38	-0.02	0.33	-0.20	-0.12	-0.42	-0.09
Caffeine	-0.10	-0.06	0.11	-0.04	0.06	0.22	-0.18	-0.07	-0.09	0.12
Epicatechin.gallate	-0.31	-0.14	-0.04	-0.55	0.76	0.65	0.12	0.21	-0.07	-0.35
Chlorogenic.acid	-0.10	0.14	0.28	-0.14	-0.27	-0.18	0.13	0.25	0.59	0.20
Cynaroside	-0.09	-0.21	0.07	-0.10	0.11	-0.16	0.30	-0.02	-0.15	0.08
Glucuronic.Acid	0.27	-0.02	-0.09	0.46	-0.30	-0.10	-0.42	-0.33	-0.27	0.46
D.Fructose	0.15	0.12	0.21	0.47	-0.27	-0.45	-0.33	-0.05	0.11	0.39
D.Gluconic.Acid	0.59	0.05	-0.26	0.79	-0.33	-0.04	-0.45	-0.34	-0.27	0.01
Lysine	0.41	-0.06	-0.02	0.68	-0.45	-0.33	-0.52	-0.29	0.00	0.57
Tyrosine	0.42	0.23	-0.08	0.72	-0.39	-0.17	-0.22	-0.32	-0.20	0.35
Trehalose	-0.62	-0.13	0.20	-0.74	0.52	0.14	0.45	0.18	0.17	-0.18
Epigallocatechin	0.41	-0.07	-0.08	0.47	0.06	0.32	-0.41	-0.59	-0.47	0.04
Esculin	-0.33	-0.24	-0.13	-0.38	0.43	0.40	0.35	-0.38	-0.10	-0.11
Gallic.acid	0.73	0.18	-0.23	0.92	-0.56	-0.35	-0.54	-0.10	-0.09	0.22
gamma.Aminobutyric.acid	-0.20	0.10	0.35	0.03	-0.20	-0.36	-0.08	0.16	0.55	0.24

Glutathione	-0.37	-0.07	0.23	-0.42	0.27	-0.16	0.30	0.39	0.10	-0.12
Guanine	0.63	-0.01	-0.11	0.86	-0.50	-0.38	-0.46	-0.21	-0.09	0.40
Isovitexin	0.06	-0.01	-0.24	0.03	0.39	0.63	-0.21	-0.43	-0.30	-0.24
Kaempferin	0.14	-0.14	0.06	-0.10	0.33	0.25	0.19	-0.21	-0.26	-0.20
kaempferol	0.67	0.41	-0.23	0.68	-0.26	-0.01	-0.30	-0.13	-0.27	-0.05
L.Serine	-0.40	-0.19	0.40	-0.27	0.10	-0.21	-0.05	0.23	0.40	0.26
L.Arginine	-0.35	-0.15	0.44	-0.20	-0.02	-0.20	-0.13	0.14	0.47	0.30
L.Aspartic.acid	-0.29	-0.11	0.22	-0.15	0.13	-0.28	-0.10	0.35	0.20	0.08
L.Glutamic.acid	-0.31	-0.11	0.23	-0.17	0.06	-0.31	0.02	0.31	0.31	0.11
L.Homoserine	-0.02	-0.26	0.24	0.15	-0.19	-0.30	-0.43	0.13	0.21	0.56
L.Isoleucine	0.45	-0.07	0.00	0.75	-0.48	-0.45	-0.45	-0.19	-0.02	0.51
L.Phenylalanine	0.17	-0.02	0.05	0.46	-0.24	-0.29	-0.12	-0.21	-0.04	0.37
L.Proline	0.26	-0.14	0.15	0.45	-0.41	-0.46	-0.20	-0.18	0.20	0.54
L.Theanine	-0.40	-0.20	0.19	-0.28	0.03	-0.37	-0.01	0.40	0.32	-0.01
L.Tryptophan	-0.29	-0.27	0.26	-0.23	0.33	0.31	0.30	-0.34	-0.17	0.06
Malic.Acid	0.06	-0.17	-0.07	-0.01	0.23	0.02	-0.11	0.31	-0.08	-0.33
Naringenin	1.00	0.11	-0.29	0.75	-0.37	-0.16	-0.27	0.00	-0.24	-0.13
Neochlorogenic.acid	0.11	1.00	-0.22	0.08	-0.16	0.00	0.11	0.36	-0.16	-0.20
Pantothenic.acid	-0.29	-0.22	1.00	-0.20	0.03	0.05	0.00	-0.14	0.54	0.38
Phloretin	0.75	0.08	-0.20	1.00	-0.50	-0.34	-0.46	-0.21	-0.15	0.12
Procyanidin.B4	-0.37	-0.16	0.03	-0.50	1.00	0.77	0.08	0.00	-0.27	-0.30
Procyanidin.B3	-0.16	0.00	0.05	-0.34	0.77	1.00	0.05	-0.14	-0.25	-0.20
Prunin	-0.27	0.11	0.00	-0.46	0.08	0.05	1.00	0.21	0.10	-0.29
Theogallin	0.00	0.36	-0.14	-0.21	0.00	-0.14	0.21	1.00	0.08	-0.38
Theophylline	-0.24	-0.16	0.54	-0.15	-0.27	-0.25	0.10	0.08	1.00	0.18
Thymine	-0.13	-0.20	0.38	0.12	-0.30	-0.20	-0.29	-0.38	0.18	1.00

Tricetin	0.25	0.03	-0.23	0.22	0.21	0.53	-0.32	-0.47	-0.44	-0.16
Xanthine	-0.24	-0.16	0.71	-0.15	0.03	-0.02	-0.11	0.02	0.72	0.23
Xylitol	-0.12	0.06	-0.01	0.13	0.00	0.19	-0.13	-0.52	-0.23	0.29
Beta.Alanine	-0.20	-0.08	0.13	0.06	-0.17	-0.54	-0.07	0.21	0.25	0.21
hydroxy.cinnamic.acid	-0.21	-0.31	0.37	-0.20	0.26	-0.05	0.10	0.16	0.09	-0.05
Citric.acid	0.26	0.27	-0.20	0.37	-0.17	-0.11	0.02	-0.02	-0.29	-0.14
Succinic.acid	0.41	0.12	-0.16	0.47	-0.38	-0.35	0.26	-0.05	0.01	-0.19
Alpha.ketoglutaric.acid	0.26	0.31	-0.26	0.26	-0.08	0.03	0.04	-0.08	-0.40	-0.21
Hydroxycoumarine	-0.14	0.16	0.25	-0.18	-0.26	-0.20	0.16	0.31	0.58	0.20
Coumarin	-0.04	-0.30	0.07	0.03	0.24	0.04	0.04	-0.20	-0.32	-0.15
Glutamine	-0.39	-0.16	0.38	-0.27	0.10	-0.21	-0.03	0.26	0.41	0.21
Delphinidin.3.O.rutinoside.chloride	-0.11	-0.15	0.25	-0.03	-0.23	-0.07	-0.25	-0.07	0.06	0.52
Eriodictyol	0.79	0.44	-0.19	0.72	-0.40	-0.17	-0.18	-0.02	-0.17	-0.02
Glycyl.L.leucine	0.37	-0.16	0.16	0.59	-0.44	-0.43	-0.53	0.02	0.19	0.49
Guanosine.monophosphate	0.53	-0.03	-0.08	0.76	-0.51	-0.43	-0.43	-0.16	-0.02	0.41
Glutathione.oxidized	-0.20	-0.16	0.30	-0.08	0.01	-0.35	-0.07	0.39	0.38	0.10
L.Histidine	-0.32	-0.15	0.62	-0.22	0.01	-0.14	-0.04	0.13	0.64	0.21
L.Pyroglutamic.acid	-0.42	-0.17	0.40	-0.30	0.10	-0.21	0.00	0.26	0.42	0.21
Myricetin	0.11	-0.21	-0.19	0.16	0.21	0.33	0.05	-0.54	-0.34	-0.16
Naringenin.chalcone	-0.30	-0.14	-0.09	-0.54	0.78	0.69	0.12	0.15	-0.10	-0.36
Quercetin	0.25	0.33	-0.08	0.15	-0.35	-0.15	0.19	0.14	0.07	-0.19
Quercetin.3beta.D.glucoside	0.10	0.12	-0.27	0.11	0.12	0.10	0.40	-0.28	-0.31	-0.17
Schaftoside	0.22	0.00	-0.12	0.02	0.16	0.46	0.29	-0.33	-0.42	-0.18
Uridine.monophosphate	0.08	-0.12	0.20	0.40	-0.50	-0.60	-0.10	0.11	0.62	0.30
Digallic.acid	-0.39	0.09	0.04	-0.40	-0.09	-0.08	0.38	0.26	0.46	-0.11
dihomomethionine	0.16	0.04	0.08	0.25	-0.02	-0.12	0.06	0.09	-0.35	-0.06

Epigallocatechin.3.O..3.O.methyl..gallate	0.14	-0.01	-0.02	0.22	-0.44	-0.11	-0.16	-0.12	0.35	0.24
Epigallocatechin..4beta..8..epicatechin.3.O .gallate.ester	0.40	-0.08	0.05	0.31	-0.07	0.30	-0.41	-0.42	-0.27	0.32
Epigallocatechin.3..glucuronide	-0.10	0.36	-0.01	-0.26	0.20	0.30	0.67	0.07	-0.23	-0.37
Gallocatechin..4alpha..8..epigallocatechin	0.47	0.05	-0.20	0.22	0.11	0.40	-0.04	-0.16	-0.26	-0.13
S.Adenosyl.L.homocysteine	-0.50	-0.25	0.51	-0.42	-0.11	-0.33	0.20	0.30	0.72	0.24
Theasinensin.B	0.43	-0.09	-0.03	0.40	-0.09	0.18	-0.38	-0.46	-0.36	0.32
Malonic.acid	0.15	-0.14	-0.29	0.14	0.21	0.31	-0.13	-0.26	0.04	-0.14
4.Dihydroxybenzoic.acid	0.09	0.31	-0.07	0.14	0.09	0.38	0.03	-0.38	-0.24	-0.17
Aminoadipic.acid	0.58	0.12	-0.25	0.43	-0.20	0.20	-0.29	-0.15	-0.34	0.19
.Adenosine.monophosphate	0.21	-0.07	0.01	0.57	-0.36	-0.36	-0.31	-0.13	0.01	0.46
Hydroxy.3.methylglutaric.acid	0.30	-0.05	-0.08	0.21	-0.12	0.10	0.13	-0.18	-0.26	-0.10
Hydroxybenzoic.acid	-0.10	-0.27	0.21	-0.03	-0.17	0.00	-0.35	0.03	0.11	0.46
Hydroxybenzaldehyde	-0.25	-0.12	-0.09	-0.48	0.76	0.74	0.08	0.09	-0.13	-0.34
Hydroxybenzoic.acid	0.13	0.54	-0.13	0.19	0.08	0.42	-0.10	-0.27	-0.28	0.00
Oxoproline	-0.27	-0.15	0.39	-0.20	0.04	-0.10	-0.13	0.15	0.29	0.28
Adenosine.diphosphate	-0.59	-0.16	0.38	-0.65	0.27	-0.12	0.36	0.34	0.34	-0.07
Ellagic.acid	-0.47	-0.03	0.10	-0.50	0.19	-0.19	0.48	0.44	0.33	-0.17
Ethylmalonic.acid	0.20	0.03	-0.05	0.31	-0.08	-0.07	0.07	-0.05	-0.23	-0.15
Fumaric.acid	0.03	0.04	0.30	0.23	-0.47	-0.36	-0.32	0.12	0.48	0.48
Cyanidin.3.O.galactoside	0.30	0.09	-0.08	0.02	-0.20	-0.03	0.21	0.41	-0.19	-0.22
Quinic.acid	-0.02	-0.35	0.41	0.04	-0.17	-0.08	0.05	-0.36	0.20	0.55
Theobromine	-0.33	-0.17	0.15	-0.36	0.37	0.19	-0.26	0.21	0.15	0.24
trans.p.Coumaric.acid	-0.10	-0.40	0.35	-0.09	0.24	-0.04	0.07	0.00	-0.10	-0.02
Shikimic.acid	-0.30	-0.40	0.42	-0.27	0.19	-0.10	0.09	0.08	0.19	0.04

Table S8-6 Corrected PCC

PCC	Tricetin	Xanthine	Xylitol	Beta.Alanine	hydroxy.cinnamic.acid	Citric.acid	Succinic.acid	Alpha.ketoglutaric.acid	Hydroxycoumarine	Coumarin
Epigallocatechin.gallate	0.39	-0.03	0.11	-0.45	0.16	-0.03	-0.26	0.05	-0.20	0.14
Catechin	0.20	0.09	0.22	-0.48	-0.10	-0.26	-0.44	-0.21	0.15	-0.26
Epicatechin	0.64	-0.25	0.22	-0.46	0.09	-0.11	-0.27	0.00	-0.64	0.38
Gallocatechin	0.05	0.12	0.24	-0.29	-0.13	-0.18	-0.27	-0.18	0.26	-0.29
Methylxanthine	-0.26	0.46	-0.15	0.26	0.13	-0.35	-0.36	-0.41	0.33	-0.33
Abscisic.acid	0.04	-0.20	-0.04	0.09	0.45	0.22	0.42	0.13	-0.20	0.63
Adenine	0.15	-0.12	0.15	0.10	-0.24	0.40	0.41	0.30	-0.09	-0.04
Avicularin	0.24	-0.19	0.38	-0.33	-0.14	0.42	0.30	0.50	-0.06	0.18
Quercetin.3.O.sophoroside	0.55	-0.17	0.74	-0.50	-0.19	0.36	-0.20	0.40	-0.16	0.06
Betaine	0.55	-0.33	0.19	-0.49	-0.35	0.26	-0.01	0.29	-0.24	-0.06
Caffeine	0.26	-0.14	0.42	-0.39	-0.07	0.19	-0.23	0.16	-0.11	-0.06
Epicatechin.gallate	0.10	-0.01	-0.19	-0.26	0.10	-0.29	-0.43	-0.20	-0.14	-0.06
Chlorogenic.acid	-0.33	0.56	-0.07	0.11	-0.10	0.06	0.15	-0.03	0.99	-0.41
Cynaroside	-0.35	0.12	-0.14	0.37	0.46	0.14	0.24	0.07	0.19	0.46
Glucuronic.Acid	0.34	-0.18	0.45	-0.20	-0.33	0.47	0.06	0.48	-0.09	-0.04
D.Fructose	-0.30	0.23	-0.05	0.59	0.07	0.14	0.19	-0.03	0.08	0.01
D.Gluconic.Acid	0.57	-0.31	0.26	-0.18	-0.44	0.35	0.36	0.35	-0.36	-0.08
Lysine	0.06	0.03	0.13	0.26	-0.27	0.14	0.16	0.05	-0.06	-0.18
Tyrosine	0.24	-0.16	0.43	0.01	-0.27	0.47	0.40	0.41	-0.14	0.04
Trehalose	-0.43	0.21	-0.26	0.29	0.40	-0.38	-0.18	-0.37	0.16	0.11
Epigallocatechin	0.81	-0.35	0.45	-0.46	-0.20	0.22	0.06	0.29	-0.58	0.28
Esculin	0.23	-0.11	0.39	-0.34	0.03	0.11	-0.07	0.18	-0.01	0.26
Gallic.acid	0.20	-0.12	0.08	0.06	-0.30	0.29	0.39	0.20	-0.05	-0.17
gamma.Aminobutyric.acid	-0.51	0.64	-0.28	0.67	0.11	-0.23	0.19	-0.34	0.47	-0.26

Glutathione	-0.63	0.21	-0.55	0.65	0.54	-0.32	-0.10	-0.37	0.02	0.27
Guanine	0.08	-0.09	0.16	0.16	-0.23	0.36	0.35	0.25	-0.09	-0.08
Isovitexin	0.77	-0.20	0.30	-0.45	-0.34	-0.01	-0.11	0.11	-0.33	-0.05
Kaempferin	0.16	-0.16	-0.07	-0.20	0.02	-0.01	0.10	0.08	-0.22	0.23
kaempferol	0.48	-0.18	0.14	-0.13	-0.25	0.41	0.41	0.43	-0.10	0.03
L.Serine	-0.60	0.56	-0.46	0.81	0.38	-0.39	-0.21	-0.50	0.26	0.03
L.Arginine	-0.49	0.64	-0.32	0.62	0.11	-0.29	-0.23	-0.37	0.34	-0.13
L.Aspartic.acid	-0.57	0.38	-0.50	0.81	0.39	-0.22	-0.17	-0.33	0.04	0.13
L.Glutamic.acid	-0.65	0.40	-0.52	0.90	0.38	-0.31	-0.04	-0.43	0.18	0.07
L.Homoserine	-0.36	0.34	-0.23	0.61	0.22	-0.28	-0.12	-0.41	0.23	-0.07
L.Isoleucine	-0.08	-0.02	0.11	0.32	-0.12	0.25	0.26	0.11	-0.09	-0.03
L.Phenylalanine	-0.08	-0.05	0.24	0.32	-0.10	0.34	0.26	0.23	-0.16	0.09
L.Proline	-0.21	0.19	-0.06	0.53	0.02	0.12	0.37	0.00	0.16	0.03
L.Theanine	-0.61	0.25	-0.46	0.75	0.33	-0.28	-0.13	-0.39	0.11	0.02
L.Tryptophan	0.14	-0.09	0.14	-0.03	0.30	-0.08	-0.11	-0.07	-0.41	0.53
Malic.Acid	-0.05	-0.11	-0.43	0.27	0.27	-0.12	-0.07	-0.18	-0.12	0.23
Naringenin	0.25	-0.24	-0.12	-0.20	-0.21	0.26	0.41	0.26	-0.14	-0.04
Neochlorogenic.acid	0.03	-0.16	0.06	-0.08	-0.31	0.27	0.12	0.31	0.16	-0.30
Pantothenic.acid	-0.23	0.71	-0.01	0.13	0.37	-0.20	-0.16	-0.26	0.25	0.07
Phloretin	0.22	-0.15	0.13	0.06	-0.20	0.37	0.47	0.26	-0.18	0.03
Procyanidin.B4	0.21	0.03	0.00	-0.17	0.26	-0.17	-0.38	-0.08	-0.26	0.24
Procyanidin.B3	0.53	-0.02	0.19	-0.54	-0.05	-0.11	-0.35	0.03	-0.20	0.04
Prunin	-0.32	-0.11	-0.13	-0.07	0.10	0.02	0.26	0.04	0.16	0.04
Theogallin	-0.47	0.02	-0.52	0.21	0.16	-0.02	-0.05	-0.08	0.31	-0.20
Theophylline	-0.44	0.72	-0.23	0.25	0.09	-0.29	0.01	-0.40	0.58	-0.32
Thymine	-0.16	0.23	0.29	0.21	-0.05	-0.14	-0.19	-0.21	0.20	-0.15

Tricetin	1.00	-0.28	0.51	-0.63	-0.41	0.26	-0.05	0.39	-0.39	0.08
Xanthine	-0.28	1.00	-0.16	0.25	0.22	-0.17	-0.14	-0.25	0.55	-0.12
Xylitol	0.51	-0.16	1.00	-0.40	-0.32	0.40	-0.05	0.44	-0.11	0.04
Beta.Alanine	-0.63	0.25	-0.40	1.00	0.27	-0.16	0.16	-0.32	0.17	0.05
hydroxy.cinnamic.acid	-0.41	0.22	-0.32	0.27	1.00	-0.34	-0.14	-0.42	-0.10	0.69
Citric.acid	0.26	-0.17	0.40	-0.16	-0.34	1.00	0.46	0.93	0.04	0.06
Succinic.acid	-0.05	-0.14	-0.05	0.16	-0.14	0.46	1.00	0.38	0.13	0.02
Alpha.ketoglutaric.acid	0.39	-0.25	0.44	-0.32	-0.42	0.93	0.38	1.00	-0.05	0.04
Hydroxycoumarine	-0.39	0.55	-0.11	0.17	-0.10	0.04	0.13	-0.05	1.00	-0.43
Coumarin	0.08	-0.12	0.04	0.05	0.69	0.06	0.02	0.04	-0.43	1.00
Glutamine	-0.60	0.57	-0.48	0.81	0.37	-0.38	-0.19	-0.49	0.27	0.03
Delphinidin.3.O.rutinoside.chloride	-0.08	0.05	0.27	-0.14	0.15	-0.08	-0.31	-0.10	0.15	-0.03
Eriodictyol	0.18	-0.16	0.05	-0.10	-0.22	0.44	0.46	0.42	0.00	-0.04
Glycyl.L.leucine	-0.16	0.26	-0.07	0.41	-0.07	0.17	0.16	0.02	0.13	-0.16
Guanosine.monophosphate	-0.02	-0.07	0.12	0.20	-0.21	0.26	0.26	0.14	-0.09	-0.13
Glutathione.oxidized	-0.59	0.48	-0.36	0.67	0.52	-0.17	0.05	-0.31	0.35	0.10
L.Histidine	-0.46	0.87	-0.31	0.52	0.24	-0.24	-0.16	-0.34	0.48	-0.09
L.Pyroglutamic.acid	-0.62	0.57	-0.48	0.81	0.38	-0.39	-0.20	-0.50	0.28	0.03
Myricetin	0.57	-0.21	0.52	-0.44	-0.06	0.43	0.12	0.47	-0.28	0.42
Naringenin.chalcone	0.15	-0.06	-0.15	-0.30	0.05	-0.33	-0.41	-0.23	-0.16	-0.09
Quercetin	-0.12	-0.20	0.06	-0.40	-0.14	0.21	0.13	0.23	0.06	-0.20
Quercetin.3beta.D.glucoside	0.16	-0.21	0.39	-0.22	-0.05	0.48	0.35	0.52	-0.04	0.28
Schaftoside	0.59	-0.28	0.27	-0.47	-0.27	0.32	0.18	0.44	-0.19	0.21
Uridine.monophosphate	-0.49	0.36	-0.20	0.58	0.04	-0.02	0.33	-0.22	0.36	-0.23
Digallic.acid	-0.38	0.02	-0.11	-0.03	0.02	-0.18	-0.06	-0.19	0.24	-0.27
dihomomethionine	0.01	0.01	0.06	0.25	0.34	0.35	0.30	0.28	-0.09	0.57

Epigallocatechin.3.O..3.O.methyl.gallate	0.06	-0.05	0.19	-0.26	-0.34	-0.07	-0.05	-0.10	0.15	-0.46
Epigallocatechin..4beta..8..epicatechin.3.O.gallate.ester	0.68	-0.15	0.32	-0.46	-0.23	-0.05	-0.11	0.04	-0.29	0.01
Epigallocatechin.3..glucuronide	0.15	-0.20	0.22	-0.47	-0.04	0.37	0.12	0.47	-0.13	0.21
Gallocatechin..4alpha..8..epigallocatechin	0.51	-0.16	0.01	-0.50	-0.15	0.04	0.09	0.16	-0.14	0.05
S.Adenosyl.L.homocysteine	-0.69	0.52	-0.32	0.50	0.41	-0.34	-0.17	-0.48	0.46	-0.10
Theasinensin.B	0.66	-0.21	0.31	-0.35	-0.23	0.11	0.05	0.19	-0.37	0.11
Malonic.acid	0.25	-0.01	0.06	-0.22	-0.19	0.04	0.05	0.09	0.02	-0.12
4.Dihydroxybenzoic.acid	0.67	-0.22	0.40	-0.46	-0.39	0.34	0.09	0.43	-0.32	0.04
Aminoadipic.acid	0.52	-0.23	0.26	-0.45	-0.42	0.21	0.09	0.28	0.01	-0.18
.Adenosine.monophosphate	-0.01	0.03	0.26	0.33	-0.12	0.35	0.29	0.21	0.03	-0.01
Hydroxy.3.methylglutaric.acid	0.42	-0.23	0.13	-0.26	-0.25	0.41	0.35	0.44	-0.13	0.16
Hydroxybenzoic.acid	-0.06	0.08	0.04	0.05	0.06	-0.21	-0.39	-0.28	0.10	-0.11
Hydroxybenzaldehyde	0.26	-0.09	-0.05	-0.40	0.00	-0.27	-0.42	-0.16	-0.19	-0.09
Hydroxybenzoic.acid	0.63	-0.23	0.59	-0.57	-0.48	0.39	-0.03	0.47	-0.15	-0.20
Oxoproline	-0.37	0.47	-0.28	0.57	0.24	-0.25	-0.20	-0.32	0.25	0.03
Adenosine.diphosphate	-0.63	0.35	-0.37	0.42	0.51	-0.40	-0.21	-0.44	0.25	0.11
Ellagic.acid	-0.72	0.19	-0.49	0.50	0.42	-0.37	0.03	-0.45	0.28	0.05
Ethylmalonic.acid	0.03	-0.19	-0.03	-0.01	0.20	0.30	0.40	0.22	-0.14	0.41
Fumaric.acid	-0.27	0.44	-0.05	0.40	0.01	0.02	-0.01	-0.12	0.50	-0.19
Cyanidin.3.O.galactoside	-0.05	-0.16	-0.19	-0.26	0.05	0.22	0.11	0.21	0.19	0.04
Quinic.acid	-0.09	0.40	0.26	0.03	0.15	0.14	0.12	0.09	0.45	0.19
Theobromine	-0.11	0.35	-0.18	0.22	0.08	-0.28	-0.45	-0.30	0.20	-0.27
trans.p.Coumaric.acid	-0.24	0.01	-0.19	0.14	0.90	-0.22	-0.07	-0.28	-0.31	0.79
Shikimic.acid	-0.39	0.25	-0.18	0.19	0.91	-0.32	-0.20	-0.39	-0.02	0.63

Table S8-7 Corrected PCC

PCC	Glutamine	Delphinidin.3.O.rutinoside.chloride	Eriodictyol	Glycyl.L.leucine	Guanosine.monophosphate	Glutathione.oxidized	L.Histidine	L.Pyroglutamic.acid	Myricetin	Naringenin.chalcone
Epigallocatechin.gallate	-0.20	-0.08	-0.16	-0.30	-0.33	-0.10	-0.16	-0.20	0.12	0.57
Catechin	-0.25	0.65	-0.20	-0.11	-0.18	-0.23	-0.10	-0.24	0.08	0.24
Epicatechin	-0.32	-0.22	-0.17	-0.37	-0.24	-0.36	-0.34	-0.32	0.47	0.57
Gallocatechin	-0.17	0.77	-0.01	0.18	0.08	-0.13	-0.03	-0.16	-0.06	-0.22
Methylxanthine	0.44	0.30	-0.33	0.38	0.04	0.50	0.44	0.44	-0.46	0.20
Abscisic.acid	-0.13	-0.05	0.32	-0.01	0.04	0.12	-0.21	-0.13	0.39	-0.32
Adenine	-0.21	0.02	0.68	0.72	0.91	-0.09	-0.18	-0.24	0.07	-0.54
Avicularin	-0.41	-0.32	0.34	-0.43	-0.17	-0.28	-0.27	-0.41	0.64	0.04
Quercetin.3.O.sophoroside	-0.55	0.53	0.18	0.05	0.15	-0.34	-0.38	-0.56	0.51	-0.08
Betaine	-0.53	0.01	0.41	-0.05	0.12	-0.53	-0.42	-0.54	0.34	-0.01
Caffeine	-0.32	0.37	-0.12	0.04	0.05	-0.16	-0.26	-0.31	0.07	0.13
Epicatechin.gallate	0.03	-0.17	-0.41	-0.42	-0.52	0.00	0.00	0.03	-0.01	0.96
Chlorogenic.acid	0.22	0.16	0.03	0.14	-0.06	0.32	0.46	0.23	-0.24	-0.19
Cynaroside	0.31	0.07	-0.03	-0.05	-0.21	0.35	0.22	0.32	0.26	-0.20
Glucuronic.Acid	-0.35	0.40	0.31	0.39	0.41	-0.15	-0.28	-0.36	0.28	-0.31
D.Fructose	0.37	-0.08	0.30	0.55	0.52	0.35	0.31	0.36	-0.22	-0.50
D.Gluconic.Acid	-0.43	-0.14	0.49	0.41	0.62	-0.33	-0.39	-0.46	0.23	-0.29
Lysine	0.07	0.11	0.38	0.76	0.84	-0.04	0.04	0.05	-0.10	-0.47
Tyrosine	-0.25	0.00	0.60	0.48	0.67	-0.20	-0.19	-0.27	0.24	-0.58
Trehalose	0.43	-0.07	-0.59	-0.49	-0.61	0.31	0.32	0.45	-0.18	0.40
Epigallocatechin	-0.53	-0.06	0.32	0.07	0.28	-0.50	-0.49	-0.55	0.46	-0.08
Esculin	-0.25	0.01	-0.26	-0.47	-0.37	-0.19	-0.19	-0.24	0.61	0.31
Gallic.acid	-0.22	0.03	0.68	0.67	0.81	-0.08	-0.20	-0.25	-0.04	-0.52
gamma.Aminobutyric.acid	0.66	-0.09	-0.07	0.34	0.09	0.61	0.71	0.66	-0.46	-0.23

Glutathione	0.75	-0.25	-0.34	-0.09	-0.31	0.58	0.47	0.76	-0.41	0.11
Guanine	-0.14	0.08	0.61	0.78	0.96	-0.08	-0.12	-0.16	0.00	-0.54
Isovitexin	-0.36	-0.16	-0.02	-0.28	-0.16	-0.49	-0.31	-0.38	0.50	0.33
Kaempferin	-0.18	-0.41	0.10	-0.35	-0.20	-0.25	-0.17	-0.17	0.17	0.30
kaempferol	-0.35	-0.20	0.83	0.26	0.40	-0.20	-0.28	-0.38	0.24	-0.31
L.Serine	1.00	-0.09	-0.33	0.30	-0.06	0.68	0.80	0.99	-0.50	-0.02
L.Arginine	0.82	-0.06	-0.27	0.30	-0.01	0.50	0.86	0.81	-0.41	-0.02
L.Aspartic.acid	0.90	-0.22	-0.23	0.31	-0.01	0.70	0.65	0.90	-0.44	-0.01
L.Glutamic.acid	0.95	-0.21	-0.24	0.28	-0.03	0.71	0.68	0.95	-0.47	-0.06
L.Homoserine	0.63	0.31	-0.12	0.61	0.30	0.54	0.44	0.61	-0.43	-0.25
L.Isoleucine	0.04	0.11	0.44	0.83	0.94	0.04	-0.01	0.02	-0.12	-0.58
L.Phenylalanine	0.09	-0.10	0.27	0.52	0.65	0.02	0.02	0.09	0.07	-0.47
L.Proline	0.29	0.00	0.36	0.65	0.55	0.30	0.22	0.28	-0.14	-0.54
L.Theanine	0.76	-0.11	-0.41	0.22	-0.06	0.63	0.49	0.77	-0.52	0.01
L.Tryptophan	0.11	-0.19	-0.26	-0.23	-0.21	-0.11	0.00	0.13	0.30	0.13
Malic.Acid	0.22	-0.19	-0.05	0.01	-0.15	0.31	-0.01	0.22	0.00	0.17
Naringenin	-0.39	-0.11	0.79	0.37	0.53	-0.20	-0.32	-0.42	0.11	-0.30
Neochlorogenic.acid	-0.16	-0.15	0.44	-0.16	-0.03	-0.16	-0.15	-0.17	-0.21	-0.14
Pantothenic.acid	0.38	0.25	-0.19	0.16	-0.08	0.30	0.62	0.40	-0.19	-0.09
Phloretin	-0.27	-0.03	0.72	0.59	0.76	-0.08	-0.22	-0.30	0.16	-0.54
Procyanidin.B4	0.10	-0.23	-0.40	-0.44	-0.51	0.01	0.01	0.10	0.21	0.78
Procyanidin.B3	-0.21	-0.07	-0.17	-0.43	-0.43	-0.35	-0.14	-0.21	0.33	0.69
Prunin	-0.03	-0.25	-0.18	-0.53	-0.43	-0.07	-0.04	0.00	0.05	0.12
Theogallin	0.26	-0.07	-0.02	0.02	-0.16	0.39	0.13	0.26	-0.54	0.15
Theophylline	0.41	0.06	-0.17	0.19	-0.02	0.38	0.64	0.42	-0.34	-0.10
Thymine	0.21	0.52	-0.02	0.49	0.41	0.10	0.21	0.21	-0.16	-0.36

Tricetin	-0.60	-0.08	0.18	-0.16	-0.02	-0.59	-0.46	-0.62	0.57	0.15
Xanthine	0.57	0.05	-0.16	0.26	-0.07	0.48	0.87	0.57	-0.21	-0.06
Xylitol	-0.48	0.27	0.05	-0.07	0.12	-0.36	-0.31	-0.48	0.52	-0.15
Beta.Alanine	0.81	-0.14	-0.10	0.41	0.20	0.67	0.52	0.81	-0.44	-0.30
hydroxy.cinnamic.acid	0.37	0.15	-0.22	-0.07	-0.21	0.52	0.24	0.38	-0.06	0.05
Citric.acid	-0.38	-0.08	0.44	0.17	0.26	-0.17	-0.24	-0.39	0.43	-0.33
Succinic.acid	-0.19	-0.31	0.46	0.16	0.26	0.05	-0.16	-0.20	0.12	-0.41
Alpha.ketoglutaric.acid	-0.49	-0.10	0.42	0.02	0.14	-0.31	-0.34	-0.50	0.47	-0.23
Hydroxycoumarine	0.27	0.15	0.00	0.13	-0.09	0.35	0.48	0.28	-0.28	-0.16
Coumarin	0.03	-0.03	-0.04	-0.16	-0.13	0.10	-0.09	0.03	0.42	-0.09
Glutamine	1.00	-0.13	-0.33	0.28	-0.08	0.68	0.81	1.00	-0.50	-0.01
Delphinidin.3.O.rutinoside.chloride	-0.13	1.00	-0.09	0.21	0.09	0.05	-0.07	-0.13	0.02	-0.23
Eriodictyol	-0.33	-0.09	1.00	0.33	0.48	-0.11	-0.23	-0.35	0.16	-0.42
Glycyl.L.leucine	0.28	0.21	0.33	1.00	0.79	0.32	0.26	0.26	-0.28	-0.48
Guanosine.monophosphate	-0.08	0.09	0.48	0.79	1.00	-0.05	-0.09	-0.10	-0.16	-0.51
Glutathione.oxidized	0.68	0.05	-0.11	0.32	-0.05	1.00	0.57	0.68	-0.34	-0.10
L.Histidine	0.81	-0.07	-0.23	0.26	-0.09	0.57	1.00	0.81	-0.34	-0.07
L.Pyroglutamic.acid	1.00	-0.13	-0.35	0.26	-0.10	0.68	0.81	1.00	-0.50	-0.01
Myricetin	-0.50	0.02	0.16	-0.28	-0.16	-0.34	-0.34	-0.50	1.00	0.00
Naringenin.chalcone	-0.01	-0.23	-0.42	-0.48	-0.51	-0.10	-0.07	-0.01	0.00	1.00
Quercetin	-0.49	0.25	0.32	-0.14	0.05	-0.21	-0.32	-0.47	0.08	-0.19
Quercetin.3beta.D.glucoside	-0.39	-0.07	0.29	-0.35	-0.14	-0.20	-0.28	-0.39	0.75	-0.12
Schaftoside	-0.42	-0.16	0.22	-0.25	-0.15	-0.48	-0.35	-0.42	0.58	0.05
Uridine.monophosphate	0.38	-0.01	0.13	0.61	0.52	0.50	0.40	0.37	-0.36	-0.42
Digallic.acid	0.00	0.07	-0.33	-0.28	-0.31	0.07	0.03	0.03	-0.20	0.12
dihomomethionine	0.15	-0.11	0.24	0.17	0.07	0.18	0.08	0.13	0.24	-0.40

Epigallocatechin.3.O.3.O.methyl..gallate	-0.31	0.45	0.11	0.21	0.29	-0.22	-0.18	-0.31	-0.05	-0.19
Epigallocatechin..4beta..8..epicatechin.3.O.gallate.ester	-0.40	0.15	0.25	0.15	0.23	-0.41	-0.31	-0.41	0.17	-0.08
Epigallocatechin.3..glucuronide	-0.38	-0.26	0.07	-0.55	-0.37	-0.38	-0.25	-0.36	0.35	0.11
Gallocatechin..4alpha..8..epigallocatechin	-0.43	-0.27	0.36	-0.14	0.04	-0.38	-0.29	-0.45	0.27	0.20
S.Adenosyl.L.homocysteine	0.65	0.19	-0.41	0.13	-0.19	0.71	0.63	0.67	-0.47	-0.02
Theasinensin.B	-0.39	0.02	0.31	0.26	0.38	-0.42	-0.34	-0.41	0.22	-0.17
Malonic.acid	-0.21	-0.19	0.13	-0.16	0.03	-0.18	-0.12	-0.23	0.33	0.33
4.Dihydroxybenzoic.acid	-0.46	-0.28	0.24	-0.26	-0.08	-0.55	-0.33	-0.47	0.47	0.02
Aminoadipic.acid	-0.47	0.16	0.44	0.16	0.23	-0.40	-0.38	-0.50	0.20	-0.12
.Adenosine.monophosphate	0.04	0.09	0.27	0.70	0.75	0.12	0.02	0.02	-0.03	-0.48
Hydroxy.3.methylglutaric.acid	-0.31	-0.24	0.26	0.08	0.19	-0.36	-0.28	-0.31	0.20	-0.11
Hydroxybenzoic.acid	0.14	0.73	-0.18	0.36	0.15	0.10	0.07	0.14	-0.13	-0.14
Hydroxybenzaldehyde	-0.12	-0.17	-0.36	-0.48	-0.48	-0.17	-0.14	-0.12	0.08	0.97
Hydroxybenzoic.acid	-0.61	0.04	0.36	-0.16	0.08	-0.56	-0.42	-0.61	0.36	0.02
Oxoproline	0.78	0.03	-0.24	0.27	0.01	0.43	0.65	0.78	-0.43	-0.09
Adenosine.diphosphate	0.59	-0.07	-0.55	-0.28	-0.49	0.56	0.51	0.62	-0.38	0.26
Ellagic.acid	0.53	-0.17	-0.43	-0.25	-0.38	0.48	0.38	0.55	-0.38	0.22
Ethylmalonic.acid	-0.16	-0.18	0.22	-0.05	-0.01	-0.02	-0.20	-0.16	0.29	-0.13
Fumaric.acid	0.43	0.29	0.15	0.56	0.32	0.36	0.45	0.42	-0.28	-0.47
Cyanidin.3.O.galactoside	-0.26	0.34	0.20	-0.03	-0.14	-0.09	-0.20	-0.25	0.12	-0.18
Quinic.acid	0.13	0.28	0.10	0.21	0.11	0.20	0.32	0.13	0.22	-0.30
Theobromine	0.46	0.07	-0.38	0.18	-0.16	0.40	0.40	0.45	-0.35	0.47
trans.p.Coumaric.acid	0.17	0.17	-0.16	-0.07	-0.09	0.31	0.03	0.18	0.06	0.03
Shikimic.acid	0.32	0.25	-0.31	-0.08	-0.22	0.49	0.25	0.34	-0.07	0.03

Table S8-8 Corrected PCC

PCC	Quer cetin	Quercetin.3beta. D.glucoside	Schaft oside	Uridine.mono phosphate	Digalli c.acid	dihomome thionine	Epigallocatechin.3.O..3 .O.methyl..gallate	Epigallocatechin..4beta..8..epic atechin.3.O.gallate.ester	Epigallocatechin. 3..glucuronide	Galocatechin..4alpha..8 ..epigallocatechin
Epigallocatechin.gallate	-0.12	-0.14	0.20	-0.43	0.04	-0.09	-0.16	0.21	0.31	0.25
Catechin	0.32	-0.18	0.12	-0.26	0.22	-0.46	0.64	0.31	-0.15	0.02
Epicatechin	-0.22	0.09	0.40	-0.56	-0.27	-0.08	-0.20	0.42	0.18	0.38
Galocatechin	0.37	-0.24	0.04	-0.03	0.13	-0.27	0.72	0.37	-0.23	-0.13
Methylxanthine	-0.38	-0.54	-0.53	0.36	0.10	-0.27	0.09	-0.01	-0.54	-0.20
Abscisic.acid	0.02	0.35	0.11	0.09	-0.19	0.58	-0.20	-0.11	0.09	0.03
Adenine	0.09	0.03	0.00	0.42	-0.40	0.22	0.24	0.31	-0.31	0.22
Avicularin	0.20	0.89	0.48	-0.26	-0.07	0.21	-0.28	-0.05	0.64	0.37
Quercetin.3.O.sophoroside	0.17	0.29	0.12	-0.27	-0.15	0.02	0.24	0.41	0.08	0.09
Betaine	0.21	0.18	0.40	-0.34	-0.23	0.11	0.09	0.51	0.23	0.50
Caffeine	0.23	-0.19	0.01	-0.21	0.13	-0.15	0.37	0.16	0.06	-0.22
Epicatechin.gallate	-0.20	-0.13	0.01	-0.38	0.16	-0.37	-0.22	-0.14	0.11	0.16
Chlorogenic.acid	0.08	-0.03	-0.15	0.35	0.22	-0.08	0.19	-0.23	-0.11	-0.11
Cynaroside	-0.22	0.50	0.09	-0.01	-0.22	0.55	-0.48	-0.33	0.08	-0.18
Glucuronic.Acid	0.06	0.10	0.14	0.04	-0.27	0.04	0.18	0.34	-0.12	0.10
D.Fructose	-0.13	-0.04	-0.31	0.53	-0.26	0.29	-0.14	-0.04	-0.30	-0.22
D.Gluconic.Acid	0.07	-0.04	0.27	0.15	-0.34	0.04	0.27	0.50	-0.15	0.37
Lysine	-0.13	-0.16	-0.13	0.46	-0.36	0.06	0.23	0.34	-0.45	0.03
Tyrosine	0.08	0.24	0.18	0.25	-0.30	0.32	0.13	0.31	0.08	0.20
Trehalose	-0.19	0.09	-0.18	-0.15	0.24	-0.09	-0.35	-0.51	0.07	-0.36
Epigallocatechin	-0.04	0.05	0.50	-0.34	-0.48	0.12	0.08	0.76	0.07	0.46
Esculin	0.03	0.58	0.40	-0.34	0.11	-0.09	-0.05	-0.16	0.31	0.01
Gallic.acid	0.14	-0.08	-0.06	0.41	-0.36	0.13	0.32	0.38	-0.37	0.19

gamma.Aminobutyric.acid	-0.28	-0.22	-0.50	0.61	0.06	0.04	-0.10	-0.33	-0.38	-0.32
Glutathione	-0.28	-0.17	-0.28	0.06	0.04	0.22	-0.51	-0.48	-0.01	-0.37
Guanine	0.05	-0.01	-0.04	0.46	-0.38	0.17	0.25	0.30	-0.33	0.13
Isovitexin	-0.14	0.14	0.50	-0.43	-0.20	-0.16	0.10	0.45	0.05	0.33
Kaempferin	-0.13	0.20	0.37	-0.35	-0.28	0.12	-0.45	0.19	0.27	0.45
kaempferol	0.04	0.22	0.31	0.04	-0.40	0.30	-0.01	0.48	0.01	0.57
L.Serine	-0.50	-0.40	-0.43	0.38	-0.01	0.14	-0.30	-0.37	-0.40	-0.43
L.Arginine	-0.40	-0.33	-0.39	0.42	0.01	0.00	-0.22	-0.31	-0.35	-0.35
L.Aspartic.acid	-0.44	-0.34	-0.42	0.35	-0.05	0.24	-0.45	-0.44	-0.31	-0.42
L.Glutamic.acid	-0.45	-0.29	-0.43	0.44	0.02	0.21	-0.37	-0.49	-0.37	-0.45
L.Homoserine	-0.39	-0.44	-0.42	0.43	-0.16	0.16	0.02	0.03	-0.69	-0.33
L.Isoleucine	-0.03	-0.12	-0.17	0.53	-0.33	0.20	0.18	0.20	-0.37	-0.03
L.Phenylalanine	-0.02	0.14	-0.03	0.36	-0.16	0.23	0.01	0.03	-0.02	-0.11
L.Proline	-0.24	-0.03	-0.13	0.54	-0.17	0.31	0.00	0.12	-0.38	0.00
L.Theanine	-0.29	-0.42	-0.50	0.41	0.18	0.01	-0.20	-0.52	-0.37	-0.60
L.Tryptophan	-0.30	0.10	0.40	-0.23	-0.09	0.25	-0.31	0.11	0.41	0.03
Malic.Acid	-0.10	-0.12	0.01	0.04	-0.04	0.15	-0.21	-0.08	-0.22	0.00
Naringenin	0.25	0.10	0.22	0.08	-0.39	0.16	0.14	0.40	-0.10	0.47
Neochlorogenic.acid	0.33	0.12	0.00	-0.12	0.09	0.04	-0.01	-0.08	0.36	0.05
Pantothenic.acid	-0.08	-0.27	-0.12	0.20	0.04	0.08	-0.02	0.05	-0.01	-0.20
Phloretin	0.15	0.11	0.02	0.40	-0.40	0.25	0.22	0.31	-0.26	0.22
Procyanidin.B4	-0.35	0.12	0.16	-0.50	-0.09	-0.02	-0.44	-0.07	0.20	0.11
Procyanidin.B3	-0.15	0.10	0.46	-0.60	-0.08	-0.12	-0.11	0.30	0.30	0.40
Prunin	0.19	0.40	0.29	-0.10	0.38	0.06	-0.16	-0.41	0.67	-0.04
Theogallin	0.14	-0.28	-0.33	0.11	0.26	0.09	-0.12	-0.42	0.07	-0.16
Theophylline	0.07	-0.31	-0.42	0.62	0.46	-0.35	0.35	-0.27	-0.23	-0.26

Thymine	-0.19	-0.17	-0.18	0.30	-0.11	-0.06	0.24	0.32	-0.37	-0.13
Tricetin	-0.12	0.16	0.59	-0.49	-0.38	0.01	0.06	0.68	0.15	0.51
Xanthine	-0.20	-0.21	-0.28	0.36	0.02	0.01	-0.05	-0.15	-0.20	-0.16
Xylitol	0.06	0.39	0.27	-0.20	-0.11	0.06	0.19	0.32	0.22	0.01
Beta.Alanine	-0.40	-0.22	-0.47	0.58	-0.03	0.25	-0.26	-0.46	-0.47	-0.50
hydroxy.cinnamic.acid	-0.14	-0.05	-0.27	0.04	0.02	0.34	-0.34	-0.23	-0.04	-0.15
Citric.acid	0.21	0.48	0.32	-0.02	-0.18	0.35	-0.07	-0.05	0.37	0.04
Succinic.acid	0.13	0.35	0.18	0.33	-0.06	0.30	-0.05	-0.11	0.12	0.09
Alpha.ketoglutaric.acid	0.23	0.52	0.44	-0.22	-0.19	0.28	-0.10	0.04	0.47	0.16
Hydroxycoumarine	0.06	-0.04	-0.19	0.36	0.24	-0.09	0.15	-0.29	-0.13	-0.14
Coumarin	-0.20	0.28	0.21	-0.23	-0.27	0.57	-0.46	0.01	0.21	0.05
Glutamine	-0.49	-0.39	-0.42	0.38	0.00	0.15	-0.31	-0.40	-0.38	-0.43
Delphinidin.3.O.rutinoside.chlo ride	0.25	-0.07	-0.16	-0.01	0.07	-0.11	0.45	0.15	-0.26	-0.27
Eriodictyol	0.32	0.29	0.22	0.13	-0.33	0.24	0.11	0.25	0.07	0.36
Glycyl.L.leucine	-0.14	-0.35	-0.25	0.61	-0.28	0.17	0.21	0.15	-0.55	-0.14
Guanosine.monophosphate	0.05	-0.14	-0.15	0.52	-0.31	0.07	0.29	0.23	-0.37	0.04
Glutathione.oxidized	-0.21	-0.20	-0.48	0.50	0.07	0.18	-0.22	-0.41	-0.38	-0.38
L.Histidine	-0.32	-0.28	-0.35	0.40	0.03	0.08	-0.18	-0.31	-0.25	-0.29
L.Pyroglutamic.acid	-0.47	-0.39	-0.42	0.37	0.03	0.13	-0.31	-0.41	-0.36	-0.45
Myricetin	0.08	0.75	0.58	-0.36	-0.20	0.24	-0.05	0.17	0.35	0.27
Naringenin.chalcone	-0.19	-0.12	0.05	-0.42	0.12	-0.40	-0.19	-0.08	0.11	0.20
Quercetin	1.00	0.24	0.00	-0.07	0.41	-0.26	0.56	-0.13	0.31	-0.05
Quercetin.3beta.D.glucoside	0.24	1.00	0.44	-0.21	-0.10	0.30	-0.20	-0.16	0.50	0.15
Schaftoside	0.00	0.44	1.00	-0.48	-0.31	0.27	-0.10	0.38	0.49	0.42
Uridine.monophosphate	-0.07	-0.21	-0.48	1.00	0.16	-0.03	0.21	-0.27	-0.42	-0.30

Digallic.acid	0.41	-0.10	-0.31	0.16	1.00	-0.43	0.37	-0.43	0.16	-0.26
dihomomethionine	-0.26	0.30	0.27	-0.03	-0.43	1.00	-0.54	-0.01	0.22	-0.02
Epigallocatechin.3.O..3.O.meth yl..gallate	0.56	-0.20	-0.10	0.21	0.37	-0.54	1.00	0.17	-0.25	-0.11
Epigallocatechin..4beta..8..epic atechin.3.O.gallate.ester	-0.13	-0.16	0.38	-0.27	-0.43	-0.01	0.17	1.00	-0.10	0.57
Epigallocatechin..3..glucuronide	0.31	0.50	0.49	-0.42	0.16	0.22	-0.25	-0.10	1.00	0.15
Gallocatechin..4alpha..8..epigal locatechin	-0.05	0.15	0.42	-0.30	-0.26	-0.02	-0.11	0.57	0.15	1.00
S.Adenosyl.L.homocysteine	-0.08	-0.38	-0.53	0.49	0.46	-0.18	0.07	-0.46	-0.24	-0.52
Theasinensin.B	-0.24	-0.07	0.39	-0.18	-0.49	0.13	0.01	0.88	-0.05	0.59
Malonic.acid	0.07	0.22	0.15	-0.03	0.05	-0.40	0.20	0.04	-0.13	0.37
4.Dihydroxybenzoic.acid	0.07	0.24	0.52	-0.31	-0.11	0.00	0.08	0.40	0.52	0.28
Aminoadipic.acid	0.06	0.09	0.39	-0.23	-0.36	0.08	0.23	0.67	-0.06	0.53
.Adenosine.monophosphate	-0.18	-0.02	-0.13	0.53	-0.20	0.32	0.10	0.16	-0.29	-0.02
Hydroxy.3.methylglutaric.acid	-0.10	0.06	0.63	-0.16	-0.30	0.27	-0.05	0.33	0.30	0.32
Hydroxybenzoic.acid	0.06	-0.42	-0.14	0.04	0.03	-0.12	0.49	0.15	-0.43	-0.34
Hydroxybenzaldehyde	-0.16	-0.09	0.08	-0.46	0.12	-0.41	-0.14	-0.01	0.13	0.25
Hydroxybenzoic.acid	0.28	0.28	0.35	-0.32	-0.06	-0.09	0.26	0.39	0.40	0.26
Oxoproline	-0.39	-0.39	-0.23	0.16	-0.08	0.16	-0.16	-0.13	-0.37	-0.33
Adenosine.diphosphate	-0.17	-0.14	-0.36	0.12	0.27	-0.03	-0.37	-0.55	0.00	-0.46
Ellagic.acid	-0.12	0.00	-0.42	0.27	0.40	-0.04	-0.33	-0.68	0.02	-0.40
Ethylmalonic.acid	0.12	0.28	0.20	-0.01	-0.04	0.41	-0.19	-0.03	0.23	0.13
Fumaric.acid	-0.08	-0.30	-0.33	0.53	0.02	0.10	0.23	0.01	-0.43	-0.20
Cyanidin.3.O.galactoside	0.45	0.15	0.29	-0.24	0.00	0.31	0.13	-0.03	0.24	-0.02
Quinic.acid	-0.18	0.25	0.24	0.18	-0.23	0.25	-0.04	0.13	-0.06	0.09

Theobromine	-0.55	-0.44	-0.35	0.09	-0.05	-0.21	-0.18	-0.04	-0.39	-0.09
trans.p.Coumaric.acid	-0.11	-0.01	-0.12	-0.08	-0.11	0.38	-0.34	-0.06	0.04	-0.07
Shikimic.acid	-0.07	-0.10	-0.30	0.05	0.12	0.23	-0.19	-0.23	-0.07	-0.27

Table S8-9 Corrected PCC

PCC	S.Adenosyl.L.hom ocysteine	Theasinen sin.B	Malonic. acid	4.Dihydroxybenz oic.acid	Aminoadipi c.acid	.Adenosine.monop hosphate	Hydroxy.3.methylgl utaric.acid	Hydroxybenz oic.acid	Hydroxybenzal dehyde	Hydroxybenz oic.acid
Epigallocatechin.gallate	-0.10	0.22	0.13	0.33	-0.03	-0.28	0.17	-0.04	0.64	0.35
Catechin	0.07	0.02	0.17	0.04	0.30	-0.25	-0.10	0.64	0.30	0.25
Epicatechin	-0.44	0.40	0.27	0.43	0.05	-0.24	0.17	-0.14	0.61	0.26
Gallocatechin	0.14	0.11	-0.10	-0.05	0.38	-0.02	-0.06	0.76	-0.16	0.18
Methylxanthine	0.60	-0.03	-0.03	-0.43	-0.10	0.14	-0.30	0.37	0.19	-0.26
Abscisic.acid	-0.17	-0.01	0.02	0.07	0.00	0.06	0.18	-0.11	-0.30	-0.13
Adenine	-0.37	0.44	0.15	0.04	0.43	0.70	0.28	0.05	-0.49	0.15
Avicularin	-0.44	0.03	0.26	0.38	0.10	-0.07	0.08	-0.64	0.07	0.42
Quercetin.3.O.sophoroside	-0.41	0.38	0.10	0.31	0.36	0.23	-0.02	0.26	0.05	0.64
Betaine	-0.68	0.43	0.09	0.46	0.63	0.09	0.17	-0.01	0.05	0.51
Caffeine	0.06	0.12	-0.02	0.15	0.09	-0.01	0.20	0.48	0.24	0.39
Epicatechin.gallate	0.06	-0.20	0.29	-0.03	-0.18	-0.46	-0.14	-0.11	0.96	-0.03
Chlorogenic.acid	0.43	-0.32	0.03	-0.28	0.04	0.04	-0.10	0.12	-0.21	-0.11
Cynaroside	0.14	-0.27	-0.16	-0.30	-0.10	-0.02	-0.07	-0.05	-0.26	-0.38
Glucuronic.Acid	-0.27	0.43	0.08	0.17	0.46	0.37	0.25	0.29	-0.20	0.33
D.Fructose	0.07	0.05	-0.18	-0.12	-0.08	0.57	-0.18	-0.02	-0.54	-0.10
D.Gluconic.Acid	-0.57	0.58	0.23	0.43	0.46	0.43	0.44	-0.02	-0.21	0.38
Lysine	-0.17	0.45	0.09	0.01	0.33	0.67	0.11	0.20	-0.45	0.08
Tyrosine	-0.39	0.48	0.02	0.36	0.31	0.60	0.29	-0.03	-0.50	0.41
Trehalose	0.42	-0.57	-0.12	-0.35	-0.59	-0.43	-0.38	-0.11	0.30	-0.36
Epigallocatechin	-0.66	0.80	0.14	0.60	0.46	0.16	0.49	0.00	0.02	0.51
Esculin	-0.07	-0.15	0.31	0.08	-0.16	-0.23	0.06	-0.08	0.34	0.16
Gallic.acid	-0.38	0.43	0.13	0.09	0.53	0.58	0.18	0.09	-0.46	0.21

gamma.Aminobutyric.acid	0.49	-0.32	-0.12	-0.32	-0.30	0.20	-0.40	-0.06	-0.32	-0.34
Glutathione	0.50	-0.47	-0.36	-0.40	-0.58	-0.20	-0.29	-0.11	-0.01	-0.60
Guanine	-0.30	0.45	0.10	0.01	0.37	0.75	0.24	0.11	-0.50	0.14
Isovitexin	-0.57	0.38	0.43	0.62	0.31	-0.18	0.18	-0.03	0.38	0.51
Kaempferin	-0.32	0.21	0.04	0.12	0.09	-0.18	0.17	-0.52	0.26	-0.09
kaempferol	-0.56	0.55	0.18	0.41	0.55	0.38	0.32	-0.29	-0.25	0.45
L.Serine	0.66	-0.37	-0.23	-0.48	-0.47	0.06	-0.31	0.18	-0.13	-0.60
L.Arginine	0.55	-0.32	-0.11	-0.37	-0.37	0.08	-0.32	0.08	-0.12	-0.49
L.Aspartic.acid	0.53	-0.37	-0.24	-0.42	-0.51	0.09	-0.30	0.03	-0.11	-0.60
L.Glutamic.acid	0.58	-0.44	-0.20	-0.46	-0.52	0.10	-0.32	0.03	-0.18	-0.63
L.Homoserine	0.39	-0.02	-0.18	-0.52	0.13	0.35	-0.22	0.51	-0.29	-0.45
L.Isoleucine	-0.14	0.38	-0.05	-0.10	0.18	0.79	0.14	0.19	-0.55	0.01
L.Phenylalanine	-0.07	0.23	-0.06	0.12	-0.08	0.60	0.15	0.03	-0.46	0.10
L.Proline	0.14	0.29	-0.04	-0.19	0.14	0.65	0.17	0.06	-0.56	-0.18
L.Theanine	0.66	-0.48	-0.25	-0.49	-0.64	0.03	-0.31	0.12	-0.11	-0.64
L.Tryptophan	0.03	0.19	-0.12	0.37	-0.24	-0.14	0.25	-0.03	0.13	0.02
Malic.Acid	0.07	-0.13	0.01	-0.19	-0.13	-0.07	-0.16	-0.03	0.10	-0.39
Naringenin	-0.50	0.43	0.15	0.09	0.58	0.21	0.30	-0.10	-0.25	0.13
Neochlorogenic.acid	-0.25	-0.09	-0.14	0.31	0.12	-0.07	-0.05	-0.27	-0.12	0.54
Pantothenic.acid	0.51	-0.03	-0.29	-0.07	-0.25	0.01	-0.08	0.21	-0.09	-0.13
Phloretin	-0.42	0.40	0.14	0.14	0.43	0.57	0.21	-0.03	-0.48	0.19
Procyanidin.B4	-0.11	-0.09	0.21	0.09	-0.20	-0.36	-0.12	-0.17	0.76	0.08
Procyanidin.B3	-0.33	0.18	0.31	0.38	0.20	-0.36	0.10	0.00	0.74	0.42
Prunin	0.20	-0.38	-0.13	0.03	-0.29	-0.31	0.13	-0.35	0.08	-0.10
Theogallin	0.30	-0.46	-0.26	-0.38	-0.15	-0.13	-0.18	0.03	0.09	-0.27
Theophylline	0.72	-0.36	0.04	-0.24	-0.34	0.01	-0.26	0.11	-0.13	-0.28

Thymine	0.24	0.32	-0.14	-0.17	0.19	0.46	-0.10	0.46	-0.34	0.00
Tricetin	-0.69	0.66	0.25	0.67	0.52	-0.01	0.42	-0.06	0.26	0.63
Xanthine	0.52	-0.21	-0.01	-0.22	-0.23	0.03	-0.23	0.08	-0.09	-0.23
Xylitol	-0.32	0.31	0.06	0.40	0.26	0.26	0.13	0.04	-0.05	0.59
Beta.Alanine	0.50	-0.35	-0.22	-0.46	-0.45	0.33	-0.26	0.05	-0.40	-0.57
hydroxy.cinnamic.acid	0.41	-0.23	-0.19	-0.39	-0.42	-0.12	-0.25	0.06	0.00	-0.48
Citric.acid	-0.34	0.11	0.04	0.34	0.21	0.35	0.41	-0.21	-0.27	0.39
Succinic.acid	-0.17	0.05	0.05	0.09	0.09	0.29	0.35	-0.39	-0.42	-0.03
Alpha.ketoglutaric.acid	-0.48	0.19	0.09	0.43	0.28	0.21	0.44	-0.28	-0.16	0.47
Hydroxycoumarine	0.46	-0.37	0.02	-0.32	0.01	0.03	-0.13	0.10	-0.19	-0.15
Coumarin	-0.10	0.11	-0.12	0.04	-0.18	-0.01	0.16	-0.11	-0.09	-0.20
Glutamine	0.65	-0.39	-0.21	-0.46	-0.47	0.04	-0.31	0.14	-0.12	-0.61
Delphinidin.3.O.rutinoside.chloride	0.19	0.02	-0.19	-0.28	0.16	0.09	-0.24	0.73	-0.17	0.04
Eriodictyol	-0.41	0.31	0.13	0.24	0.44	0.27	0.26	-0.18	-0.36	0.36
Glycyl.L.leucine	0.13	0.26	-0.16	-0.26	0.16	0.70	0.08	0.36	-0.48	-0.16
Guanosine.monophosphate	-0.19	0.38	0.03	-0.08	0.23	0.75	0.19	0.15	-0.48	0.08
Glutathione.oxidized	0.71	-0.42	-0.18	-0.55	-0.40	0.12	-0.36	0.10	-0.17	-0.56
L.Histidine	0.63	-0.34	-0.12	-0.33	-0.38	0.02	-0.28	0.07	-0.14	-0.42
L.Pyroglutamic.acid	0.67	-0.41	-0.23	-0.47	-0.50	0.02	-0.31	0.14	-0.12	-0.61
Myricetin	-0.47	0.22	0.33	0.47	0.20	-0.03	0.20	-0.13	0.08	0.36
Naringenin.chalcone	-0.02	-0.17	0.33	0.02	-0.12	-0.48	-0.11	-0.14	0.97	0.02
Quercetin	-0.08	-0.24	0.07	0.07	0.06	-0.18	-0.10	0.06	-0.16	0.28
Quercetin.3beta.D.glucoside	-0.38	-0.07	0.22	0.24	0.09	-0.02	0.06	-0.42	-0.09	0.28
Schaftoside	-0.53	0.39	0.15	0.52	0.39	-0.13	0.63	-0.14	0.08	0.35
Uridine.monophosphate	0.49	-0.18	-0.03	-0.31	-0.23	0.53	-0.16	0.04	-0.46	-0.32
Digallic.acid	0.46	-0.49	0.05	-0.11	-0.36	-0.20	-0.30	0.03	0.12	-0.06

dihomomethionine	-0.18	0.13	-0.40	0.00	0.08	0.32	0.27	-0.12	-0.41	-0.09
Epigallocatechin.3.O..3.O.methyl.gal late	0.07	0.01	0.20	0.08	0.23	0.10	-0.05	0.49	-0.14	0.26
Epigallocatechin.4beta..8..epicatechi n.3.O.gallate.ester	-0.46	0.88	0.04	0.40	0.67	0.16	0.33	0.15	-0.01	0.39
Epigallocatechin.3..glucuronide	-0.24	-0.05	-0.13	0.52	-0.06	-0.29	0.30	-0.43	0.13	0.40
Gallocatechin..4alpha..8..epigallocate chin	-0.52	0.59	0.37	0.28	0.53	-0.02	0.32	-0.34	0.25	0.26
S.Adenosyl.L.homocysteine	1.00	-0.52	-0.24	-0.49	-0.56	-0.08	-0.35	0.26	-0.08	-0.53
Theasinensin.B	-0.52	1.00	0.02	0.41	0.54	0.32	0.48	0.01	-0.09	0.37
Malonic.acid	-0.24	0.02	1.00	0.17	0.17	-0.07	0.08	-0.18	0.37	0.15
4.Dihydroxybenzoic.acid	-0.49	0.41	0.17	1.00	0.24	-0.09	0.40	-0.23	0.09	0.74
Aminoadipic.acid	-0.56	0.54	0.17	0.24	1.00	0.15	0.31	0.11	-0.06	0.37
.Adenosine.monophosphate	-0.08	0.32	-0.07	-0.09	0.15	1.00	0.16	0.10	-0.46	0.05
Hydroxy.3.methylglutaric.acid	-0.35	0.48	0.08	0.40	0.31	0.16	1.00	-0.07	-0.06	0.21
Hydroxybenzoic.acid	0.26	0.01	-0.18	-0.23	0.11	0.10	-0.07	1.00	-0.10	-0.06
Hydroxybenzaldehyde	-0.08	-0.09	0.37	0.09	-0.06	-0.46	-0.06	-0.10	1.00	0.12
Hydroxybenzoic.acid	-0.53	0.37	0.15	0.74	0.37	0.05	0.21	-0.06	0.12	1.00
Oxoproline	0.47	-0.18	-0.17	-0.35	-0.14	0.07	-0.07	0.29	-0.17	-0.39
Adenosine.diphosphate	0.71	-0.61	-0.26	-0.46	-0.64	-0.36	-0.40	-0.08	0.16	-0.56
Ellagic.acid	0.55	-0.69	-0.19	-0.47	-0.62	-0.23	-0.45	-0.20	0.10	-0.57
Ethylmalonic.acid	-0.23	0.06	0.11	0.20	0.11	0.08	0.26	-0.21	-0.12	-0.02
Fumaric.acid	0.40	-0.06	-0.04	-0.24	0.14	0.40	-0.16	0.35	-0.47	-0.17
Cyanidin.3.O.galactoside	-0.12	-0.13	-0.26	-0.14	0.32	-0.18	0.12	0.31	-0.17	-0.08
Quinic.acid	0.23	0.14	0.05	-0.17	0.17	0.23	0.21	0.13	-0.29	-0.13
Theobromine	0.40	-0.05	0.04	-0.28	-0.07	-0.04	-0.27	0.19	0.45	-0.18

trans.p.Coumaric.acid	0.22	-0.03	-0.22	-0.27	-0.32	-0.04	-0.06	0.06	0.01	-0.39
Shikimic.acid	0.54	-0.26	-0.20	-0.41	-0.43	-0.13	-0.21	0.17	-0.01	-0.44

Table S8-10 Corrected PCC

PCC	Oxoproline	Adenosine.diphosphate	Ellagic.acid	Ethylmalonic.acid	Fumaric.acid	Cyanidin.3.O.galactoside	Quinic.acid	Theobromine	trans.p.Coumaric.acid	Shikimic.acid
Epigallocatechin.gallate	-0.17	0.01	-0.13	0.04	-0.37	-0.09	-0.18	0.27	0.19	0.14
Catechin	-0.02	-0.13	-0.28	-0.22	0.05	0.24	0.17	0.11	-0.09	0.05
Epicatechin	-0.27	-0.16	-0.29	0.06	-0.56	-0.23	-0.20	0.00	0.26	0.04
Gallocatechin	0.08	-0.20	-0.34	-0.20	0.32	0.37	0.28	-0.05	-0.11	0.02
Methylxanthine	0.33	0.29	0.12	-0.38	0.38	-0.26	0.19	0.87	-0.02	0.23
Abscisic.acid	-0.18	-0.15	-0.01	0.59	-0.02	0.23	0.09	-0.40	0.47	0.34
Adenine	-0.09	-0.65	-0.51	0.19	0.35	0.00	0.14	-0.27	-0.11	-0.28
Avicularin	-0.45	-0.17	-0.03	0.25	-0.35	-0.01	0.16	-0.39	-0.11	-0.22
Quercetin.3.O.sophoroside	-0.36	-0.52	-0.56	-0.06	0.01	0.05	0.09	-0.07	-0.08	-0.13
Betaine	-0.36	-0.60	-0.51	0.24	-0.07	0.32	-0.20	-0.27	-0.22	-0.47
Caffeine	-0.06	-0.15	-0.42	-0.03	-0.03	0.10	0.01	0.13	0.05	0.16
Epicatechin.gallate	-0.10	0.29	0.24	-0.14	-0.44	-0.15	-0.28	0.54	0.07	0.08
Chlorogenic.acid	0.22	0.20	0.22	-0.12	0.49	0.20	0.48	0.16	-0.30	-0.01
Cynaroside	0.21	0.33	0.37	0.28	0.03	0.27	0.47	-0.01	0.41	0.38
Glucuronic.Acid	-0.19	-0.52	-0.61	0.17	0.19	0.02	0.32	0.07	-0.17	-0.26
D.Fructose	0.27	0.03	0.07	0.14	0.43	-0.21	0.11	-0.06	0.04	-0.03
D.Gluconic.Acid	-0.29	-0.73	-0.67	0.23	0.02	-0.11	-0.12	-0.28	-0.25	-0.50
Lysine	0.14	-0.49	-0.40	0.02	0.48	-0.20	0.18	0.03	-0.19	-0.30
Tyrosine	-0.17	-0.61	-0.47	0.25	0.21	-0.09	0.18	-0.35	-0.15	-0.33
Trehalose	0.26	0.76	0.76	-0.19	-0.30	-0.10	-0.04	0.20	0.27	0.39
Epigallocatechin	-0.29	-0.66	-0.79	0.20	-0.21	-0.12	-0.03	-0.28	0.05	-0.21
Esculin	-0.21	0.09	0.05	-0.02	-0.34	-0.05	0.28	-0.10	0.04	0.16
Gallic.acid	-0.10	-0.66	-0.51	0.18	0.37	0.04	0.00	-0.20	-0.22	-0.35
gamma.Aminobutyric.acid	0.45	0.37	0.47	-0.13	0.45	-0.30	0.12	0.26	-0.11	0.05

Glutathione	0.48	0.72	0.68	-0.01	-0.03	-0.06	-0.09	0.21	0.41	0.43
Guanine	-0.03	-0.60	-0.46	0.12	0.36	-0.06	0.17	-0.20	-0.11	-0.27
Isovitexin	-0.24	-0.43	-0.43	-0.03	-0.30	-0.13	-0.24	-0.05	-0.29	-0.41
Kaempferin	-0.20	0.07	0.02	0.15	-0.39	-0.01	0.07	-0.16	0.20	-0.06
kaempferol	-0.25	-0.64	-0.52	0.26	0.13	0.03	0.03	-0.24	-0.18	-0.39
L.Serine	0.79	0.59	0.52	-0.17	0.44	-0.27	0.16	0.48	0.19	0.33
L.Arginine	0.62	0.51	0.45	-0.21	0.43	-0.29	0.20	0.42	-0.05	0.12
L.Aspartic.acid	0.62	0.55	0.48	-0.04	0.31	-0.23	-0.04	0.45	0.22	0.30
L.Glutamic.acid	0.68	0.60	0.61	-0.06	0.36	-0.25	0.02	0.36	0.19	0.28
L.Homoserine	0.65	0.20	0.13	-0.08	0.62	-0.04	0.24	0.43	0.11	0.21
L.Isoleucine	0.08	-0.45	-0.33	0.07	0.41	-0.12	0.16	-0.14	-0.02	-0.15
L.Phenylalanine	0.09	-0.22	-0.11	0.14	0.21	-0.23	0.11	-0.28	0.00	-0.14
L.Proline	0.31	-0.15	-0.09	0.16	0.49	-0.18	0.41	0.03	0.02	0.02
L.Theanine	0.56	0.67	0.59	-0.15	0.29	-0.18	-0.13	0.31	0.19	0.34
L.Tryptophan	0.08	0.14	0.04	0.23	-0.27	-0.19	0.15	-0.10	0.43	0.27
Malic.Acid	0.09	0.20	0.21	0.18	0.09	0.22	-0.28	0.03	0.26	0.14
Naringenin	-0.27	-0.59	-0.47	0.20	0.03	0.30	-0.02	-0.33	-0.10	-0.30
Neochlorogenic.acid	-0.15	-0.16	-0.03	0.03	0.04	0.09	-0.35	-0.17	-0.40	-0.40
Pantothenic.acid	0.39	0.38	0.10	-0.05	0.30	-0.08	0.41	0.15	0.35	0.42
Phloretin	-0.20	-0.65	-0.50	0.31	0.23	0.02	0.04	-0.36	-0.09	-0.27
Procyanidin.B4	0.04	0.27	0.19	-0.08	-0.47	-0.20	-0.17	0.37	0.24	0.19
Procyanidin.B3	-0.10	-0.12	-0.19	-0.07	-0.36	-0.03	-0.08	0.19	-0.04	-0.10
Prunin	-0.13	0.36	0.48	0.07	-0.32	0.21	0.05	-0.26	0.07	0.09
Theogallin	0.15	0.34	0.44	-0.05	0.12	0.41	-0.36	0.21	0.00	0.08
Theophylline	0.29	0.34	0.33	-0.23	0.48	-0.19	0.20	0.15	-0.10	0.19
Thymine	0.28	-0.07	-0.17	-0.15	0.48	-0.22	0.55	0.24	-0.02	0.04

Tricetin	-0.37	-0.63	-0.72	0.03	-0.27	-0.05	-0.09	-0.11	-0.24	-0.39
Xanthine	0.47	0.35	0.19	-0.19	0.44	-0.16	0.40	0.35	0.01	0.25
Xylitol	-0.28	-0.37	-0.49	-0.03	-0.05	-0.19	0.26	-0.18	-0.19	-0.18
Beta.Alanine	0.57	0.42	0.50	-0.01	0.40	-0.26	0.03	0.22	0.14	0.19
hydroxy.cinnamic.acid	0.24	0.51	0.42	0.20	0.01	0.05	0.15	0.08	0.90	0.91
Citric.acid	-0.25	-0.40	-0.37	0.30	0.02	0.22	0.14	-0.28	-0.22	-0.32
Succinic.acid	-0.20	-0.21	0.03	0.40	-0.01	0.11	0.12	-0.45	-0.07	-0.20
Alpha.ketoglutaric.acid	-0.32	-0.44	-0.45	0.22	-0.12	0.21	0.09	-0.30	-0.28	-0.39
Hydroxycoumarine	0.25	0.25	0.28	-0.14	0.50	0.19	0.45	0.20	-0.31	-0.02
Coumarin	0.03	0.11	0.05	0.41	-0.19	0.04	0.19	-0.27	0.79	0.63
Glutamine	0.78	0.59	0.53	-0.16	0.43	-0.26	0.13	0.46	0.17	0.32
Delphinidin.3.O.rutinoside.chloride	0.03	-0.07	-0.17	-0.18	0.29	0.34	0.28	0.07	0.17	0.25
Eriodictyol	-0.24	-0.55	-0.43	0.22	0.15	0.20	0.10	-0.38	-0.16	-0.31
Glycyl.L.leucine	0.27	-0.28	-0.25	-0.05	0.56	-0.03	0.21	0.18	-0.07	-0.08
Guanosine.monophosphate	0.01	-0.49	-0.38	-0.01	0.32	-0.14	0.11	-0.16	-0.09	-0.22
Glutathione.oxidized	0.43	0.56	0.48	-0.02	0.36	-0.09	0.20	0.40	0.31	0.49
L.Histidine	0.65	0.51	0.38	-0.20	0.45	-0.20	0.32	0.40	0.03	0.25
L.Pyroglutamic.acid	0.78	0.62	0.55	-0.16	0.42	-0.25	0.13	0.45	0.18	0.34
Myricetin	-0.43	-0.38	-0.38	0.29	-0.28	0.12	0.22	-0.35	0.06	-0.07
Naringenin.chalcone	-0.09	0.26	0.22	-0.13	-0.47	-0.18	-0.30	0.47	0.03	0.03
Quercetin	-0.39	-0.17	-0.12	0.12	-0.08	0.45	-0.18	-0.55	-0.11	-0.07
Quercetin.3beta.D.glucoside	-0.39	-0.14	0.00	0.28	-0.30	0.15	0.25	-0.44	-0.01	-0.10
Schaftoside	-0.23	-0.36	-0.42	0.20	-0.33	0.29	0.24	-0.35	-0.12	-0.30
Uridine.monophosphate	0.16	0.12	0.27	-0.01	0.53	-0.24	0.18	0.09	-0.08	0.05
Digallic.acid	-0.08	0.27	0.40	-0.04	0.02	0.00	-0.23	-0.05	-0.11	0.12
dihomomethionine	0.16	-0.03	-0.04	0.41	0.10	0.31	0.25	-0.21	0.38	0.23

Epigallocatechin.3.O..3.O.methyl..gallate	-0.16	-0.37	-0.33	-0.19	0.23	0.13	-0.04	-0.18	-0.34	-0.19
Epigallocatechin..4beta..8..epicatechin.3.O.gallate.ester	-0.13	-0.55	-0.68	-0.03	0.01	-0.03	0.13	-0.04	-0.06	-0.23
Epigallocatechin.3..glucuronide	-0.37	0.00	0.02	0.23	-0.43	0.24	-0.06	-0.39	0.04	-0.07
Gallocatechin..4alpha..8..epigallocatechin	-0.33	-0.46	-0.40	0.13	-0.20	-0.02	0.09	-0.09	-0.07	-0.27
S.Adenosyl.L.homocysteine	0.47	0.71	0.55	-0.23	0.40	-0.12	0.23	0.40	0.22	0.54
Theasinensin.B	-0.18	-0.61	-0.69	0.06	-0.06	-0.13	0.14	-0.05	-0.03	-0.26
Malonic.acid	-0.17	-0.26	-0.19	0.11	-0.04	-0.26	0.05	0.04	-0.22	-0.20
4.Dihydroxybenzoic.acid	-0.35	-0.46	-0.47	0.20	-0.24	-0.14	-0.17	-0.28	-0.27	-0.41
Aminoadipic.acid	-0.14	-0.64	-0.62	0.11	0.14	0.32	0.17	-0.07	-0.32	-0.43
.Adenosine.monophosphate	0.07	-0.36	-0.23	0.08	0.40	-0.18	0.23	-0.04	-0.04	-0.13
Hydroxy.3.methylglutaric.acid	-0.07	-0.40	-0.45	0.26	-0.16	0.12	0.21	-0.27	-0.06	-0.21
Hydroxybenzoic.acid	0.29	-0.08	-0.20	-0.21	0.35	0.31	0.13	0.19	0.06	0.17
Hydroxybenzaldehyde	-0.17	0.16	0.10	-0.12	-0.47	-0.17	-0.29	0.45	0.01	-0.01
Hydroxybenzoic.acid	-0.39	-0.56	-0.57	-0.02	-0.17	-0.08	-0.13	-0.18	-0.39	-0.44
Oxoproline	1.00	0.36	0.21	-0.16	0.48	-0.15	0.24	0.32	0.12	0.28
Adenosine.diphosphate	0.36	1.00	0.80	-0.14	-0.02	-0.10	0.05	0.31	0.35	0.53
Ellagic.acid	0.21	0.80	1.00	-0.02	-0.06	-0.06	-0.10	0.12	0.24	0.34
Ethylmalonic.acid	-0.16	-0.14	-0.02	1.00	-0.05	0.18	0.10	-0.31	0.27	0.09
Fumaric.acid	0.48	-0.02	-0.06	-0.05	1.00	0.04	0.34	0.18	-0.12	0.05
Cyanidin.3.O.galactoside	-0.15	-0.10	-0.06	0.18	0.04	1.00	0.02	-0.29	0.09	0.02
Quinic.acid	0.24	0.05	-0.10	0.10	0.34	0.02	1.00	0.05	0.14	0.27
Theobromine	0.32	0.31	0.12	-0.31	0.18	-0.29	0.05	1.00	-0.06	0.10
trans.p.Coumaric.acid	0.12	0.35	0.24	0.27	-0.12	0.09	0.14	-0.06	1.00	0.84
Shikimic.acid	0.28	0.53	0.34	0.09	0.05	0.02	0.27	0.10	0.84	1.00

Table S9-1 Corrected *p*-value

<i>p</i> -value	Epigallocatechin.gallate	Catechin	Epicatechin	Gallocatechin	Methylxanthine	Abscisic.acid	Adenine	Avicularin	Quercetin.3.O.sophoroside	Betaine
Epigallocatechin.gallate	0.00	0.14	0.00	0.48	0.44	0.83	0.01	0.78	0.03	0.51
Catechin	0.08	0.00	0.25	0.00	0.09	0.01	0.08	0.03	0.00	0.26
Epicatechin	0.00	0.17	0.00	0.14	0.09	0.92	0.14	0.08	0.02	0.01
Gallocatechin	0.38	0.00	0.08	0.00	0.11	0.07	0.79	0.00	0.00	0.28
Methylxanthine	0.33	0.05	0.05	0.06	0.00	0.00	0.39	0.00	0.88	0.00
Abscisic.acid	0.76	0.00	0.90	0.04	0.00	0.00	0.02	0.15	0.80	0.56
Adenine	0.00	0.04	0.08	0.72	0.29	0.01	0.00	0.96	0.07	0.01
Avicularin	0.70	0.01	0.04	0.00	0.00	0.09	0.95	0.00	0.06	0.02
Quercetin.3.O.sophoroside	0.01	0.00	0.01	0.00	0.84	0.73	0.03	0.03	0.00	0.00
Betaine	0.41	0.18	0.01	0.19	0.00	0.46	0.00	0.01	0.00	0.00
Caffeine	0.00	0.00	0.09	0.00	0.05	0.41	1.00	0.02	0.00	0.89
Epicatechin.gallate	0.00	0.04	0.00	0.03	0.01	0.00	0.00	0.88	0.50	0.53
Chlorogenic.acid	0.11	0.10	0.00	0.00	0.00	0.11	0.57	0.68	0.28	0.05
Cynaroside	0.01	0.02	0.07	0.10	0.32	0.00	0.24	0.01	0.09	0.04
Glucuronic.Acid	0.89	0.11	0.65	0.00	0.31	0.54	0.00	0.93	0.00	0.01
D.Fructose	0.00	0.00	0.01	0.19	0.63	0.53	0.00	0.70	0.52	0.88
D.Gluconic.Acid	0.90	0.47	0.06	0.86	0.01	0.05	0.00	0.91	0.02	0.00
Lysine	0.00	0.23	0.04	0.23	0.07	0.90	0.00	0.08	0.10	0.13
Tyrosine	0.12	0.04	0.36	0.84	0.02	0.01	0.00	0.01	0.00	0.00
Trehalose	0.79	0.81	0.68	0.05	0.37	0.08	0.00	0.74	0.00	0.00
Epigallocatechin	0.00	0.39	0.00	0.45	0.00	0.08	0.00	0.19	0.00	0.00
Esculin	0.06	0.08	0.00	0.52	0.08	0.86	0.00	0.00	0.02	0.16
Gallic.acid	0.01	0.20	0.03	0.23	0.62	0.02	0.00	0.36	0.04	0.00
gamma.Aminobutyric.acid	0.00	0.01	0.00	0.33	0.00	0.20	0.88	0.04	0.00	0.00

Glutathione	0.51	0.00	0.24	0.00	0.41	0.93	0.00	0.10	0.00	0.00
Guanine	0.00	0.08	0.05	0.46	0.80	0.11	0.00	0.60	0.03	0.02
Isovitexin	0.00	0.02	0.00	0.88	0.02	0.87	0.71	0.04	0.00	0.00
Kaempferin	0.56	0.07	0.00	0.00	0.00	0.92	0.33	0.00	0.11	0.04
kaempferol	0.88	0.03	0.71	0.24	0.01	0.01	0.00	0.00	0.02	0.00
L.Serine	0.07	0.03	0.00	0.18	0.00	0.22	0.07	0.00	0.00	0.00
L.Arginine	0.01	0.13	0.00	0.41	0.00	0.00	0.20	0.00	0.00	0.00
L.Aspartic.acid	0.13	0.00	0.02	0.00	0.00	0.89	0.27	0.00	0.00	0.00
L.Glutamic.acid	0.01	0.00	0.00	0.00	0.00	0.97	0.20	0.00	0.00	0.00
L.Homoserine	0.01	0.66	0.00	0.01	0.00	0.86	0.03	0.00	0.15	0.04
L.Isoleucine	0.00	0.02	0.02	0.61	0.54	0.28	0.00	0.12	0.13	0.22
L.Phenylalanine	0.01	0.00	0.32	0.22	0.13	0.36	0.00	0.31	0.32	0.87
L.Proline	0.00	0.00	0.00	0.77	0.05	0.15	0.00	0.31	0.39	0.26
L.Theanine	0.07	0.01	0.01	0.03	0.00	0.33	0.03	0.00	0.00	0.00
L.Tryptophan	0.00	0.55	0.00	0.19	0.04	0.10	0.02	0.16	0.41	0.76
Malic.Acid	0.98	0.11	0.04	0.03	0.52	0.06	0.66	0.28	0.02	0.55
Naringenin	0.08	0.16	0.77	0.84	0.01	0.01	0.00	0.27	0.50	0.00
Neochlorogenic.acid	0.41	0.08	0.00	0.34	0.01	0.45	0.85	0.01	0.36	0.00
Pantothenic.acid	0.36	0.02	0.78	0.00	0.00	0.17	0.09	0.03	0.56	0.02
Phloretin	0.01	0.04	0.29	0.86	0.03	0.00	0.00	0.56	0.04	0.00
Procyanidin.B4	0.00	0.50	0.00	0.00	0.53	0.21	0.00	0.03	0.42	0.82
Procyanidin.B3	0.00	0.00	0.00	0.61	0.57	0.06	0.00	0.01	0.00	0.00
Prunin	0.94	0.18	0.16	0.06	0.00	0.85	0.00	0.00	0.00	0.05
Theogallin	0.47	0.12	0.00	0.20	0.11	0.82	0.09	0.02	0.00	0.26
Theophylline	0.08	0.15	0.00	0.04	0.00	0.04	0.28	0.00	0.00	0.00
Thymine	0.01	0.01	0.02	0.00	0.00	0.01	0.01	0.03	0.02	0.39

Tricetin	0.00	0.05	0.00	0.61	0.01	0.73	0.17	0.02	0.00	0.00
Xanthine	0.77	0.41	0.02	0.26	0.00	0.06	0.26	0.07	0.11	0.00
Xylitol	0.31	0.03	0.04	0.03	0.16	0.73	0.16	0.00	0.00	0.07
Beta.Alanine	0.00	0.00	0.00	0.01	0.01	0.40	0.36	0.00	0.00	0.00
hydroxy.cinnamic.acid	0.13	0.36	0.42	0.21	0.22	0.00	0.02	0.19	0.07	0.00
Citric.acid	0.80	0.01	0.31	0.09	0.00	0.04	0.00	0.00	0.00	0.01
Succinic.acid	0.01	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.06	0.94
Alpha.ketoglutaric.acid	0.62	0.05	0.97	0.09	0.00	0.24	0.00	0.00	0.00	0.01
Hydroxycoumarine	0.06	0.17	0.00	0.01	0.00	0.06	0.38	0.59	0.13	0.02
Coumarin	0.17	0.01	0.00	0.00	0.00	0.00	0.72	0.09	0.59	0.58
Glutamine	0.06	0.02	0.00	0.11	0.00	0.24	0.05	0.00	0.00	0.00
Delphinidin.3.O.rutinoside.chloride	0.46	0.00	0.04	0.00	0.00	0.65	0.88	0.00	0.00	0.93
Eriodictyol	0.14	0.06	0.11	0.96	0.00	0.00	0.00	0.00	0.08	0.00
Glycyl.L.leucine	0.00	0.31	0.00	0.09	0.00	0.89	0.00	0.00	0.66	0.67
Guanosine.monophosphate	0.00	0.09	0.02	0.44	0.72	0.68	0.00	0.11	0.16	0.28
Glutathione.oxidized	0.37	0.03	0.00	0.21	0.00	0.27	0.41	0.01	0.00	0.00
L.Histidine	0.13	0.37	0.00	0.79	0.00	0.05	0.09	0.01	0.00	0.00
L.Pyroglutamic.acid	0.06	0.02	0.00	0.13	0.00	0.21	0.03	0.00	0.00	0.00
Myricetin	0.26	0.43	0.00	0.59	0.00	0.00	0.54	0.00	0.00	0.00
Naringenin.chalcone	0.00	0.02	0.00	0.04	0.05	0.00	0.00	0.70	0.47	0.94
Quercetin	0.26	0.00	0.04	0.00	0.00	0.84	0.39	0.05	0.11	0.05
Quercetin.3beta.D.glucoside	0.20	0.09	0.42	0.02	0.00	0.00	0.79	0.00	0.01	0.10
Schaftoside	0.06	0.27	0.00	0.73	0.00	0.32	0.97	0.00	0.25	0.00
Uridine.monophosphate	0.00	0.01	0.00	0.79	0.00	0.41	0.00	0.01	0.01	0.00
Digallic.acid	0.74	0.04	0.01	0.23	0.36	0.07	0.00	0.49	0.14	0.03
dihomomethionine	0.42	0.00	0.46	0.01	0.01	0.00	0.04	0.04	0.88	0.28

Epigallocatechin.3.O..3.O.methyl..gallate	0.12	0.00	0.05	0.00	0.40	0.06	0.02	0.01	0.02	0.39
Epigallocatechin..4beta..8..epicatechin.3.O.gallate.ester	0.05	0.00	0.00	0.00	0.89	0.31	0.00	0.64	0.00	0.00
Epigallocatechin.3..glucuronide	0.00	0.17	0.10	0.03	0.00	0.41	0.00	0.00	0.43	0.03
Gallocatechin..4alpha..8..epigallocatechin	0.02	0.84	0.00	0.23	0.06	0.79	0.04	0.00	0.38	0.00
S.Adenosyl.L.homocysteine	0.37	0.51	0.00	0.19	0.00	0.11	0.00	0.00	0.00	0.00
Theasinensin.B	0.04	0.85	0.00	0.31	0.76	0.93	0.00	0.78	0.00	0.00
Malonic.acid	0.23	0.10	0.01	0.37	0.76	0.84	0.16	0.01	0.35	0.41
4.Dihydroxybenzoic.acid	0.00	0.72	0.00	0.67	0.00	0.52	0.69	0.00	0.00	0.00
Aminoadipic.acid	0.75	0.00	0.61	0.00	0.37	1.00	0.00	0.33	0.00	0.00
.Adenosine.monophosphate	0.01	0.02	0.02	0.84	0.18	0.59	0.00	0.52	0.03	0.38
Hydroxy.3.methylglutaric.acid	0.11	0.34	0.11	0.56	0.00	0.09	0.01	0.46	0.82	0.11
Hydroxybenzoic.acid	0.73	0.00	0.19	0.00	0.00	0.29	0.67	0.00	0.01	0.96
Hydroxybenzaldehyde	0.00	0.00	0.00	0.13	0.07	0.00	0.00	0.52	0.63	0.62
Hydroxybenzoic.acid	0.00	0.02	0.01	0.10	0.01	0.22	0.17	0.00	0.00	0.00
Oxoproline	0.12	0.86	0.01	0.46	0.00	0.08	0.38	0.00	0.00	0.00
Adenosine.diphosphate	0.94	0.22	0.14	0.06	0.01	0.17	0.00	0.11	0.00	0.00
Ellagic.acid	0.21	0.01	0.01	0.00	0.26	0.91	0.00	0.76	0.00	0.00
Ethylmalonic.acid	0.69	0.04	0.60	0.06	0.00	0.00	0.08	0.02	0.57	0.02
Fumaric.acid	0.00	0.64	0.00	0.00	0.00	0.88	0.00	0.00	0.92	0.51
Cyanidin.3.O.galactoside	0.40	0.02	0.03	0.00	0.01	0.03	1.00	0.92	0.61	0.00
Quinic.acid	0.09	0.12	0.06	0.01	0.08	0.40	0.18	0.14	0.40	0.05
Theobromine	0.01	0.32	0.96	0.67	0.00	0.00	0.01	0.00	0.48	0.01
trans.p.Coumaric.acid	0.07	0.40	0.01	0.30	0.86	0.00	0.31	0.30	0.48	0.04
Shikimic.acid	0.20	0.65	0.71	0.86	0.03	0.00	0.01	0.04	0.21	0.00

Table S9-2 Corrected *p*-value

<i>p</i> -value	Caffeine	Epicatechin.gallate	Chlorogenic.acid	Cynaroside	Glucuronic.Acid	D.Fructose	D.Gluconic.Acid	Lysine	Tyrosine	Trehalose
Epigallocatechin.gallate	0.00	0.00	0.18	0.02	0.92	0.00	0.92	0.00	0.19	0.84
Catechin	0.00	0.07	0.17	0.04	0.18	0.00	0.57	0.33	0.08	0.86
Epicatechin	0.15	0.00	0.00	0.12	0.73	0.02	0.11	0.09	0.46	0.76
Gallocatechin	0.00	0.07	0.01	0.17	0.01	0.28	0.90	0.32	0.88	0.09
Methylxanthine	0.10	0.02	0.01	0.43	0.41	0.71	0.03	0.12	0.04	0.47
Abscisic.acid	0.51	0.01	0.18	0.00	0.63	0.62	0.10	0.92	0.03	0.14
Adenine	1.00	0.00	0.66	0.33	0.00	0.00	0.00	0.00	0.00	0.00
Avicularin	0.04	0.91	0.76	0.03	0.95	0.78	0.93	0.13	0.03	0.81
Quercetin.3.O.sophoroside	0.00	0.60	0.38	0.15	0.00	0.62	0.04	0.16	0.00	0.00
Betaine	0.92	0.62	0.09	0.07	0.02	0.91	0.00	0.20	0.01	0.00
Caffeine	0.00	0.29	0.61	0.01	0.00	0.03	0.34	0.95	0.71	0.06
Epicatechin.gallate	0.20	0.00	0.18	0.22	0.04	0.00	0.01	0.00	0.00	0.00
Chlorogenic.acid	0.51	0.11	0.00	0.17	0.63	0.51	0.01	0.69	0.45	0.37
Cynaroside	0.00	0.14	0.11	0.00	0.79	0.23	0.00	0.22	0.68	0.00
Glucuronic.Acid	0.00	0.02	0.54	0.72	0.00	0.43	0.00	0.00	0.00	0.00
D.Fructose	0.01	0.00	0.41	0.15	0.33	0.00	0.17	0.00	0.00	0.29
D.Gluconic.Acid	0.24	0.00	0.00	0.00	0.00	0.10	0.00	0.00	0.00	0.00
Lysine	0.93	0.00	0.60	0.14	0.00	0.00	0.00	0.00	0.00	0.00
Tyrosine	0.62	0.00	0.34	0.59	0.00	0.00	0.00	0.00	0.00	0.00
Trehalose	0.03	0.00	0.27	0.00	0.00	0.20	0.00	0.00	0.00	0.00
Epigallocatechin	0.00	0.20	0.00	0.00	0.00	0.92	0.00	0.01	0.00	0.00
Esculin	0.06	0.01	0.91	0.02	0.73	0.00	0.02	0.00	0.05	0.00
Gallic.acid	0.77	0.00	0.90	0.03	0.00	0.00	0.00	0.00	0.00	0.00
gamma.Aminobutyric.acid	0.00	0.05	0.00	0.21	0.03	0.00	0.06	0.04	0.96	0.03

Glutathione	0.00	0.15	0.78	0.00	0.00	0.03	0.00	0.00	0.00	0.00
Guanine	0.84	0.00	0.57	0.26	0.00	0.00	0.00	0.00	0.00	0.00
Isovitexin	0.39	0.02	0.01	0.00	0.85	0.01	0.00	0.94	0.72	0.16
Kaempferin	0.00	0.02	0.05	0.23	0.04	0.74	0.57	0.03	0.30	0.11
kaempferol	0.06	0.00	0.51	0.27	0.00	0.01	0.00	0.00	0.00	0.00
L.Serine	0.01	0.84	0.04	0.00	0.00	0.00	0.00	0.37	0.03	0.00
L.Arginine	0.00	0.75	0.01	0.22	0.08	0.00	0.00	0.10	0.09	0.01
L.Aspartic.acid	0.01	0.50	0.93	0.01	0.02	0.00	0.00	0.49	0.10	0.00
L.Glutamic.acid	0.00	0.88	0.24	0.00	0.00	0.00	0.00	0.50	0.06	0.00
L.Homoserine	0.99	0.03	0.05	0.02	0.19	0.00	0.66	0.00	0.76	0.83
L.Isoleucine	0.85	0.00	0.50	0.50	0.00	0.00	0.00	0.00	0.00	0.00
L.Phenylalanine	0.96	0.00	0.18	0.63	0.01	0.00	0.00	0.00	0.00	0.01
L.Proline	0.08	0.00	0.12	0.02	0.01	0.00	0.04	0.00	0.00	0.02
L.Theanine	0.16	0.71	0.62	0.33	0.00	0.00	0.00	0.75	0.00	0.00
L.Tryptophan	0.25	0.25	0.00	0.06	0.45	0.39	0.65	0.13	0.25	0.21
Malic.Acid	0.01	0.08	0.20	0.60	0.01	0.19	0.92	0.37	0.00	0.21
Naringenin	0.34	0.00	0.33	0.40	0.01	0.16	0.00	0.00	0.00	0.00
Neochlorogenic.acid	0.60	0.18	0.18	0.05	0.88	0.25	0.64	0.57	0.03	0.21
Pantothenic.acid	0.28	0.71	0.01	0.49	0.38	0.05	0.01	0.82	0.48	0.06
Phloretin	0.73	0.00	0.20	0.34	0.00	0.00	0.00	0.00	0.00	0.00
Procyanidin.B4	0.56	0.00	0.01	0.30	0.00	0.01	0.00	0.00	0.00	0.00
Procyanidin.B3	0.04	0.00	0.08	0.14	0.33	0.00	0.69	0.00	0.12	0.18
Prunin	0.08	0.26	0.22	0.00	0.00	0.00	0.00	0.00	0.04	0.00
Theogallin	0.51	0.05	0.02	0.85	0.00	0.66	0.00	0.01	0.00	0.09
Theophylline	0.41	0.49	0.00	0.16	0.01	0.30	0.01	0.96	0.06	0.12
Thymine	0.26	0.00	0.05	0.45	0.00	0.00	0.95	0.00	0.00	0.08

Tricetin	0.01	0.34	0.00	0.00	0.00	0.00	0.00	0.59	0.02	0.00
Xanthine	0.19	0.95	0.00	0.26	0.09	0.03	0.00	0.76	0.13	0.05
Xylitol	0.00	0.07	0.49	0.18	0.00	0.62	0.01	0.23	0.00	0.01
Beta.Alanine	0.00	0.01	0.28	0.00	0.05	0.00	0.09	0.02	0.92	0.01
hydroxy.cinnamic.acid	0.54	0.33	0.34	0.00	0.00	0.53	0.00	0.01	0.01	0.00
Citric.acid	0.07	0.01	0.58	0.20	0.00	0.19	0.00	0.18	0.00	0.00
Succinic.acid	0.03	0.00	0.15	0.02	0.59	0.07	0.00	0.14	0.00	0.09
Alpha.ketoglutaric.acid	0.13	0.06	0.76	0.53	0.00	0.79	0.00	0.63	0.00	0.00
Hydroxycoumarine	0.29	0.18	0.00	0.07	0.40	0.45	0.00	0.56	0.18	0.14
Coumarin	0.59	0.58	0.00	0.00	0.69	0.96	0.48	0.08	0.71	0.31
Glutamine	0.00	0.76	0.04	0.00	0.00	0.00	0.00	0.51	0.02	0.00
Delphinidin.3.O.rutinoside.chloride	0.00	0.10	0.14	0.54	0.00	0.48	0.19	0.32	0.97	0.53
Eriodictyol	0.27	0.00	0.76	0.79	0.00	0.00	0.00	0.00	0.00	0.00
Glycyl.L.leucine	0.68	0.00	0.19	0.61	0.00	0.00	0.00	0.00	0.00	0.00
Guanosine.monophosphate	0.61	0.00	0.55	0.05	0.00	0.00	0.00	0.00	0.00	0.00
Glutathione.oxidized	0.12	0.99	0.00	0.00	0.15	0.00	0.00	0.71	0.06	0.00
L.Histidine	0.01	0.97	0.00	0.04	0.01	0.00	0.00	0.69	0.07	0.00
L.Pyroglutamic.acid	0.00	0.76	0.03	0.00	0.00	0.00	0.00	0.67	0.01	0.00
Myricetin	0.49	0.94	0.02	0.01	0.01	0.04	0.03	0.34	0.02	0.09
Naringenin.chalcone	0.23	0.00	0.08	0.05	0.00	0.00	0.01	0.00	0.00	0.00
Quercetin	0.03	0.07	0.46	0.03	0.60	0.23	0.52	0.24	0.46	0.07
Quercetin.3beta.D.glucoside	0.07	0.21	0.75	0.00	0.33	0.70	0.74	0.14	0.02	0.42
Schaftoside	0.89	0.95	0.15	0.40	0.18	0.00	0.01	0.24	0.10	0.09
Uridine.monophosphate	0.05	0.00	0.00	0.95	0.69	0.00	0.15	0.00	0.02	0.16
Digallic.acid	0.23	0.14	0.04	0.04	0.01	0.01	0.00	0.00	0.00	0.03
dihomomethionine	0.15	0.00	0.44	0.00	0.68	0.01	0.68	0.56	0.00	0.40

Epigallocatechin.3.O..3.O.methyl..gallate	0.00	0.03	0.08	0.00	0.09	0.18	0.01	0.03	0.22	0.00
Epigallocatechin..4beta..8..epicatechin.3.O.gallate.ester	0.12	0.20	0.03	0.00	0.00	0.70	0.00	0.00	0.00	0.00
Epigallocatechin.3..glucuronide	0.60	0.31	0.28	0.47	0.27	0.00	0.15	0.00	0.47	0.54
Gallocatechin..4alpha..8..epigallocatechin	0.04	0.13	0.32	0.09	0.35	0.04	0.00	0.80	0.06	0.00
S.Adenosyl.L.homocysteine	0.57	0.55	0.00	0.20	0.01	0.50	0.00	0.10	0.00	0.00
Theasinensin.B	0.24	0.06	0.00	0.01	0.00	0.61	0.00	0.00	0.00	0.00
Malonic.acid	0.83	0.00	0.81	0.13	0.45	0.09	0.03	0.38	0.88	0.24
4.Dihydroxybenzoic.acid	0.15	0.81	0.01	0.00	0.11	0.25	0.00	0.95	0.00	0.00
Aminoadipic.acid	0.40	0.09	0.72	0.33	0.00	0.43	0.00	0.00	0.00	0.00
.Adenosine.monophosphate	0.93	0.00	0.71	0.84	0.00	0.00	0.00	0.00	0.00	0.00
Hydroxy.3.methylglutaric.acid	0.06	0.18	0.32	0.52	0.02	0.09	0.00	0.30	0.01	0.00
Hydroxybenzoic.acid	0.00	0.30	0.28	0.66	0.01	0.83	0.82	0.05	0.81	0.30
Hydroxybenzaldehyde	0.03	0.00	0.05	0.02	0.06	0.00	0.05	0.00	0.00	0.00
Hydroxybenzoic.acid	0.00	0.77	0.30	0.00	0.00	0.34	0.00	0.46	0.00	0.00
Oxoproline	0.57	0.34	0.04	0.05	0.07	0.01	0.00	0.20	0.11	0.01
Adenosine.diphosphate	0.17	0.00	0.07	0.00	0.00	0.78	0.00	0.00	0.00	0.00
Ellagic.acid	0.00	0.03	0.04	0.00	0.00	0.52	0.00	0.00	0.00	0.00
Ethylmalonic.acid	0.81	0.17	0.28	0.01	0.10	0.19	0.03	0.84	0.02	0.07
Fumaric.acid	0.77	0.00	0.00	0.80	0.08	0.00	0.85	0.00	0.04	0.00
Cyanidin.3.O.galactoside	0.36	0.16	0.05	0.01	0.82	0.05	0.29	0.06	0.38	0.36
Quinic.acid	0.92	0.01	0.00	0.00	0.00	0.31	0.25	0.09	0.08	0.72
Theobromine	0.22	0.00	0.13	0.91	0.50	0.57	0.01	0.76	0.00	0.06
trans.p.Coumaric.acid	0.65	0.50	0.00	0.00	0.11	0.72	0.02	0.08	0.15	0.01
Shikimic.acid	0.13	0.46	0.90	0.00	0.01	0.76	0.00	0.00	0.00	0.00

Table S9-3 Corrected *p*-value

<i>p</i> -value	Epigallocatechin	Esculin	Gallic.acid	gamma.Aminobutyric.acid	Glutathione	Guanine	Isovitexin	Kaempferin	kaempferol	L.Serine
Epigallocatechin.gallate	0.01	0.11	0.02	0.01	0.61	0.01	0.00	0.65	0.91	0.12
Catechin	0.49	0.14	0.30	0.03	0.00	0.13	0.04	0.13	0.06	0.06
Epicatechin	0.00	0.00	0.07	0.00	0.34	0.09	0.00	0.00	0.79	0.01
Gallocatechin	0.55	0.62	0.32	0.43	0.00	0.56	0.91	0.00	0.34	0.27
Methylxanthine	0.00	0.14	0.71	0.00	0.51	0.85	0.05	0.00	0.02	0.00
Abscisic.acid	0.14	0.90	0.04	0.29	0.95	0.18	0.91	0.94	0.01	0.31
Adenine	0.00	0.00	0.00	0.91	0.00	0.00	0.78	0.43	0.00	0.12
Avicularin	0.28	0.00	0.47	0.08	0.17	0.69	0.08	0.00	0.00	0.00
Quercetin.3.O.sophoroside	0.00	0.05	0.09	0.00	0.00	0.06	0.00	0.18	0.03	0.00
Betaine	0.00	0.25	0.00	0.00	0.00	0.05	0.00	0.09	0.00	0.00
Caffeine	0.01	0.11	0.83	0.00	0.00	0.88	0.49	0.00	0.11	0.01
Epicatechin.gallate	0.29	0.01	0.00	0.09	0.23	0.00	0.05	0.04	0.01	0.88
Chlorogenic.acid	0.00	0.93	0.93	0.00	0.84	0.67	0.01	0.10	0.60	0.09
Cynaroside	0.01	0.05	0.07	0.30	0.00	0.36	0.01	0.33	0.37	0.01
Glucuronic.Acid	0.00	0.80	0.00	0.05	0.00	0.00	0.89	0.08	0.01	0.01
D.Fructose	0.94	0.00	0.00	0.00	0.07	0.00	0.02	0.81	0.03	0.00
D.Gluconic.Acid	0.00	0.03	0.00	0.11	0.00	0.00	0.00	0.67	0.00	0.00
Lysine	0.01	0.00	0.00	0.08	0.01	0.00	0.95	0.05	0.00	0.48
Tyrosine	0.00	0.09	0.00	0.97	0.00	0.00	0.79	0.40	0.00	0.06
Trehalose	0.00	0.00	0.00	0.06	0.00	0.00	0.25	0.18	0.00	0.00
Epigallocatechin	0.00	0.76	0.00	0.00	0.00	0.00	0.00	0.05	0.00	0.00
Esculin	0.68	0.00	0.00	0.00	0.21	0.00	0.02	0.50	0.02	0.04
Gallic.acid	0.00	0.00	0.00	0.58	0.00	0.00	0.75	0.06	0.00	0.09
gamma.Aminobutyric.acid	0.00	0.00	0.48	0.00	0.00	0.64	0.01	0.03	0.57	0.00

Glutathione	0.00	0.13	0.00	0.00	0.00	0.00	0.00	0.31	0.00	0.00
Guanine	0.00	0.00	0.00	0.54	0.00	0.00	0.58	0.26	0.00	0.38
Isovitexin	0.00	0.01	0.67	0.00	0.00	0.48	0.00	0.44	0.04	0.00
Kaempferin	0.02	0.40	0.03	0.01	0.22	0.18	0.34	0.00	0.20	0.15
kaempferol	0.00	0.01	0.00	0.47	0.00	0.00	0.02	0.13	0.00	0.00
L.Serine	0.00	0.02	0.05	0.00	0.00	0.28	0.00	0.09	0.00	0.00
L.Arginine	0.00	0.03	0.14	0.00	0.00	0.58	0.00	0.22	0.00	0.00
L.Aspartic.acid	0.00	0.00	0.18	0.00	0.00	0.55	0.00	0.27	0.01	0.00
L.Glutamic.acid	0.00	0.01	0.15	0.00	0.00	0.47	0.00	0.15	0.01	0.00
L.Homoserine	0.04	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.22	0.00
L.Isoleucine	0.01	0.00	0.00	0.10	0.06	0.00	0.05	0.07	0.00	0.50
L.Phenylalanine	0.06	0.26	0.00	0.29	0.90	0.00	0.20	0.22	0.09	0.27
L.Proline	0.71	0.01	0.00	0.00	0.72	0.00	0.00	0.43	0.00	0.00
L.Theanine	0.00	0.06	0.02	0.00	0.00	0.11	0.00	0.05	0.00	0.00
L.Tryptophan	0.00	0.01	0.00	0.02	0.01	0.05	0.18	0.05	0.05	0.23
Malic.Acid	0.83	0.44	0.65	0.70	0.00	0.29	0.49	0.02	0.52	0.05
Naringenin	0.00	0.00	0.00	0.05	0.00	0.00	0.56	0.18	0.00	0.00
Neochlorogenic.acid	0.52	0.02	0.09	0.35	0.51	0.94	0.90	0.19	0.00	0.08
Pantothenic.acid	0.43	0.22	0.03	0.00	0.03	0.32	0.02	0.57	0.03	0.00
Phloretin	0.00	0.00	0.00	0.81	0.00	0.00	0.76	0.34	0.00	0.01
Procyanidin.B4	0.60	0.00	0.00	0.07	0.01	0.00	0.00	0.00	0.01	0.36
Procyanidin.B3	0.00	0.00	0.00	0.00	0.12	0.00	0.00	0.02	0.93	0.05
Prunin	0.00	0.00	0.00	0.44	0.00	0.00	0.05	0.07	0.00	0.64
Theogallin	0.00	0.00	0.35	0.13	0.00	0.04	0.00	0.04	0.21	0.03
Theophylline	0.00	0.35	0.37	0.00	0.36	0.41	0.00	0.01	0.01	0.00
Thymine	0.71	0.28	0.04	0.02	0.27	0.00	0.02	0.06	0.66	0.01

Tricetin	0.00	0.03	0.05	0.00	0.00	0.47	0.00	0.13	0.00	0.00
Xanthine	0.00	0.32	0.25	0.00	0.04	0.42	0.06	0.12	0.09	0.00
Xylitol	0.00	0.00	0.43	0.01	0.00	0.12	0.00	0.50	0.20	0.00
Beta.Alanine	0.00	0.00	0.59	0.00	0.00	0.14	0.00	0.06	0.21	0.00
hydroxy.cinnamic.acid	0.06	0.81	0.00	0.30	0.00	0.03	0.00	0.83	0.02	0.00
Citric.acid	0.04	0.28	0.01	0.03	0.00	0.00	0.94	0.92	0.00	0.00
Succinic.acid	0.57	0.49	0.00	0.07	0.33	0.00	0.31	0.35	0.00	0.05
Alpha.ketoglutaric.acid	0.01	0.09	0.06	0.00	0.00	0.02	0.28	0.48	0.00	0.00
Hydroxycoumarine	0.00	0.93	0.62	0.00	0.86	0.41	0.00	0.04	0.35	0.01
Coumarin	0.01	0.01	0.11	0.01	0.01	0.46	0.63	0.03	0.75	0.78
Glutamine	0.00	0.02	0.04	0.00	0.00	0.20	0.00	0.10	0.00	0.00
Delphinidin.3.O.rutinoside.chloride	0.56	0.94	0.76	0.40	0.02	0.44	0.13	0.00	0.06	0.37
Eriodictyol	0.00	0.01	0.00	0.49	0.00	0.00	0.82	0.36	0.00	0.00
Glycyl.L.leucine	0.53	0.00	0.00	0.00	0.42	0.00	0.01	0.00	0.01	0.00
Guanosine.monophosphate	0.01	0.00	0.00	0.39	0.00	0.00	0.14	0.07	0.00	0.60
Glutathione.oxidized	0.00	0.08	0.47	0.00	0.00	0.47	0.00	0.02	0.06	0.00
L.Histidine	0.00	0.08	0.06	0.00	0.00	0.25	0.00	0.11	0.01	0.00
L.Pyroglutamic.acid	0.00	0.02	0.02	0.00	0.00	0.13	0.00	0.11	0.00	0.00
Myricetin	0.00	0.00	0.70	0.00	0.00	0.98	0.00	0.11	0.02	0.00
Naringenin.chalcone	0.45	0.00	0.00	0.03	0.32	0.00	0.00	0.00	0.00	0.87
Quercetin	0.68	0.76	0.18	0.01	0.01	0.62	0.20	0.20	0.72	0.00
Quercetin.3beta.D.glucoside	0.61	0.00	0.44	0.04	0.10	0.89	0.19	0.05	0.04	0.00
Schaftoside	0.00	0.00	0.58	0.00	0.01	0.69	0.00	0.00	0.00	0.00
Uridine.monophosphate	0.00	0.00	0.00	0.00	0.55	0.00	0.00	0.00	0.68	0.00
Digallic.acid	0.00	0.30	0.00	0.56	0.68	0.00	0.06	0.01	0.00	0.96
dihomomethionine	0.25	0.40	0.23	0.71	0.03	0.10	0.13	0.28	0.00	0.18

Epigallocatechin.3.O..3.O.methyl..gallate	0.45	0.64	0.00	0.33	0.00	0.02	0.34	0.00	0.92	0.00
Epigallocatechin..4beta..8..epicatechin.3.O. gallate.ester	0.00	0.14	0.00	0.00	0.00	0.00	0.00	0.07	0.00	0.00
Epigallocatechin.3..glucuronide	0.50	0.00	0.00	0.00	0.95	0.00	0.64	0.01	0.96	0.00
Gallocatechin..4alpha..8..epigallocatechin	0.00	0.92	0.07	0.00	0.00	0.22	0.00	0.00	0.00	0.00
S.Adenosyl.L.homocysteine	0.00	0.54	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Theasinensin.B	0.00	0.17	0.00	0.00	0.00	0.00	0.00	0.05	0.00	0.00
Malonic.acid	0.17	0.00	0.23	0.24	0.00	0.33	0.00	0.68	0.09	0.03
4.Dihydroxybenzoic.acid	0.00	0.46	0.41	0.00	0.00	0.90	0.00	0.24	0.00	0.00
Aminoadipic.acid	0.00	0.14	0.00	0.00	0.00	0.00	0.00	0.41	0.00	0.00
.Adenosine.monophosphate	0.12	0.03	0.00	0.06	0.06	0.00	0.08	0.09	0.00	0.55
Hydroxy.3.methylglutaric.acid	0.00	0.58	0.08	0.00	0.01	0.02	0.09	0.12	0.00	0.00
Hydroxybenzoic.acid	0.99	0.44	0.37	0.59	0.32	0.29	0.76	0.00	0.01	0.09
Hydroxybenzaldehyde	0.87	0.00	0.00	0.00	0.94	0.00	0.00	0.01	0.02	0.24
Hydroxybenzoic.acid	0.00	0.13	0.04	0.00	0.00	0.20	0.00	0.42	0.00	0.00
Oxoproline	0.00	0.05	0.34	0.00	0.00	0.75	0.02	0.06	0.02	0.00
Adenosine.diphosphate	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.53	0.00	0.00
Ellagic.acid	0.00	0.64	0.00	0.00	0.00	0.00	0.00	0.83	0.00	0.00
Ethylmalonic.acid	0.06	0.88	0.09	0.21	0.94	0.24	0.78	0.17	0.01	0.12
Fumaric.acid	0.05	0.00	0.00	0.00	0.76	0.00	0.00	0.00	0.21	0.00
Cyanidin.3.O.galactoside	0.27	0.64	0.74	0.00	0.59	0.57	0.23	0.93	0.81	0.01
Quinic.acid	0.81	0.01	0.96	0.28	0.42	0.11	0.02	0.50	0.78	0.14
Theobromine	0.01	0.34	0.06	0.01	0.05	0.06	0.64	0.14	0.02	0.00
trans.p.Coumaric.acid	0.62	0.71	0.04	0.28	0.00	0.30	0.01	0.05	0.09	0.08
Shikimic.acid	0.05	0.14	0.00	0.67	0.00	0.01	0.00	0.58	0.00	0.00

Table S9-4 Corrected *p*-value

<i>p</i> -value	L.Arginine	L.Aspartic.acid	L.Glutamic.acid	L.Homoserine	L.Isoleucine	L.Phenylalanine	L.Proline	L.Theanine	L.Tryptophan	Malic.Acid
Epigallocatechin.gallate	0.02	0.21	0.02	0.02	0.00	0.02	0.00	0.12	0.00	0.99
Catechin	0.21	0.00	0.00	0.74	0.04	0.00	0.01	0.01	0.65	0.18
Epicatechin	0.00	0.05	0.00	0.00	0.05	0.42	0.00	0.02	0.00	0.08
Gallocatechin	0.51	0.00	0.01	0.03	0.70	0.31	0.83	0.06	0.28	0.06
Methylxanthine	0.00	0.00	0.01	0.00	0.63	0.20	0.09	0.00	0.07	0.62
Abscisic.acid	0.01	0.92	0.98	0.90	0.38	0.46	0.23	0.43	0.17	0.11
Adenine	0.29	0.37	0.30	0.07	0.00	0.00	0.00	0.06	0.04	0.74
Avicularin	0.01	0.00	0.00	0.00	0.19	0.42	0.41	0.00	0.24	0.38
Quercetin.3.O.sophoroside	0.00	0.00	0.00	0.23	0.20	0.42	0.49	0.00	0.51	0.04
Betaine	0.00	0.00	0.00	0.09	0.32	0.90	0.36	0.00	0.83	0.64
Caffeine	0.00	0.01	0.00	0.99	0.89	0.97	0.14	0.25	0.35	0.03
Epicatechin.gallate	0.81	0.60	0.91	0.07	0.00	0.00	0.00	0.78	0.35	0.14
Chlorogenic.acid	0.01	0.95	0.34	0.09	0.60	0.27	0.20	0.70	0.00	0.29
Cynaroside	0.32	0.01	0.00	0.05	0.60	0.72	0.04	0.44	0.11	0.69
Glucuronic.Acid	0.14	0.05	0.00	0.28	0.00	0.03	0.02	0.00	0.56	0.02
D.Fructose	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.49	0.28
D.Gluconic.Acid	0.00	0.01	0.00	0.74	0.00	0.00	0.08	0.00	0.73	0.94
Lysine	0.17	0.59	0.60	0.00	0.00	0.00	0.00	0.82	0.20	0.47
Tyrosine	0.15	0.17	0.11	0.83	0.00	0.00	0.00	0.00	0.35	0.01
Trehalose	0.02	0.01	0.00	0.87	0.00	0.01	0.04	0.00	0.31	0.30
Epigallocatechin	0.00	0.00	0.00	0.08	0.03	0.11	0.78	0.00	0.01	0.87
Esculin	0.06	0.01	0.02	0.00	0.00	0.36	0.03	0.10	0.02	0.55
Gallic.acid	0.21	0.27	0.23	0.01	0.00	0.00	0.00	0.04	0.00	0.74
gamma.Aminobutyric.acid	0.00	0.00	0.00	0.00	0.17	0.39	0.00	0.00	0.04	0.78

Glutathione	0.00	0.00	0.00	0.02	0.10	0.93	0.79	0.00	0.02	0.01
Guanine	0.67	0.65	0.57	0.01	0.00	0.00	0.00	0.17	0.09	0.40
Isovitexin	0.00	0.00	0.00	0.02	0.10	0.29	0.01	0.00	0.27	0.59
Kaempferin	0.31	0.37	0.23	0.00	0.12	0.31	0.54	0.10	0.09	0.05
kaempferol	0.01	0.02	0.02	0.32	0.00	0.15	0.00	0.00	0.10	0.62
L.Serine	0.00	0.00	0.00	0.00	0.60	0.37	0.01	0.00	0.33	0.10
L.Arginine	0.00	0.00	0.00	0.00	0.58	0.49	0.08	0.00	0.78	0.46
L.Aspartic.acid	0.00	0.00	0.00	0.00	0.35	0.17	0.02	0.00	0.30	0.00
L.Glutamic.acid	0.00	0.00	0.00	0.00	0.48	0.17	0.00	0.00	0.47	0.01
L.Homoserine	0.00	0.00	0.00	0.00	0.00	0.11	0.00	0.00	0.32	0.35
L.Isoleucine	0.48	0.25	0.38	0.00	0.00	0.00	0.00	0.95	0.39	0.55
L.Phenylalanine	0.38	0.10	0.11	0.06	0.00	0.00	0.00	0.48	0.03	0.53
L.Proline	0.04	0.01	0.00	0.00	0.00	0.00	0.00	0.35	0.52	0.84
L.Theanine	0.00	0.00	0.00	0.00	0.93	0.38	0.25	0.00	0.84	0.00
L.Tryptophan	0.70	0.21	0.37	0.22	0.29	0.01	0.42	0.79	0.00	0.87
Malic.Acid	0.36	0.00	0.00	0.26	0.45	0.43	0.78	0.00	0.83	0.00
Naringenin	0.00	0.01	0.00	0.85	0.00	0.10	0.02	0.00	0.01	0.56
Neochlorogenic.acid	0.17	0.30	0.31	0.01	0.50	0.83	0.18	0.06	0.01	0.11
Pantothenic.acid	0.00	0.03	0.03	0.02	0.99	0.63	0.16	0.08	0.01	0.49
Phloretin	0.06	0.15	0.10	0.16	0.00	0.00	0.00	0.01	0.03	0.96
Procyanidin.B4	0.85	0.23	0.56	0.07	0.00	0.02	0.00	0.80	0.00	0.03
Procyanidin.B3	0.05	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.83
Prunin	0.21	0.37	0.87	0.00	0.00	0.24	0.05	0.90	0.00	0.29
Theogallin	0.19	0.00	0.00	0.24	0.07	0.04	0.08	0.00	0.00	0.00
Theophylline	0.00	0.06	0.00	0.05	0.88	0.69	0.06	0.00	0.11	0.47
Thymine	0.00	0.45	0.30	0.00	0.00	0.00	0.00	0.94	0.57	0.00

Tricetin	0.00	0.00	0.00	0.00	0.48	0.46	0.05	0.00	0.19	0.62
Xanthine	0.00	0.00	0.00	0.00	0.89	0.61	0.07	0.02	0.38	0.30
Xylitol	0.00	0.00	0.00	0.03	0.30	0.02	0.60	0.00	0.20	0.00
Beta.Alanine	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.77	0.01
hydroxy.cinnamic.acid	0.28	0.00	0.00	0.04	0.24	0.34	0.84	0.00	0.00	0.01
Citric.acid	0.01	0.04	0.00	0.01	0.02	0.00	0.26	0.01	0.44	0.24
Succinic.acid	0.03	0.10	0.71	0.25	0.01	0.02	0.00	0.24	0.28	0.49
Alpha.ketoglutaric.acid	0.00	0.00	0.00	0.00	0.32	0.03	0.98	0.00	0.54	0.08
Hydroxycoumarine	0.00	0.70	0.09	0.03	0.38	0.13	0.13	0.31	0.00	0.25
Coumarin	0.21	0.23	0.50	0.50	0.76	0.39	0.78	0.83	0.00	0.03
Glutamine	0.00	0.00	0.00	0.00	0.69	0.39	0.01	0.00	0.28	0.04
Delphinidin.3.O.rutinoside.chloride	0.56	0.04	0.05	0.00	0.31	0.35	0.99	0.29	0.08	0.07
Eriodictyol	0.01	0.03	0.02	0.28	0.00	0.01	0.00	0.00	0.02	0.67
Glycyl.L.leucine	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.04	0.03	0.93
Guanosine.monophosphate	0.90	0.90	0.80	0.00	0.00	0.00	0.00	0.60	0.05	0.17
Glutathione.oxidized	0.00	0.00	0.00	0.00	0.70	0.83	0.00	0.00	0.30	0.00
L.Histidine	0.00	0.00	0.00	0.00	0.96	0.84	0.04	0.00	0.98	0.95
L.Pyroglutamic.acid	0.00	0.00	0.00	0.00	0.83	0.42	0.01	0.00	0.24	0.04
Myricetin	0.00	0.00	0.00	0.00	0.26	0.49	0.20	0.00	0.00	0.98
Naringenin.chalcone	0.83	0.94	0.60	0.02	0.00	0.00	0.00	0.96	0.24	0.11
Quercetin	0.00	0.00	0.00	0.00	0.76	0.88	0.02	0.01	0.00	0.36
Quercetin.3beta.D.glucoside	0.00	0.00	0.01	0.00	0.27	0.18	0.79	0.00	0.37	0.26
Schaftoside	0.00	0.00	0.00	0.00	0.10	0.77	0.24	0.00	0.00	0.91
Uridine.monophosphate	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.71
Digallic.acid	0.92	0.64	0.88	0.13	0.00	0.13	0.11	0.09	0.42	0.71
dihomomethionine	0.96	0.03	0.05	0.14	0.06	0.03	0.00	0.89	0.02	0.16

Epigallocatechin.3.O.3.methyl..gallate	0.04	0.00	0.00	0.88	0.08	0.89	0.98	0.07	0.00	0.04
Epigallocatechin..4beta..8..epicatechin.3.O .gallate.ester	0.00	0.00	0.00	0.76	0.06	0.80	0.25	0.00	0.29	0.43
Epigallocatechin.3..glucuronide	0.00	0.00	0.00	0.00	0.00	0.89	0.00	0.00	0.00	0.03
Galocatechin..4alpha..8..epigallocatechin	0.00	0.00	0.00	0.00	0.77	0.32	0.99	0.00	0.79	0.99
S.Adenosyl.L.homocysteine	0.00	0.00	0.00	0.00	0.18	0.51	0.18	0.00	0.81	0.52
Theasinensin.B	0.00	0.00	0.00	0.88	0.00	0.03	0.01	0.00	0.08	0.23
Malonic.acid	0.29	0.02	0.05	0.10	0.61	0.56	0.72	0.02	0.26	0.89
4.Dihydroxybenzoic.acid	0.00	0.00	0.00	0.00	0.34	0.24	0.07	0.00	0.00	0.07
Aminoadipic.acid	0.00	0.00	0.00	0.21	0.09	0.44	0.18	0.00	0.02	0.21
.Adenosine.monophosphate	0.43	0.38	0.37	0.00	0.00	0.00	0.00	0.78	0.20	0.50
Hydroxy.3.methylglutaric.acid	0.00	0.00	0.00	0.04	0.19	0.16	0.11	0.00	0.02	0.14
Hydroxybenzoic.acid	0.47	0.78	0.80	0.00	0.07	0.81	0.55	0.27	0.81	0.80
Hydroxybenzaldehyde	0.27	0.31	0.09	0.01	0.00	0.00	0.00	0.31	0.24	0.35
Hydroxybenzoic.acid	0.00	0.00	0.00	0.00	0.92	0.37	0.09	0.00	0.87	0.00
Oxoproline	0.00	0.00	0.00	0.00	0.45	0.42	0.00	0.00	0.46	0.40
Adenosine.diphosphate	0.00	0.00	0.00	0.06	0.00	0.04	0.16	0.00	0.18	0.06
Ellagic.acid	0.00	0.00	0.00	0.24	0.00	0.32	0.38	0.00	0.72	0.04
Ethylmalonic.acid	0.04	0.71	0.56	0.46	0.50	0.18	0.13	0.16	0.03	0.10
Fumaric.acid	0.00	0.00	0.00	0.00	0.00	0.04	0.00	0.01	0.01	0.42
Cyanidin.3.O.galactoside	0.01	0.03	0.02	0.73	0.25	0.03	0.10	0.09	0.08	0.04
Quinic.acid	0.06	0.68	0.87	0.02	0.13	0.29	0.00	0.21	0.17	0.01
Theobromine	0.00	0.00	0.00	0.00	0.20	0.01	0.80	0.00	0.37	0.79
trans.p.Coumaric.acid	0.66	0.04	0.07	0.29	0.87	0.98	0.86	0.08	0.00	0.01
Shikimic.acid	0.27	0.00	0.01	0.05	0.14	0.18	0.87	0.00	0.01	0.19

Table S9-5 Corrected *p*-value

<i>p</i> -value	Naringenin	Neochlorogenic.acid	Pantothenic.acid	Phloretin	Procyanidin.B4	Procyanidin.B3	Prunin	Theogallin	Theophylline	Thymine
Epigallocatechin.gallate	0.14	0.51	0.46	0.02	0.00	0.00	0.95	0.57	0.13	0.03
Catechin	0.25	0.13	0.04	0.08	0.59	0.00	0.27	0.20	0.22	0.02
Epicatechin	0.83	0.01	0.84	0.39	0.00	0.00	0.24	0.00	0.00	0.04
Gallocatechin	0.88	0.45	0.01	0.90	0.00	0.70	0.11	0.29	0.08	0.00
Methylxanthine	0.02	0.02	0.01	0.06	0.62	0.66	0.01	0.18	0.00	0.00
Abscisic.acid	0.02	0.56	0.26	0.00	0.30	0.11	0.89	0.87	0.08	0.02
Adenine	0.00	0.89	0.16	0.00	0.00	0.00	0.00	0.15	0.38	0.03
Avicularin	0.37	0.02	0.06	0.65	0.06	0.03	0.00	0.04	0.01	0.06
Quercetin.3.O.sophoroside	0.60	0.46	0.65	0.08	0.52	0.01	0.00	0.00	0.01	0.03
Betaine	0.00	0.01	0.05	0.00	0.87	0.01	0.10	0.35	0.00	0.49
Caffeine	0.44	0.68	0.38	0.80	0.65	0.08	0.14	0.61	0.51	0.36
Epicatechin.gallate	0.01	0.27	0.78	0.00	0.00	0.00	0.36	0.10	0.59	0.00
Chlorogenic.acid	0.43	0.27	0.02	0.29	0.02	0.14	0.31	0.04	0.00	0.10
Cynaroside	0.50	0.09	0.59	0.44	0.40	0.22	0.01	0.89	0.24	0.55
Glucuronic.Acid	0.02	0.91	0.48	0.00	0.01	0.44	0.00	0.01	0.02	0.00
D.Fructose	0.25	0.35	0.09	0.00	0.02	0.00	0.00	0.74	0.40	0.00
D.Gluconic.Acid	0.00	0.72	0.03	0.00	0.01	0.77	0.00	0.00	0.03	0.97
Lysine	0.00	0.66	0.87	0.00	0.00	0.00	0.00	0.02	0.97	0.00
Tyrosine	0.00	0.07	0.58	0.00	0.00	0.19	0.07	0.01	0.11	0.00
Trehalose	0.00	0.30	0.11	0.00	0.00	0.26	0.00	0.15	0.19	0.14
Epigallocatechin	0.00	0.62	0.54	0.00	0.69	0.01	0.00	0.00	0.00	0.78
Esculin	0.00	0.05	0.32	0.00	0.00	0.00	0.00	0.00	0.46	0.38
Gallic.acid	0.00	0.16	0.07	0.00	0.00	0.00	0.00	0.46	0.48	0.07
gamma.Aminobutyric.acid	0.10	0.46	0.00	0.86	0.12	0.00	0.54	0.20	0.00	0.05

Glutathione	0.00	0.60	0.06	0.00	0.02	0.20	0.01	0.00	0.47	0.37
Guanine	0.00	0.96	0.42	0.00	0.00	0.00	0.00	0.09	0.51	0.00
Isovitexin	0.65	0.93	0.05	0.82	0.00	0.00	0.09	0.00	0.01	0.05
Kaempferin	0.26	0.27	0.66	0.45	0.00	0.04	0.12	0.08	0.03	0.11
kaempferol	0.00	0.00	0.06	0.00	0.03	0.94	0.01	0.30	0.02	0.74
L.Serine	0.00	0.13	0.00	0.03	0.46	0.09	0.73	0.06	0.00	0.03
L.Arginine	0.00	0.25	0.00	0.10	0.89	0.10	0.31	0.28	0.00	0.01
L.Aspartic.acid	0.02	0.40	0.07	0.23	0.33	0.02	0.47	0.00	0.10	0.56
L.Glutamic.acid	0.01	0.41	0.06	0.16	0.65	0.01	0.90	0.01	0.01	0.40
L.Homoserine	0.89	0.03	0.05	0.24	0.12	0.01	0.00	0.33	0.09	0.00
L.Isoleucine	0.00	0.60	0.99	0.00	0.00	0.00	0.00	0.12	0.91	0.00
L.Phenylalanine	0.17	0.87	0.71	0.00	0.04	0.02	0.34	0.08	0.76	0.00
L.Proline	0.03	0.27	0.25	0.00	0.00	0.00	0.10	0.14	0.11	0.00
L.Theanine	0.00	0.11	0.14	0.02	0.85	0.00	0.92	0.00	0.01	0.95
L.Tryptophan	0.01	0.03	0.03	0.06	0.00	0.01	0.01	0.00	0.18	0.66
Malic.Acid	0.65	0.18	0.59	0.97	0.07	0.88	0.39	0.01	0.57	0.00
Naringenin	0.00	0.40	0.01	0.00	0.00	0.22	0.03	1.00	0.05	0.33
Neochlorogenic.acid	0.30	0.00	0.07	0.56	0.21	0.98	0.40	0.00	0.20	0.10
Pantothenic.acid	0.01	0.03	0.00	0.10	0.84	0.71	0.99	0.28	0.00	0.00
Phloretin	0.00	0.46	0.06	0.00	0.00	0.00	0.00	0.10	0.24	0.36
Procyanidin.B4	0.00	0.13	0.78	0.00	0.00	0.00	0.57	1.00	0.03	0.01
Procyanidin.B3	0.14	0.97	0.62	0.00	0.00	0.00	0.72	0.28	0.04	0.11
Prunin	0.01	0.30	0.98	0.00	0.47	0.64	0.00	0.09	0.44	0.02
Theogallin	1.00	0.00	0.19	0.05	1.00	0.19	0.05	0.00	0.58	0.00
Theophylline	0.02	0.13	0.00	0.16	0.01	0.02	0.33	0.48	0.00	0.15
Thymine	0.24	0.06	0.00	0.26	0.00	0.06	0.01	0.00	0.09	0.00

Tricetin	0.02	0.76	0.03	0.04	0.04	0.00	0.00	0.00	0.00	0.12
Xanthine	0.02	0.14	0.00	0.15	0.77	0.85	0.28	0.86	0.00	0.03
Xylitol	0.27	0.59	0.92	0.22	0.98	0.07	0.24	0.00	0.03	0.01
Beta.Alanine	0.06	0.45	0.23	0.59	0.11	0.00	0.53	0.05	0.02	0.04
hydroxy.cinnamic.acid	0.05	0.00	0.00	0.06	0.01	0.66	0.36	0.13	0.40	0.61
Citric.acid	0.01	0.01	0.06	0.00	0.10	0.29	0.85	0.83	0.01	0.18
Succinic.acid	0.00	0.26	0.13	0.00	0.00	0.00	0.01	0.67	0.95	0.07
Alpha.ketoglutaric.acid	0.01	0.00	0.01	0.01	0.46	0.81	0.69	0.45	0.00	0.05
Hydroxycoumarine	0.18	0.14	0.02	0.09	0.01	0.06	0.13	0.00	0.00	0.06
Coumarin	0.68	0.00	0.50	0.79	0.02	0.70	0.71	0.06	0.00	0.16
Glutamine	0.00	0.12	0.00	0.01	0.35	0.05	0.77	0.01	0.00	0.05
Delphinidin.3.O.rutinoside.chloride	0.30	0.15	0.02	0.78	0.03	0.50	0.02	0.52	0.59	0.00
Eriodictyol	0.00	0.00	0.08	0.00	0.00	0.11	0.09	0.89	0.12	0.85
Glycyl.L.leucine	0.00	0.14	0.12	0.00	0.00	0.00	0.00	0.83	0.07	0.00
Guanosine.monophosphate	0.00	0.74	0.48	0.00	0.00	0.00	0.00	0.12	0.88	0.00
Glutathione.oxidized	0.06	0.13	0.00	0.47	0.90	0.00	0.49	0.00	0.00	0.36
L.Histidine	0.00	0.17	0.00	0.04	0.93	0.20	0.69	0.22	0.00	0.05
L.Pyroglutamic.acid	0.00	0.10	0.00	0.00	0.36	0.04	1.00	0.01	0.00	0.05
Myricetin	0.31	0.05	0.07	0.12	0.05	0.00	0.61	0.00	0.00	0.12
Naringenin.chalcone	0.00	0.20	0.42	0.00	0.00	0.00	0.24	0.16	0.35	0.00
Quercetin	0.02	0.00	0.43	0.15	0.00	0.17	0.07	0.18	0.49	0.08
Quercetin.3beta.D.glucoside	0.36	0.27	0.01	0.31	0.27	0.35	0.00	0.01	0.00	0.12
Schaftoside	0.04	0.99	0.26	0.82	0.13	0.00	0.01	0.00	0.00	0.08
Uridine.monophosphate	0.46	0.27	0.06	0.00	0.00	0.00	0.37	0.31	0.00	0.00
Digallic.acid	0.00	0.40	0.69	0.00	0.37	0.47	0.00	0.01	0.00	0.32
dihomomethionine	0.14	0.67	0.43	0.02	0.82	0.25	0.55	0.42	0.00	0.59

Epigallocatechin.3.O.3.O.methyl..gallate	0.20	0.90	0.87	0.04	0.00	0.32	0.13	0.24	0.00	0.02
Epigallocatechin..4beta..8..epicatechin.3.O .gallate.ester	0.00	0.44	0.62	0.00	0.54	0.00	0.00	0.00	0.01	0.00
Epigallocatechin.3..glucuronide	0.37	0.00	0.96	0.01	0.06	0.00	0.00	0.53	0.03	0.00
Gallocatechin..4alpha..8..epigallocatechin	0.00	0.63	0.05	0.04	0.30	0.00	0.73	0.12	0.01	0.21
S.Adenosyl.L.homocysteine	0.00	0.02	0.00	0.00	0.32	0.00	0.05	0.00	0.00	0.03
Theasinensin.B	0.00	0.39	0.81	0.00	0.40	0.08	0.00	0.00	0.00	0.00
Malonic.acid	0.15	0.20	0.01	0.20	0.05	0.00	0.24	0.01	0.71	0.18
4.Dihydroxybenzoic.acid	0.39	0.00	0.52	0.18	0.40	0.00	0.75	0.00	0.02	0.11
Aminoadipic.acid	0.00	0.26	0.02	0.00	0.05	0.06	0.00	0.15	0.00	0.08
.Adenosine.monophosphate	0.05	0.49	0.95	0.00	0.00	0.00	0.00	0.23	0.92	0.00
Hydroxy.3.methylglutaric.acid	0.00	0.64	0.44	0.04	0.26	0.33	0.22	0.09	0.01	0.34
Hydroxybenzoic.acid	0.33	0.01	0.05	0.75	0.11	1.00	0.00	0.81	0.32	0.00
Hydroxybenzaldehyde	0.02	0.28	0.38	0.00	0.00	0.00	0.45	0.37	0.23	0.00
Hydroxybenzoic.acid	0.21	0.00	0.23	0.07	0.47	0.00	0.37	0.01	0.01	0.98
Oxoproline	0.01	0.17	0.00	0.06	0.72	0.35	0.24	0.16	0.01	0.01
Adenosine.diphosphate	0.00	0.13	0.00	0.00	0.01	0.28	0.00	0.00	0.00	0.49
Ellagic.acid	0.00	0.79	0.33	0.00	0.08	0.07	0.00	0.00	0.00	0.12
Ethylmalonic.acid	0.05	0.77	0.61	0.00	0.43	0.53	0.50	0.66	0.03	0.17
Fumaric.acid	0.78	0.73	0.00	0.03	0.00	0.00	0.00	0.27	0.00	0.00
Cyanidin.3.O.galactoside	0.00	0.41	0.47	0.87	0.06	0.79	0.05	0.00	0.07	0.03
Quinic.acid	0.82	0.00	0.00	0.69	0.11	0.46	0.61	0.00	0.05	0.00
Theobromine	0.00	0.12	0.17	0.00	0.00	0.08	0.01	0.05	0.15	0.02
trans.p.Coumaric.acid	0.33	0.00	0.00	0.41	0.02	0.74	0.51	0.97	0.33	0.86
Shikimic.acid	0.00	0.00	0.00	0.01	0.07	0.35	0.39	0.43	0.07	0.74

Table S9-6 Corrected *p*-value

<i>p</i> -value	Tricetin	Xanthine	Xylitol	Beta.Alanine	hydroxy.cinnamic.acid	Citric.acid	Succinic.acid	Alpha.ketoglutaric.acid	Hydroxycoumarine	Coumarin
Epigallocatechin.gallate	0.00	0.83	0.41	0.00	0.21	0.85	0.03	0.70	0.11	0.26
Catechin	0.10	0.52	0.07	0.00	0.46	0.03	0.00	0.10	0.25	0.03
Epicatechin	0.00	0.04	0.07	0.00	0.52	0.41	0.03	0.98	0.00	0.00
Gallocatechin	0.70	0.35	0.05	0.02	0.31	0.15	0.02	0.15	0.03	0.01
Methylxanthine	0.03	0.00	0.25	0.03	0.31	0.00	0.00	0.00	0.00	0.00
Abscisic.acid	0.80	0.11	0.80	0.50	0.00	0.07	0.00	0.33	0.11	0.00
Adenine	0.25	0.35	0.24	0.46	0.05	0.00	0.00	0.01	0.48	0.79
Avicularin	0.05	0.12	0.00	0.00	0.28	0.00	0.01	0.00	0.68	0.16
Quercetin.3.O.sophoroside	0.00	0.19	0.00	0.00	0.12	0.00	0.10	0.00	0.20	0.68
Betaine	0.00	0.01	0.13	0.00	0.00	0.03	0.95	0.01	0.05	0.67
Caffeine	0.03	0.28	0.00	0.00	0.63	0.12	0.06	0.20	0.39	0.68
Epicatechin.gallate	0.45	0.97	0.13	0.03	0.43	0.01	0.00	0.11	0.27	0.67
Chlorogenic.acid	0.00	0.00	0.59	0.38	0.45	0.67	0.23	0.83	0.00	0.00
Cynaroside	0.00	0.36	0.27	0.00	0.00	0.30	0.05	0.63	0.12	0.00
Glucuronic.Acid	0.00	0.15	0.00	0.10	0.00	0.00	0.68	0.00	0.50	0.77
D.Fructose	0.01	0.06	0.71	0.00	0.62	0.28	0.12	0.85	0.55	0.97
D.Gluconic.Acid	0.00	0.01	0.03	0.15	0.00	0.00	0.00	0.00	0.00	0.58
Lysine	0.68	0.83	0.33	0.03	0.02	0.27	0.22	0.71	0.66	0.14
Tyrosine	0.05	0.21	0.00	0.94	0.02	0.00	0.00	0.00	0.27	0.78
Trehalose	0.00	0.09	0.03	0.01	0.00	0.00	0.15	0.00	0.21	0.41
Epigallocatechin	0.00	0.00	0.00	0.00	0.11	0.08	0.66	0.01	0.00	0.02
Esculin	0.06	0.42	0.00	0.00	0.86	0.38	0.59	0.16	0.95	0.03
Gallic.acid	0.10	0.35	0.54	0.68	0.01	0.01	0.00	0.11	0.71	0.18
gamma.Aminobutyric.acid	0.00	0.00	0.02	0.00	0.40	0.06	0.12	0.00	0.00	0.03

Glutathione	0.00	0.08	0.00	0.00	0.00	0.01	0.43	0.00	0.90	0.03
Guanine	0.57	0.52	0.20	0.22	0.06	0.00	0.00	0.04	0.51	0.56
Isovitexin	0.00	0.11	0.01	0.00	0.00	0.96	0.42	0.38	0.00	0.72
Kaempferin	0.20	0.20	0.60	0.11	0.88	0.94	0.45	0.58	0.08	0.06
kaempferol	0.00	0.15	0.29	0.31	0.04	0.00	0.00	0.00	0.45	0.81
L.Serine	0.00	0.00	0.00	0.00	0.00	0.00	0.09	0.00	0.03	0.84
L.Arginine	0.00	0.00	0.01	0.00	0.38	0.01	0.06	0.00	0.00	0.30
L.Aspartic.acid	0.00	0.00	0.00	0.00	0.00	0.07	0.17	0.01	0.77	0.32
L.Glutamic.acid	0.00	0.00	0.00	0.00	0.00	0.01	0.78	0.00	0.14	0.60
L.Homoserine	0.00	0.00	0.06	0.00	0.07	0.02	0.34	0.00	0.06	0.60
L.Isoleucine	0.58	0.92	0.40	0.01	0.34	0.04	0.03	0.42	0.48	0.83
L.Phenylalanine	0.56	0.70	0.05	0.01	0.44	0.00	0.03	0.06	0.20	0.49
L.Proline	0.10	0.13	0.69	0.00	0.88	0.36	0.00	0.98	0.20	0.84
L.Theanine	0.00	0.04	0.00	0.00	0.00	0.02	0.33	0.00	0.41	0.88
L.Tryptophan	0.27	0.48	0.29	0.83	0.01	0.54	0.38	0.63	0.00	0.00
Malic.Acid	0.71	0.41	0.00	0.03	0.03	0.34	0.59	0.14	0.35	0.06
Naringenin	0.04	0.05	0.37	0.11	0.09	0.03	0.00	0.03	0.27	0.76
Neochlorogenic.acid	0.82	0.21	0.68	0.56	0.01	0.03	0.36	0.01	0.21	0.01
Pantothenic.acid	0.06	0.00	0.94	0.33	0.00	0.11	0.20	0.03	0.04	0.60
Phloretin	0.08	0.23	0.31	0.68	0.11	0.00	0.00	0.03	0.15	0.85
Procyanidin.B4	0.08	0.83	0.99	0.18	0.03	0.17	0.00	0.56	0.03	0.05
Procyanidin.B3	0.00	0.89	0.13	0.00	0.74	0.39	0.00	0.86	0.10	0.77
Prunin	0.01	0.38	0.34	0.62	0.46	0.89	0.03	0.77	0.20	0.78
Theogallin	0.00	0.90	0.00	0.09	0.20	0.87	0.75	0.56	0.01	0.11
Theophylline	0.00	0.00	0.06	0.04	0.51	0.02	0.97	0.00	0.00	0.01
Thymine	0.19	0.06	0.01	0.08	0.70	0.27	0.13	0.10	0.11	0.24

Tricetin	0.00	0.02	0.00	0.00	0.00	0.03	0.75	0.00	0.00	0.55
Xanthine	0.01	0.00	0.21	0.04	0.07	0.17	0.27	0.04	0.00	0.34
Xylitol	0.00	0.14	0.00	0.00	0.01	0.00	0.71	0.00	0.39	0.78
Beta.Alanine	0.00	0.02	0.00	0.00	0.02	0.20	0.20	0.01	0.18	0.74
hydroxy.cinnamic.acid	0.00	0.03	0.00	0.01	0.00	0.00	0.27	0.00	0.46	0.00
Citric.acid	0.01	0.10	0.00	0.13	0.00	0.00	0.00	0.00	0.80	0.65
Succinic.acid	0.67	0.18	0.62	0.12	0.19	0.00	0.00	0.00	0.30	0.89
Alpha.ketoglutaric.acid	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.70	0.78
Hydroxycoumarine	0.00	0.00	0.29	0.11	0.36	0.73	0.21	0.61	0.00	0.00
Coumarin	0.45	0.25	0.70	0.65	0.00	0.56	0.84	0.71	0.00	0.00
Glutamine	0.00	0.00	0.00	0.00	0.00	0.00	0.07	0.00	0.01	0.80
Delphinidin.3.O.rutinoside.chloride	0.47	0.65	0.01	0.18	0.17	0.43	0.00	0.37	0.17	0.78
Eriodictyol	0.09	0.14	0.67	0.37	0.03	0.00	0.00	0.00	1.00	0.72
Glycyl.L.leucine	0.14	0.01	0.53	0.00	0.49	0.10	0.14	0.82	0.23	0.13
Guanosine.monophosphate	0.85	0.50	0.26	0.05	0.05	0.01	0.01	0.18	0.40	0.24
Glutathione.oxidized	0.00	0.00	0.00	0.00	0.00	0.12	0.62	0.00	0.00	0.37
L.Histidine	0.00	0.00	0.00	0.00	0.02	0.03	0.14	0.00	0.00	0.41
L.Pyroglutamic.acid	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.00	0.01	0.78
Myricetin	0.00	0.05	0.00	0.00	0.58	0.00	0.27	0.00	0.01	0.00
Naringenin.chalcone	0.15	0.57	0.15	0.00	0.61	0.00	0.00	0.03	0.13	0.42
Quercetin	0.26	0.06	0.56	0.00	0.19	0.05	0.24	0.03	0.60	0.06
Quercetin.3beta.D.glucoside	0.13	0.04	0.00	0.03	0.66	0.00	0.00	0.00	0.72	0.01
Schaftoside	0.00	0.01	0.01	0.00	0.01	0.00	0.09	0.00	0.08	0.05
Uridine.monophosphate	0.00	0.00	0.06	0.00	0.68	0.88	0.00	0.03	0.00	0.03
Digallic.acid	0.00	0.85	0.29	0.81	0.88	0.09	0.56	0.07	0.03	0.01
dihomomethionine	0.89	0.89	0.55	0.02	0.00	0.00	0.00	0.01	0.39	0.00

Epigallocatechin.3.O.3.O.methyl..gallate	0.60	0.67	0.07	0.01	0.00	0.52	0.64	0.34	0.15	0.00
Epigallocatechin..4beta..8..epicatechin.3.O .gallate.ester	0.00	0.16	0.00	0.00	0.03	0.63	0.29	0.69	0.01	0.91
Epigallocatechin.3..glucuronide	0.17	0.06	0.04	0.00	0.68	0.00	0.25	0.00	0.24	0.04
Gallocatechin..4alpha..8..epigallocatechin	0.00	0.12	0.89	0.00	0.17	0.74	0.39	0.14	0.20	0.65
S.Adenosyl.L.homocysteine	0.00	0.00	0.00	0.00	0.00	0.00	0.12	0.00	0.00	0.36
Theasinensin.B	0.00	0.05	0.00	0.00	0.03	0.29	0.65	0.07	0.00	0.32
Malonic.acid	0.02	0.92	0.56	0.04	0.08	0.74	0.64	0.39	0.87	0.26
4.Dihydroxybenzoic.acid	0.00	0.04	0.00	0.00	0.00	0.00	0.41	0.00	0.00	0.69
Aminoadipic.acid	0.00	0.03	0.01	0.00	0.00	0.04	0.38	0.01	0.90	0.09
.Adenosine.monophosphate	0.91	0.78	0.01	0.00	0.26	0.00	0.01	0.05	0.75	0.92
Hydroxy.3.methylglutaric.acid	0.00	0.03	0.24	0.01	0.02	0.00	0.00	0.00	0.21	0.12
Hydroxybenzoic.acid	0.55	0.47	0.73	0.66	0.55	0.05	0.00	0.01	0.35	0.29
Hydroxybenzaldehyde	0.01	0.41	0.65	0.00	0.97	0.01	0.00	0.13	0.08	0.42
Hydroxybenzoic.acid	0.00	0.03	0.00	0.00	0.00	0.00	0.81	0.00	0.15	0.06
Oxoproline	0.00	0.00	0.01	0.00	0.02	0.02	0.06	0.00	0.02	0.76
Adenosine.diphosphate	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.00	0.02	0.30
Ellagic.acid	0.00	0.07	0.00	0.00	0.00	0.00	0.80	0.00	0.01	0.63
Ethylmalonic.acid	0.75	0.07	0.81	0.91	0.06	0.00	0.00	0.04	0.20	0.00
Fumaric.acid	0.01	0.00	0.63	0.00	0.92	0.85	0.92	0.28	0.00	0.07
Cyanidin.3.O.galactoside	0.62	0.13	0.08	0.01	0.67	0.03	0.29	0.05	0.07	0.71
Quinic.acid	0.40	0.00	0.01	0.79	0.17	0.19	0.26	0.38	0.00	0.07
Theobromine	0.32	0.00	0.09	0.04	0.48	0.01	0.00	0.00	0.06	0.01
trans.p.Coumaric.acid	0.02	0.92	0.08	0.18	0.00	0.04	0.49	0.01	0.00	0.00
Shikimic.acid	0.00	0.02	0.09	0.07	0.00	0.00	0.06	0.00	0.89	0.00

Table S9-7 Corrected *p*-value

<i>p</i> -value	Glutamine	Delphinidin.3.O.rutinoside. chloride	Eriodictyol	Glycyl.L.leucine	Guanosine.monophosphate	Glutathione.oxidized	L.Histidine	L.Pyroglutamic. acid	Myricetin	Naringenin. chalcone
Epigallocatechin.gallate	0.11	0.56	0.21	0.01	0.00	0.47	0.20	0.11	0.36	0.00
Catechin	0.04	0.00	0.11	0.41	0.15	0.06	0.47	0.05	0.54	0.05
Epicatechin	0.01	0.08	0.17	0.00	0.04	0.00	0.00	0.01	0.00	0.00
Gallocatechin	0.17	0.00	0.97	0.15	0.54	0.31	0.84	0.20	0.68	0.07
Methylxanthine	0.00	0.01	0.01	0.00	0.79	0.00	0.00	0.00	0.00	0.10
Abscisic.acid	0.33	0.73	0.01	0.92	0.76	0.37	0.10	0.31	0.00	0.01
Adenine	0.09	0.91	0.00	0.00	0.00	0.51	0.16	0.05	0.63	0.00
Avicularin	0.00	0.01	0.00	0.00	0.18	0.02	0.03	0.00	0.00	0.78
Quercetin.3.O.sophoroside	0.00	0.00	0.14	0.74	0.24	0.00	0.00	0.00	0.00	0.57
Betaine	0.00	0.95	0.00	0.75	0.38	0.00	0.00	0.00	0.00	0.96
Caffeine	0.01	0.00	0.37	0.75	0.70	0.19	0.03	0.01	0.59	0.32
Epicatechin.gallate	0.83	0.17	0.00	0.00	0.00	0.99	0.97	0.82	0.95	0.00
Chlorogenic.acid	0.08	0.22	0.82	0.28	0.64	0.01	0.00	0.07	0.05	0.14
Cynaroside	0.01	0.63	0.84	0.70	0.09	0.00	0.08	0.01	0.03	0.10
Glucuronic.Acid	0.00	0.00	0.01	0.00	0.00	0.24	0.02	0.00	0.02	0.01
D.Fructose	0.00	0.58	0.01	0.00	0.00	0.00	0.01	0.00	0.07	0.00
D.Gluconic.Acid	0.00	0.27	0.00	0.00	0.00	0.00	0.00	0.00	0.07	0.02
Lysine	0.61	0.42	0.00	0.00	0.00	0.79	0.77	0.75	0.45	0.00
Tyrosine	0.04	0.98	0.00	0.00	0.00	0.11	0.13	0.02	0.05	0.00
Trehalose	0.00	0.62	0.00	0.00	0.00	0.01	0.01	0.00	0.15	0.00
Epigallocatechin	0.00	0.65	0.01	0.63	0.02	0.00	0.00	0.00	0.00	0.55
Esculin	0.04	0.95	0.03	0.00	0.00	0.13	0.14	0.05	0.00	0.01
Gallic.acid	0.07	0.82	0.00	0.00	0.00	0.57	0.11	0.04	0.78	0.00

gamma.Aminobutyric.acid	0.00	0.50	0.59	0.00	0.49	0.00	0.00	0.00	0.00	0.05
Glutathione	0.00	0.04	0.00	0.52	0.01	0.00	0.00	0.00	0.00	0.42
Guanine	0.29	0.54	0.00	0.00	0.00	0.57	0.35	0.20	0.98	0.00
Isovitexin	0.00	0.20	0.87	0.02	0.21	0.00	0.01	0.00	0.00	0.01
Kaempferin	0.16	0.00	0.47	0.00	0.12	0.04	0.18	0.18	0.17	0.01
kaempferol	0.00	0.11	0.00	0.03	0.00	0.11	0.02	0.00	0.05	0.01
L.Serine	0.00	0.48	0.00	0.01	0.69	0.00	0.00	0.00	0.00	0.91
L.Arginine	0.00	0.65	0.02	0.01	0.92	0.00	0.00	0.00	0.00	0.87
L.Aspartic.acid	0.00	0.08	0.06	0.01	0.93	0.00	0.00	0.00	0.00	0.96
L.Glutamic.acid	0.00	0.09	0.05	0.02	0.85	0.00	0.00	0.00	0.00	0.69
L.Homoserine	0.00	0.01	0.38	0.00	0.01	0.00	0.00	0.00	0.00	0.04
L.Isoleucine	0.77	0.41	0.00	0.00	0.00	0.77	0.97	0.88	0.36	0.00
L.Phenylalanine	0.49	0.46	0.03	0.00	0.00	0.88	0.88	0.53	0.59	0.00
L.Proline	0.01	0.99	0.00	0.00	0.00	0.01	0.08	0.02	0.29	0.00
L.Theanine	0.00	0.39	0.00	0.07	0.69	0.00	0.00	0.00	0.00	0.97
L.Tryptophan	0.38	0.14	0.03	0.06	0.10	0.40	0.99	0.33	0.01	0.33
Malic.Acid	0.07	0.13	0.75	0.95	0.26	0.01	0.96	0.08	0.99	0.17
Naringenin	0.00	0.40	0.00	0.00	0.00	0.12	0.01	0.00	0.42	0.01
Neochlorogenic.acid	0.19	0.23	0.00	0.22	0.81	0.20	0.26	0.17	0.09	0.29
Pantothenic.acid	0.00	0.04	0.14	0.20	0.58	0.01	0.00	0.00	0.12	0.52
Phloretin	0.02	0.84	0.00	0.00	0.00	0.57	0.07	0.01	0.19	0.00
Procyanidin.B4	0.45	0.06	0.00	0.00	0.00	0.92	0.95	0.46	0.09	0.00
Procyanidin.B3	0.10	0.60	0.17	0.00	0.00	0.00	0.29	0.08	0.00	0.00
Prunin	0.83	0.04	0.16	0.00	0.00	0.59	0.76	1.00	0.70	0.34
Theogallin	0.03	0.61	0.92	0.88	0.20	0.00	0.32	0.03	0.00	0.24
Theophylline	0.00	0.68	0.19	0.13	0.91	0.00	0.00	0.00	0.00	0.46

Thymine	0.09	0.00	0.89	0.00	0.00	0.46	0.09	0.09	0.19	0.00
Tricetin	0.00	0.57	0.15	0.22	0.89	0.00	0.00	0.00	0.00	0.23
Xanthine	0.00	0.73	0.22	0.03	0.60	0.00	0.00	0.00	0.09	0.66
Xylitol	0.00	0.03	0.75	0.63	0.36	0.00	0.01	0.00	0.00	0.23
Beta.Alanine	0.00	0.27	0.47	0.00	0.10	0.00	0.00	0.00	0.00	0.01
hydroxy.cinnamic.acid	0.00	0.26	0.07	0.59	0.09	0.00	0.04	0.00	0.67	0.70
Citric.acid	0.00	0.53	0.00	0.17	0.03	0.19	0.05	0.00	0.00	0.01
Succinic.acid	0.12	0.01	0.00	0.22	0.03	0.70	0.21	0.11	0.36	0.00
Alpha.ketoglutaric.acid	0.00	0.47	0.00	0.87	0.27	0.01	0.00	0.00	0.00	0.06
Hydroxycoumarine	0.03	0.25	1.00	0.33	0.50	0.00	0.00	0.02	0.02	0.21
Coumarin	0.85	0.83	0.79	0.21	0.33	0.47	0.51	0.84	0.00	0.52
Glutamine	0.00	0.30	0.01	0.02	0.56	0.00	0.00	0.00	0.00	0.96
Delphinidin.3.O.rutinoside.chloride	0.21	0.00	0.51	0.10	0.49	0.74	0.63	0.33	0.89	0.06
Eriodictyol	0.00	0.41	0.00	0.01	0.00	0.40	0.06	0.00	0.20	0.00
Glycyl.L.leucine	0.01	0.05	0.00	0.00	0.00	0.01	0.03	0.03	0.02	0.00
Guanosine.monophosphate	0.46	0.39	0.00	0.00	0.00	0.73	0.50	0.46	0.22	0.00
Glutathione.oxidized	0.00	0.66	0.30	0.00	0.65	0.00	0.00	0.00	0.00	0.44
L.Histidine	0.00	0.54	0.03	0.01	0.39	0.00	0.00	0.00	0.00	0.61
L.Pyroglutamic.acid	0.00	0.24	0.00	0.01	0.35	0.00	0.00	0.00	0.00	0.97
Myricetin	0.00	0.85	0.13	0.01	0.14	0.00	0.00	0.00	0.00	0.98
Naringenin.chalcone	0.94	0.03	0.00	0.00	0.00	0.34	0.51	0.95	0.97	0.00
Quercetin	0.00	0.02	0.00	0.18	0.61	0.05	0.00	0.00	0.45	0.07
Quercetin.3beta.D.glucoside	0.00	0.51	0.01	0.00	0.18	0.06	0.01	0.00	0.00	0.25
Schaftoside	0.00	0.13	0.04	0.02	0.17	0.00	0.00	0.00	0.00	0.66
Uridine.monophosphate	0.00	0.92	0.22	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Digallic.acid	0.97	0.53	0.00	0.01	0.00	0.50	0.79	0.77	0.06	0.28

dihomomethionine	0.17	0.30	0.02	0.11	0.53	0.08	0.48	0.21	0.02	0.00
Epigallocatechin.3.O..3.O.methyl..gallate	0.00	0.00	0.32	0.05	0.01	0.04	0.08	0.00	0.64	0.08
Epigallocatechin..4beta..8..epicatechin.3.O.g allate.ester	0.00	0.17	0.02	0.15	0.03	0.00	0.00	0.00	0.10	0.46
Epigallocatechin.3..glucuronide	0.00	0.01	0.54	0.00	0.00	0.00	0.02	0.00	0.00	0.31
Galocatechin..4alpha..8..epigallocatechin	0.00	0.01	0.00	0.19	0.72	0.00	0.00	0.00	0.01	0.06
S.Adenosyl.L.homocysteine	0.00	0.08	0.00	0.23	0.07	0.00	0.00	0.00	0.00	0.88
Theasinensin.B	0.00	0.87	0.00	0.01	0.00	0.00	0.00	0.00	0.04	0.11
Malonic.acid	0.04	0.07	0.22	0.12	0.78	0.09	0.24	0.03	0.00	0.00
4.Dihydroxybenzoic.acid	0.00	0.01	0.03	0.01	0.46	0.00	0.00	0.00	0.00	0.84
Aminoadipic.acid	0.00	0.12	0.00	0.12	0.03	0.00	0.00	0.00	0.06	0.24
.Adenosine.monophosphate	0.71	0.39	0.01	0.00	0.00	0.27	0.85	0.82	0.79	0.00
Hydroxy.3.methylglutaric.acid	0.00	0.02	0.01	0.44	0.07	0.00	0.01	0.00	0.05	0.28
Hydroxybenzoic.acid	0.18	0.00	0.08	0.00	0.16	0.35	0.51	0.18	0.22	0.19
Hydroxybenzaldehyde	0.26	0.11	0.00	0.00	0.00	0.11	0.20	0.26	0.45	0.00
Hydroxybenzoic.acid	0.00	0.73	0.00	0.14	0.46	0.00	0.00	0.00	0.00	0.87
Oxoproline	0.00	0.78	0.02	0.01	0.95	0.00	0.00	0.00	0.00	0.38
Adenosine.diphosphate	0.00	0.53	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.01
Ellagic.acid	0.00	0.11	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.04
Ethylmalonic.acid	0.13	0.08	0.03	0.64	0.91	0.86	0.06	0.13	0.01	0.21
Fumaric.acid	0.00	0.01	0.15	0.00	0.00	0.00	0.00	0.00	0.01	0.00
Cyanidin.3.O.galactoside	0.01	0.00	0.06	0.76	0.18	0.41	0.06	0.02	0.25	0.09
Quinic.acid	0.23	0.01	0.37	0.04	0.29	0.06	0.00	0.21	0.04	0.00
Theobromine	0.00	0.50	0.00	0.10	0.13	0.00	0.00	0.00	0.00	0.00
trans.p.Coumaric.acid	0.11	0.12	0.12	0.51	0.38	0.00	0.77	0.09	0.59	0.75
Shikimic.acid	0.00	0.02	0.00	0.47	0.04	0.00	0.02	0.00	0.51	0.78

Table S9-8 Corrected *p*-value

<i>p</i> -value	Quercetin	Quercetin.3beta. D.glucoside	Schaftoside	Uridine.mono phosphate	Digallic.acid	dihomomet hionine	Epigallocatechin.3.O..3.O. methyl..gallate	Epigallocatechin..4beta..8..e picatechin.3.O.gallate.ester	Epigallocatechin. 3..glucuronide	Gallocatechin..4alpha.. 8..epigallocatechin
Epigallocatechin.gallate	0.35	0.29	0.11	0.00	0.80	0.52	0.20	0.09	0.01	0.04
Catechin	0.01	0.15	0.37	0.03	0.08	0.00	0.00	0.01	0.26	0.89
Epicatechin	0.08	0.52	0.00	0.00	0.02	0.56	0.10	0.00	0.16	0.00
Gallocatechin	0.00	0.05	0.80	0.84	0.32	0.03	0.00	0.00	0.06	0.33
Methylxanthine	0.00	0.00	0.00	0.00	0.47	0.03	0.50	0.92	0.00	0.10
Abscisic.acid	0.88	0.00	0.42	0.51	0.13	0.00	0.11	0.41	0.51	0.85
Adenine	0.49	0.85	0.97	0.00	0.00	0.08	0.05	0.01	0.01	0.07
Avicularin	0.10	0.00	0.00	0.03	0.59	0.08	0.02	0.73	0.00	0.00
Quercetin.3.O.sophoroside	0.18	0.01	0.34	0.02	0.22	0.92	0.05	0.00	0.54	0.48
Betaine	0.09	0.16	0.00	0.00	0.05	0.38	0.49	0.00	0.07	0.00
Caffeine	0.06	0.12	0.92	0.09	0.33	0.23	0.00	0.19	0.69	0.08
Epicatechin.gallate	0.12	0.30	0.96	0.00	0.22	0.00	0.07	0.29	0.41	0.21
Chlorogenic.acid	0.56	0.82	0.24	0.00	0.07	0.55	0.14	0.06	0.38	0.42
Cynaroside	0.07	0.00	0.51	0.96	0.07	0.00	0.00	0.00	0.57	0.15
Glucuronic.Acid	0.69	0.44	0.27	0.76	0.02	0.76	0.16	0.00	0.37	0.46
D.Fructose	0.33	0.77	0.01	0.00	0.03	0.01	0.26	0.78	0.01	0.08
D.Gluconic.Acid	0.62	0.81	0.02	0.23	0.00	0.76	0.03	0.00	0.23	0.00
Lysine	0.34	0.22	0.33	0.00	0.00	0.65	0.06	0.00	0.00	0.85
Tyrosine	0.56	0.05	0.16	0.04	0.01	0.01	0.32	0.01	0.57	0.11
Trehalose	0.12	0.52	0.15	0.24	0.05	0.51	0.00	0.00	0.64	0.00
Epigallocatechin	0.76	0.70	0.00	0.00	0.00	0.35	0.56	0.00	0.60	0.00
Esculin	0.82	0.00	0.00	0.00	0.40	0.50	0.73	0.22	0.01	0.94
Gallic.acid	0.27	0.55	0.67	0.00	0.00	0.33	0.01	0.00	0.00	0.12

gamma.Aminobutyric.acid	0.02	0.07	0.00	0.00	0.65	0.78	0.43	0.01	0.00	0.01
Glutathione	0.02	0.17	0.02	0.64	0.76	0.07	0.00	0.00	0.96	0.00
Guanine	0.71	0.92	0.77	0.00	0.00	0.17	0.04	0.01	0.00	0.31
Isovitexin	0.29	0.28	0.00	0.00	0.11	0.20	0.44	0.00	0.72	0.00
Kaempferin	0.30	0.10	0.00	0.00	0.02	0.38	0.00	0.13	0.02	0.00
kaempferol	0.79	0.07	0.01	0.76	0.00	0.01	0.94	0.00	0.97	0.00
L.Serine	0.00	0.00	0.00	0.00	0.97	0.27	0.01	0.00	0.00	0.00
L.Arginine	0.00	0.00	0.00	0.00	0.94	0.97	0.08	0.01	0.00	0.00
L.Aspartic.acid	0.00	0.00	0.00	0.00	0.73	0.05	0.00	0.00	0.01	0.00
L.Glutamic.acid	0.00	0.02	0.00	0.00	0.92	0.09	0.00	0.00	0.00	0.00
L.Homoserine	0.00	0.00	0.00	0.00	0.21	0.22	0.91	0.82	0.00	0.00
L.Isoleucine	0.82	0.37	0.17	0.00	0.01	0.10	0.14	0.11	0.00	0.83
L.Phenylalanine	0.91	0.27	0.83	0.00	0.21	0.06	0.92	0.85	0.92	0.42
L.Proline	0.05	0.84	0.33	0.00	0.17	0.01	0.99	0.35	0.00	0.99
L.Theanine	0.02	0.00	0.00	0.00	0.15	0.92	0.12	0.00	0.00	0.00
L.Tryptophan	0.01	0.47	0.00	0.06	0.52	0.04	0.01	0.39	0.00	0.85
Malic.Acid	0.46	0.35	0.93	0.78	0.78	0.25	0.08	0.54	0.07	1.00
Naringenin	0.04	0.47	0.08	0.56	0.00	0.22	0.29	0.00	0.47	0.00
Neochlorogenic.acid	0.01	0.37	0.99	0.37	0.50	0.75	0.92	0.55	0.00	0.72
Pantothenic.acid	0.53	0.03	0.36	0.11	0.77	0.53	0.91	0.71	0.97	0.10
Phloretin	0.23	0.42	0.87	0.00	0.00	0.04	0.07	0.01	0.03	0.08
Procyanidin.B4	0.00	0.37	0.20	0.00	0.48	0.87	0.00	0.63	0.11	0.40
Procyanidin.B3	0.25	0.45	0.00	0.00	0.57	0.34	0.42	0.01	0.01	0.00
Prunin	0.13	0.00	0.02	0.47	0.00	0.64	0.21	0.00	0.00	0.80
Theogallin	0.27	0.02	0.01	0.41	0.03	0.52	0.34	0.00	0.62	0.20
Theophylline	0.59	0.01	0.00	0.00	0.00	0.00	0.00	0.02	0.06	0.03

Thymine	0.13	0.19	0.14	0.01	0.42	0.68	0.05	0.01	0.00	0.30
Tricetin	0.35	0.21	0.00	0.00	0.00	0.92	0.69	0.00	0.26	0.00
Xanthine	0.11	0.08	0.02	0.00	0.89	0.92	0.75	0.24	0.10	0.19
Xylitol	0.65	0.00	0.02	0.11	0.39	0.65	0.12	0.01	0.08	0.92
Beta.Alanine	0.00	0.07	0.00	0.00	0.86	0.04	0.03	0.00	0.00	0.00
hydroxy.cinnamic.acid	0.28	0.74	0.02	0.76	0.91	0.00	0.00	0.06	0.76	0.25
Citric.acid	0.09	0.00	0.01	0.91	0.16	0.00	0.62	0.71	0.00	0.80
Succinic.acid	0.33	0.00	0.15	0.00	0.65	0.01	0.73	0.39	0.35	0.49
Alpha.ketoglutaric.acid	0.06	0.00	0.00	0.07	0.13	0.02	0.44	0.76	0.00	0.22
Hydroxycoumarine	0.69	0.79	0.13	0.00	0.05	0.49	0.22	0.02	0.34	0.29
Coumarin	0.11	0.02	0.09	0.06	0.02	0.00	0.00	0.93	0.08	0.74
Glutamine	0.00	0.00	0.00	0.00	0.98	0.26	0.01	0.00	0.00	0.00
Delphinidin.3.O.rutinoside.chloride	0.04	0.61	0.20	0.94	0.62	0.40	0.00	0.25	0.03	0.02
Eriodictyol	0.01	0.01	0.07	0.32	0.00	0.05	0.42	0.04	0.63	0.00
Glycyl.L.leucine	0.27	0.00	0.03	0.00	0.02	0.18	0.09	0.24	0.00	0.28
Guanosine.monophosphate	0.70	0.27	0.25	0.00	0.01	0.63	0.02	0.06	0.00	0.79
Glutathione.oxidized	0.10	0.11	0.00	0.00	0.60	0.14	0.08	0.00	0.00	0.00
L.Histidine	0.01	0.02	0.00	0.00	0.85	0.58	0.14	0.01	0.04	0.01
L.Pyroglutamic.acid	0.00	0.00	0.00	0.00	0.83	0.30	0.01	0.00	0.00	0.00
Myricetin	0.55	0.00	0.00	0.00	0.11	0.05	0.72	0.16	0.00	0.03
Naringenin.chalcone	0.12	0.34	0.74	0.00	0.38	0.00	0.13	0.56	0.42	0.10
Quercetin	0.00	0.05	0.99	0.59	0.00	0.03	0.00	0.32	0.01	0.72
Quercetin.3beta.D.glucoside	0.02	0.00	0.00	0.09	0.47	0.01	0.11	0.22	0.00	0.24
Schaftoside	0.98	0.00	0.00	0.00	0.01	0.03	0.43	0.00	0.00	0.00
Uridine.monophosphate	0.49	0.04	0.00	0.00	0.19	0.86	0.08	0.03	0.00	0.01
Digallic.acid	0.00	0.36	0.00	0.12	0.00	0.00	0.00	0.00	0.22	0.03

dihomomethionine	0.01	0.00	0.01	0.81	0.00	0.00	0.00	0.97	0.07	0.89
Epigallocatechin.3.O..3.O.methyl.gallate	0.00	0.06	0.33	0.04	0.00	0.00	0.00	0.17	0.04	0.41
Epigallocatechin.4beta..8..epicatechin.3.O.gallate.ester	0.23	0.14	0.00	0.01	0.00	0.95	0.10	0.00	0.47	0.00
Epigallocatechin.3..glucuronide	0.00	0.00	0.00	0.00	0.14	0.04	0.02	0.36	0.00	0.22
Galocatechin..4alpha..8..epigallocatechin	0.63	0.16	0.00	0.00	0.01	0.86	0.30	0.00	0.15	0.00
S.Adenosyl.L.homocysteine	0.48	0.00	0.00	0.00	0.00	0.09	0.50	0.00	0.03	0.00
Theasinensin.B	0.03	0.51	0.00	0.08	0.00	0.21	0.96	0.00	0.65	0.00
Malonic.acid	0.50	0.03	0.16	0.78	0.67	0.00	0.06	0.74	0.21	0.00
4.Dihydroxybenzoic.acid	0.49	0.02	0.00	0.00	0.31	0.99	0.46	0.00	0.00	0.01
Aminoadipic.acid	0.55	0.40	0.00	0.03	0.00	0.47	0.03	0.00	0.55	0.00
.Adenosine.monophosphate	0.09	0.85	0.22	0.00	0.06	0.00	0.34	0.12	0.01	0.85
Hydroxy.3.methylglutaric.acid	0.37	0.58	0.00	0.13	0.00	0.01	0.61	0.00	0.00	0.00
Hydroxybenzoic.acid	0.56	0.00	0.19	0.73	0.76	0.28	0.00	0.15	0.00	0.00
Hydroxybenzaldehyde	0.14	0.38	0.43	0.00	0.27	0.00	0.20	0.96	0.21	0.02
Hydroxybenzoic.acid	0.01	0.01	0.00	0.00	0.56	0.40	0.01	0.00	0.00	0.01
Oxoproline	0.00	0.00	0.03	0.12	0.45	0.14	0.14	0.22	0.00	0.00
Adenosine.diphosphate	0.10	0.18	0.00	0.25	0.01	0.76	0.00	0.00	1.00	0.00
Ellagic.acid	0.24	0.98	0.00	0.01	0.00	0.74	0.00	0.00	0.84	0.00
Ethylmalonic.acid	0.25	0.01	0.06	0.91	0.70	0.00	0.08	0.79	0.03	0.22
Fumaric.acid	0.47	0.00	0.00	0.00	0.82	0.36	0.03	0.96	0.00	0.05
Cyanidin.3.O.galactoside	0.00	0.15	0.01	0.02	0.99	0.00	0.24	0.78	0.02	0.83
Quinic.acid	0.10	0.02	0.02	0.09	0.03	0.02	0.69	0.21	0.57	0.40
Theobromine	0.00	0.00	0.00	0.39	0.64	0.05	0.08	0.68	0.00	0.42

trans.p.Coumaric.acid	0.29	0.91	0.26	0.47	0.28	0.00	0.00	0.60	0.74	0.52
Shikimic.acid	0.51	0.34	0.00	0.62	0.26	0.03	0.08	0.03	0.53	0.01

Table S9-9 Corrected p-value

<i>p</i> -value	S.Adenosyl.L.ho mocysteine	Theasinensin.B	Malonic.a cid	4.Dihydroxybenz oic.acid	Aminoadic.ac id	Adenosine.monophos phate	Hydroxy.3.methylglutar ic.acid	Hydroxybenzoic .acid	Hydroxybenzalde hyde	Hydroxybenzoic .acid
Epigallocatechin.gallate	0.48	0.08	0.32	0.00	0.82	0.02	0.18	0.80	0.00	0.00
Catechin	0.61	0.89	0.17	0.79	0.01	0.04	0.44	0.00	0.01	0.04
Epicatechin	0.00	0.00	0.02	0.00	0.70	0.05	0.17	0.28	0.00	0.03
Galocatechin	0.28	0.42	0.47	0.75	0.00	0.88	0.65	0.00	0.20	0.16
Methylxanthine	0.00	0.83	0.83	0.00	0.47	0.27	0.01	0.00	0.13	0.03
Abscisic.acid	0.18	0.94	0.88	0.62	1.00	0.68	0.16	0.39	0.01	0.32
Adenine	0.00	0.00	0.24	0.76	0.00	0.00	0.02	0.75	0.00	0.25
Avicularin	0.00	0.84	0.03	0.00	0.43	0.62	0.56	0.00	0.62	0.00
Quercetin.3.O.sophoroside	0.00	0.00	0.46	0.01	0.00	0.06	0.87	0.03	0.71	0.00
Betaine	0.00	0.00	0.51	0.00	0.00	0.48	0.18	0.97	0.71	0.00
Caffeine	0.66	0.34	0.88	0.24	0.50	0.95	0.11	0.00	0.05	0.00
Epicatechin.gallate	0.64	0.10	0.01	0.86	0.15	0.00	0.27	0.40	0.00	0.83
Chlorogenic.acid	0.00	0.01	0.86	0.02	0.79	0.78	0.43	0.38	0.10	0.40
Cynaroside	0.29	0.02	0.20	0.01	0.44	0.88	0.62	0.74	0.03	0.00
Glucuronic.Acid	0.02	0.00	0.56	0.18	0.00	0.00	0.04	0.01	0.12	0.01
D.Fructose	0.59	0.70	0.15	0.35	0.53	0.00	0.15	0.88	0.00	0.44
D.Gluconic.Acid	0.00	0.00	0.06	0.00	0.00	0.00	0.00	0.87	0.09	0.00
Lysine	0.17	0.00	0.48	0.96	0.00	0.00	0.40	0.10	0.00	0.56
Tyrosine	0.00	0.00	0.91	0.00	0.01	0.00	0.01	0.86	0.00	0.00
Trehalose	0.00	0.00	0.34	0.00	0.00	0.00	0.00	0.40	0.01	0.00
Epigallocatechin	0.00	0.00	0.26	0.00	0.00	0.19	0.00	0.99	0.90	0.00
Esculin	0.63	0.25	0.01	0.56	0.22	0.06	0.67	0.55	0.00	0.21
Gallic.acid	0.00	0.00	0.32	0.51	0.00	0.00	0.14	0.48	0.00	0.08

gamma.Aminobutyric.acid	0.00	0.01	0.34	0.01	0.01	0.10	0.00	0.68	0.01	0.00
Glutathione	0.00	0.00	0.00	0.00	0.00	0.11	0.02	0.42	0.96	0.00
Guanine	0.01	0.00	0.44	0.93	0.00	0.00	0.04	0.39	0.00	0.29
Isovitexin	0.00	0.00	0.00	0.00	0.01	0.14	0.15	0.82	0.00	0.00
Kaempferin	0.01	0.09	0.76	0.34	0.51	0.15	0.19	0.00	0.03	0.52
kaempferol	0.00	0.00	0.15	0.00	0.00	0.00	0.01	0.01	0.04	0.00
L.Serine	0.00	0.00	0.06	0.00	0.00	0.64	0.01	0.15	0.34	0.00
L.Arginine	0.00	0.01	0.39	0.00	0.00	0.54	0.01	0.57	0.37	0.00
L.Aspartic.acid	0.00	0.00	0.05	0.00	0.00	0.48	0.01	0.84	0.41	0.00
L.Glutamic.acid	0.00	0.00	0.10	0.00	0.00	0.47	0.01	0.86	0.15	0.00
L.Homoserine	0.00	0.91	0.16	0.00	0.30	0.00	0.07	0.00	0.01	0.00
L.Isoleucine	0.27	0.00	0.70	0.44	0.16	0.00	0.28	0.12	0.00	0.94
L.Phenylalanine	0.61	0.07	0.66	0.34	0.54	0.00	0.25	0.86	0.00	0.47
L.Proline	0.27	0.02	0.79	0.12	0.27	0.00	0.18	0.64	0.00	0.15
L.Theanine	0.00	0.00	0.04	0.00	0.00	0.84	0.01	0.37	0.42	0.00
L.Tryptophan	0.86	0.13	0.36	0.00	0.04	0.29	0.04	0.86	0.34	0.91
Malic.Acid	0.62	0.33	0.92	0.13	0.31	0.60	0.22	0.85	0.45	0.00
Naringenin	0.00	0.00	0.24	0.49	0.00	0.09	0.01	0.43	0.04	0.30
Neochlorogenic.acid	0.04	0.49	0.29	0.01	0.36	0.59	0.72	0.02	0.38	0.00
Pantothenic.acid	0.00	0.86	0.02	0.61	0.04	0.97	0.54	0.09	0.48	0.33
Phloretin	0.00	0.00	0.30	0.27	0.00	0.00	0.09	0.82	0.00	0.12
Procyanidin.B4	0.42	0.50	0.09	0.50	0.10	0.00	0.35	0.18	0.00	0.57
Procyanidin.B3	0.00	0.14	0.01	0.00	0.11	0.00	0.43	1.00	0.00	0.00
Prunin	0.10	0.00	0.33	0.81	0.01	0.01	0.31	0.00	0.55	0.47
Theogallin	0.01	0.00	0.03	0.00	0.23	0.32	0.15	0.86	0.48	0.02
Theophylline	0.00	0.00	0.78	0.05	0.00	0.94	0.03	0.42	0.33	0.02

Thymine	0.05	0.01	0.27	0.18	0.14	0.00	0.44	0.00	0.00	0.99
Tricetin	0.00	0.00	0.04	0.00	0.00	0.94	0.00	0.64	0.03	0.00
Xanthine	0.00	0.09	0.94	0.08	0.06	0.84	0.06	0.57	0.51	0.06
Xylitol	0.01	0.01	0.65	0.00	0.03	0.03	0.33	0.79	0.73	0.00
Beta.Alanine	0.00	0.00	0.08	0.00	0.00	0.00	0.03	0.74	0.00	0.00
hydroxy.cinnamic.acid	0.00	0.06	0.13	0.00	0.00	0.35	0.04	0.64	0.98	0.00
Citric.acid	0.00	0.39	0.81	0.00	0.08	0.00	0.00	0.09	0.03	0.00
Succinic.acid	0.19	0.74	0.73	0.51	0.48	0.01	0.00	0.00	0.00	0.86
Alpha.ketoglutaric.acid	0.00	0.13	0.49	0.00	0.02	0.09	0.00	0.02	0.21	0.00
Hydroxycoumarine	0.00	0.00	0.91	0.01	0.92	0.82	0.30	0.46	0.13	0.22
Coumarin	0.46	0.42	0.36	0.76	0.14	0.94	0.19	0.39	0.52	0.11
Glutamine	0.00	0.00	0.09	0.00	0.00	0.78	0.01	0.27	0.36	0.00
Delphinidin.3.O.rutinoside.chloride	0.14	0.90	0.12	0.02	0.19	0.50	0.04	0.00	0.18	0.80
Eriodictyol	0.00	0.01	0.32	0.05	0.00	0.02	0.03	0.14	0.00	0.00
Glycyl.L.leucine	0.33	0.03	0.20	0.03	0.20	0.00	0.54	0.00	0.00	0.22
Guanosine.monophosphate	0.12	0.00	0.84	0.56	0.06	0.00	0.12	0.25	0.00	0.56
Glutathione.oxidized	0.00	0.00	0.16	0.00	0.00	0.37	0.00	0.45	0.17	0.00
L.Histidine	0.00	0.00	0.34	0.00	0.00	0.89	0.02	0.61	0.29	0.00
L.Pyroglutamic.acid	0.00	0.00	0.07	0.00	0.00	0.86	0.01	0.27	0.36	0.00
Myricetin	0.00	0.08	0.01	0.00	0.10	0.85	0.10	0.31	0.55	0.00
Naringenin.chalcone	0.91	0.19	0.00	0.88	0.34	0.00	0.38	0.28	0.00	0.91
Quercetin	0.58	0.05	0.59	0.59	0.64	0.15	0.47	0.66	0.22	0.02
Quercetin.3beta.D.glucoside	0.00	0.60	0.07	0.05	0.50	0.89	0.67	0.00	0.48	0.02
Schaftoside	0.00	0.00	0.24	0.00	0.00	0.32	0.00	0.28	0.53	0.00
Uridine.monophosphate	0.00	0.14	0.84	0.01	0.06	0.00	0.21	0.80	0.00	0.01
Digallic.acid	0.00	0.00	0.75	0.42	0.00	0.11	0.01	0.82	0.36	0.65

dihomomethionine	0.15	0.30	0.00	0.99	0.57	0.01	0.02	0.38	0.00	0.50
Epigallocatechin.3.O..3.O.methyl..gallate	0.60	0.97	0.10	0.56	0.05	0.44	0.70	0.00	0.29	0.03
Epigallocatechin..4beta..8..epicatechin.3.O.g allate.ester	0.00	0.00	0.81	0.00	0.00	0.20	0.00	0.22	0.97	0.00
Epigallocatechin.3..glucuronide	0.05	0.74	0.30	0.00	0.65	0.01	0.01	0.00	0.30	0.00
Galocatechin..4alpha..8..epigallocatechin	0.00	0.00	0.00	0.02	0.00	0.89	0.01	0.00	0.04	0.03
S.Adenosyl.L.homocysteine	0.00	0.00	0.05	0.00	0.00	0.58	0.00	0.03	0.56	0.00
Theasinensin.B	0.00	0.00	0.88	0.00	0.00	0.01	0.00	0.92	0.50	0.00
Malonic.acid	0.03	0.84	0.00	0.19	0.19	0.59	0.55	0.15	0.00	0.25
4.Dihydroxybenzoic.acid	0.00	0.00	0.11	0.00	0.05	0.48	0.00	0.07	0.50	0.00
Aminoadipic.acid	0.00	0.00	0.12	0.02	0.00	0.25	0.01	0.39	0.68	0.00
.Adenosine.monophosphate	0.48	0.00	0.49	0.38	0.16	0.00	0.22	0.45	0.00	0.70
Hydroxy.3.methylglutaric.acid	0.00	0.00	0.45	0.00	0.00	0.14	0.00	0.62	0.65	0.09
Hydroxybenzoic.acid	0.01	0.90	0.09	0.03	0.29	0.35	0.53	0.00	0.44	0.66
Hydroxybenzaldehyde	0.46	0.40	0.00	0.40	0.59	0.00	0.56	0.33	0.00	0.34
Hydroxybenzoic.acid	0.00	0.00	0.17	0.00	0.00	0.61	0.05	0.56	0.25	0.00
Oxoproline	0.00	0.09	0.12	0.00	0.18	0.53	0.50	0.01	0.12	0.00
Adenosine.diphosphate	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.43	0.14	0.00
Ellagic.acid	0.00	0.00	0.07	0.00	0.00	0.03	0.00	0.05	0.36	0.00
Ethylmalonic.acid	0.03	0.58	0.31	0.06	0.29	0.46	0.01	0.04	0.26	0.88
Fumaric.acid	0.00	0.57	0.68	0.02	0.19	0.00	0.12	0.00	0.00	0.10
Cyanidin.3.O.galactoside	0.24	0.21	0.01	0.19	0.00	0.09	0.28	0.00	0.11	0.47
Quinic.acid	0.03	0.18	0.66	0.11	0.11	0.03	0.05	0.21	0.01	0.21
Theobromine	0.00	0.63	0.70	0.01	0.51	0.70	0.01	0.07	0.00	0.08
trans.p.Coumaric.acid	0.04	0.80	0.03	0.01	0.00	0.69	0.55	0.55	0.94	0.00
Shikimic.acid	0.00	0.01	0.07	0.00	0.00	0.24	0.05	0.10	0.95	0.00

Table S9-10 Corrected *p*-value

<i>p</i> -value	Oxoproline	Adenosine.diphosphate	Ellagic.acid	Ethylmalonic.acid	Fumaric.acid	Cyanidin.3.O.galactoside	Quinic.acid	Theobromine	trans.p.Coumaric.acid	Shikimic.acid
Epigallocatechin.gallate	0.19	0.96	0.31	0.76	0.00	0.50	0.16	0.02	0.13	0.29
Catechin	0.90	0.32	0.02	0.08	0.73	0.04	0.19	0.42	0.50	0.73
Epicatechin	0.03	0.22	0.01	0.69	0.00	0.06	0.11	0.97	0.03	0.78
Gallocatechin	0.56	0.10	0.00	0.11	0.01	0.00	0.02	0.75	0.41	0.90
Methylxanthine	0.01	0.01	0.36	0.00	0.00	0.03	0.14	0.00	0.90	0.06
Abscisic.acid	0.14	0.25	0.94	0.00	0.92	0.05	0.50	0.00	0.00	0.00
Adenine	0.48	0.00	0.00	0.13	0.00	1.00	0.26	0.03	0.41	0.02
Avicularin	0.00	0.18	0.82	0.04	0.00	0.94	0.22	0.00	0.40	0.07
Quercetin.3.O.sophoroside	0.00	0.00	0.00	0.66	0.94	0.70	0.50	0.58	0.58	0.30
Betaine	0.00	0.00	0.00	0.04	0.61	0.01	0.10	0.02	0.08	0.00
Caffeine	0.66	0.25	0.00	0.86	0.83	0.47	0.94	0.32	0.73	0.20
Epicatechin.gallate	0.45	0.01	0.05	0.26	0.00	0.25	0.02	0.00	0.60	0.56
Chlorogenic.acid	0.08	0.12	0.07	0.38	0.00	0.10	0.00	0.21	0.01	0.93
Cynaroside	0.09	0.00	0.00	0.02	0.85	0.02	0.00	0.93	0.00	0.00
Glucuronic.acid	0.12	0.00	0.00	0.17	0.13	0.87	0.01	0.60	0.18	0.03
D.Fructose	0.03	0.83	0.62	0.28	0.00	0.09	0.41	0.66	0.79	0.83
D.Gluconic.acid	0.01	0.00	0.00	0.06	0.89	0.39	0.34	0.02	0.04	0.00
Lysine	0.29	0.00	0.00	0.88	0.00	0.10	0.16	0.83	0.13	0.01
Tyrosine	0.18	0.00	0.00	0.04	0.08	0.48	0.14	0.00	0.23	0.00
Trehalose	0.03	0.00	0.00	0.12	0.01	0.47	0.79	0.11	0.03	0.00
Epigallocatechin	0.01	0.00	0.00	0.11	0.09	0.37	0.86	0.02	0.70	0.09
Esculin	0.09	0.50	0.72	0.92	0.00	0.72	0.02	0.45	0.78	0.22
Gallic.acid	0.44	0.00	0.00	0.15	0.00	0.81	0.97	0.11	0.07	0.00
Gamma.aminobutyric.acid	0.00	0.00	0.00	0.30	0.00	0.01	0.38	0.03	0.38	0.75

Glutathione	0.00	0.00	0.00	0.96	0.83	0.68	0.52	0.09	0.00	0.00
Guanine	0.82	0.00	0.00	0.34	0.00	0.66	0.17	0.11	0.40	0.02
Isovitexin	0.05	0.00	0.00	0.84	0.01	0.32	0.04	0.72	0.02	0.00
Kaempferin	0.11	0.63	0.87	0.25	0.00	0.94	0.60	0.22	0.10	0.67
Kaempferol	0.03	0.00	0.00	0.03	0.31	0.86	0.84	0.04	0.15	0.00
L.serine	0.00	0.00	0.00	0.19	0.00	0.03	0.22	0.00	0.13	0.00
L.arginine	0.00	0.00	0.00	0.08	0.00	0.02	0.11	0.00	0.74	0.37
L.aspartic.acid	0.00	0.00	0.00	0.78	0.01	0.06	0.75	0.00	0.07	0.01
L.glutamic.acid	0.00	0.00	0.00	0.65	0.00	0.04	0.90	0.00	0.12	0.02
L.homoserine	0.00	0.11	0.33	0.56	0.00	0.80	0.04	0.00	0.40	0.10
L.isoleucine	0.55	0.00	0.00	0.60	0.00	0.34	0.21	0.29	0.91	0.22
L.phenylalanine	0.52	0.07	0.42	0.27	0.08	0.06	0.39	0.02	0.99	0.26
L.proline	0.01	0.24	0.48	0.20	0.00	0.16	0.00	0.86	0.90	0.91
L.theanine	0.00	0.00	0.00	0.24	0.02	0.16	0.30	0.01	0.13	0.00
L.tryptophan	0.56	0.26	0.79	0.06	0.03	0.14	0.25	0.48	0.00	0.03
Malic.acid	0.50	0.10	0.08	0.16	0.52	0.08	0.02	0.85	0.03	0.29
Naringenin	0.02	0.00	0.00	0.10	0.84	0.01	0.87	0.01	0.43	0.01
Neochlorogenic.acid	0.26	0.21	0.85	0.83	0.80	0.51	0.00	0.19	0.00	0.00
Pantothenic.acid	0.00	0.00	0.44	0.70	0.01	0.57	0.00	0.25	0.00	0.00
Phloretin	0.11	0.00	0.00	0.01	0.06	0.90	0.77	0.00	0.51	0.02
Procyanidin.B4	0.79	0.02	0.13	0.53	0.00	0.11	0.18	0.00	0.05	0.12
Procyanidin.B3	0.45	0.38	0.12	0.62	0.00	0.85	0.56	0.13	0.81	0.46
Prunin	0.34	0.00	0.00	0.60	0.01	0.09	0.70	0.03	0.60	0.50
Theogallin	0.25	0.00	0.00	0.74	0.37	0.00	0.00	0.09	0.97	0.54
Theophylline	0.02	0.00	0.00	0.06	0.00	0.13	0.10	0.23	0.43	0.13
Thymine	0.02	0.59	0.19	0.26	0.00	0.07	0.00	0.05	0.90	0.81

Tricetin	0.00	0.00	0.00	0.82	0.02	0.71	0.51	0.42	0.05	0.00
Xanthine	0.00	0.00	0.12	0.12	0.00	0.20	0.00	0.00	0.94	0.04
Xylitol	0.02	0.00	0.00	0.86	0.72	0.14	0.03	0.15	0.13	0.15
Beta.alanine	0.00	0.00	0.00	0.93	0.00	0.03	0.84	0.08	0.26	0.12
hydroxy.cinnamic.acid	0.04	0.00	0.00	0.11	0.94	0.75	0.26	0.58	0.00	0.00
Citric.acid	0.04	0.00	0.00	0.01	0.89	0.07	0.28	0.02	0.08	0.01
Succinic.acid	0.11	0.09	0.85	0.00	0.94	0.39	0.35	0.00	0.59	0.11
Alpha.ketoglutaric.acid	0.01	0.00	0.00	0.08	0.38	0.09	0.48	0.01	0.02	0.00
Hydroxycoumarine	0.04	0.04	0.02	0.29	0.00	0.12	0.00	0.10	0.01	0.92
Coumarin	0.82	0.40	0.71	0.00	0.12	0.78	0.12	0.02	0.00	0.00
Glutamine	0.00	0.00	0.00	0.20	0.00	0.03	0.33	0.00	0.18	0.01
Delphinidin.3.O.rutinoside.chloride	0.84	0.63	0.18	0.14	0.02	0.00	0.02	0.60	0.19	0.04
Eriodictyol	0.05	0.00	0.00	0.07	0.23	0.11	0.47	0.00	0.19	0.01
Glycyl.L.leucine	0.03	0.02	0.04	0.72	0.00	0.82	0.08	0.16	0.60	0.57
Guanosine.monophosphate	0.96	0.00	0.00	0.94	0.01	0.27	0.39	0.21	0.48	0.08
Glutathione.oxidized	0.00	0.00	0.00	0.90	0.00	0.51	0.11	0.00	0.01	0.00
L.histidine	0.00	0.00	0.00	0.11	0.00	0.10	0.01	0.00	0.83	0.04
L.pyroglutamic.acid	0.00	0.00	0.00	0.20	0.00	0.04	0.30	0.00	0.15	0.00
Myricetin	0.00	0.00	0.00	0.01	0.02	0.34	0.08	0.00	0.68	0.61
Naringenin.chalcone	0.49	0.03	0.08	0.30	0.00	0.15	0.01	0.00	0.81	0.84
Quercetin	0.00	0.16	0.34	0.35	0.57	0.00	0.16	0.00	0.40	0.61
Quercetin.3beta.D.glucoside	0.00	0.26	0.99	0.02	0.01	0.24	0.03	0.00	0.93	0.45
Schaftoside	0.06	0.00	0.00	0.10	0.01	0.02	0.05	0.00	0.36	0.01
Uridine.monophosphate	0.19	0.35	0.03	0.94	0.00	0.05	0.15	0.50	0.57	0.71
Digallic.acid	0.55	0.02	0.00	0.78	0.87	0.99	0.06	0.73	0.38	0.36
Dihomomethionine	0.22	0.82	0.81	0.00	0.47	0.01	0.04	0.09	0.00	0.06

Epigallocatechin.3.O..3.O.methyl..gallate	0.22	0.00	0.00	0.14	0.06	0.33	0.77	0.14	0.00	0.14
Epigallocatechin..4beta..8..epicatechin.3.O.gallate.ester	0.32	0.00	0.00	0.85	0.97	0.84	0.30	0.75	0.69	0.07
Epigallocatechin.3..glucuronide	0.00	1.00	0.88	0.07	0.00	0.05	0.66	0.00	0.81	0.62
Galocatechin..4alpha..8..epigallocatechin	0.01	0.00	0.00	0.32	0.10	0.88	0.50	0.52	0.62	0.03
S.adenosyl.L.homocysteine	0.00	0.00	0.00	0.06	0.00	0.34	0.06	0.00	0.07	0.00
Theasinensin.B	0.16	0.00	0.00	0.67	0.66	0.31	0.27	0.71	0.85	0.03
Malonic.acid	0.19	0.03	0.12	0.41	0.75	0.03	0.74	0.77	0.07	0.12
4.Dihydroxybenzoic.acid	0.00	0.00	0.00	0.11	0.04	0.28	0.17	0.02	0.03	0.00
Aminoadipic.acid	0.26	0.00	0.00	0.39	0.28	0.01	0.18	0.61	0.01	0.00
.Adenosine.monophosphate	0.62	0.00	0.06	0.56	0.00	0.15	0.06	0.77	0.76	0.33
Hydroxy.3.methylglutaric.acid	0.60	0.00	0.00	0.03	0.19	0.38	0.10	0.03	0.65	0.09
Hydroxybenzoic.acid	0.02	0.54	0.10	0.09	0.00	0.01	0.31	0.12	0.64	0.17
Hydroxybenzaldehyde	0.19	0.22	0.47	0.36	0.00	0.18	0.01	0.00	0.96	0.96
Hydroxybenzoic.acid	0.00	0.00	0.00	0.91	0.17	0.57	0.30	0.14	0.00	0.00
Oxoproline	0.00	0.00	0.08	0.19	0.00	0.23	0.05	0.01	0.37	0.02
Adenosine.diphosphate	0.00	0.00	0.00	0.30	0.89	0.47	0.73	0.01	0.00	0.00
Ellagic.acid	0.04	0.00	0.00	0.90	0.64	0.66	0.44	0.34	0.05	0.00
Ethylmalonic.acid	0.12	0.20	0.86	0.00	0.72	0.15	0.44	0.01	0.03	0.48
Fumaric.acid	0.00	0.85	0.54	0.63	0.00	0.75	0.00	0.15	0.36	0.71
Cyanidin.3.O.galactoside	0.15	0.36	0.57	0.09	0.68	0.00	0.88	0.02	0.51	0.88
Quinic.acid	0.02	0.65	0.33	0.34	0.00	0.84	0.00	0.72	0.26	0.03
Theobromine	0.00	0.00	0.25	0.00	0.09	0.01	0.63	0.00	0.66	0.43
trans.p.Coumaric.acid	0.27	0.00	0.02	0.01	0.26	0.41	0.18	0.57	0.00	0.00
Shikimic.acid	0.01	0.00	0.00	0.38	0.63	0.84	0.01	0.33	0.00	0.00

Table S10 WGCNA

From node	To node	Weight	Direction	Group
TEA009266	TEA027807	0.530007568	undirected	ANR
TEA009266	TEA010670	0.529935851	undirected	ANR
TEA009266	TEA000421	0.527295398	undirected	ANR
TEA009266	TEA013916	0.526285014	undirected	ANR
TEA009266	TEA016550	0.525832098	undirected	ANR
TEA009266	TEA014700	0.52577796	undirected	ANR
TEA009266	TEA026179	0.524311062	undirected	ANR
TEA009266	TEA010994	0.524188278	undirected	ANR
TEA009266	TEA000468	0.523154971	undirected	ANR
TEA009266	TEA024196	0.522834224	undirected	ANR
TEA009266	TEA003322	0.522814158	undirected	ANR
TEA009266	TEA001183	0.522452363	undirected	ANR
TEA009266	TEA016836	0.522221793	undirected	ANR
TEA009266	novel.2571	0.522197173	undirected	ANR
TEA009266	TEA007471	0.522100986	undirected	ANR
TEA009266	novel.6346	0.521974073	undirected	ANR
TEA009266	TEA024531	0.521542701	undirected	ANR
TEA009266	TEA015852	0.521256899	undirected	ANR
TEA009266	TEA009821	0.521165398	undirected	ANR
TEA009266	TEA021242	0.521055314	undirected	ANR
TEA009266	TEA011328	0.520037373	undirected	ANR
TEA009266	TEA029957	0.519876161	undirected	ANR
TEA009266	TEA028082	0.519616157	undirected	ANR
TEA009266	TEA029178	0.518720716	undirected	ANR

TEA009266	TEA016145	0.518572401	undirected	ANR
TEA009266	TEA011052	0.518569058	undirected	ANR
TEA009266	TEA022720	0.518213662	undirected	ANR
TEA009266	TEA025042	0.518182227	undirected	ANR
TEA009266	TEA001161	0.518078854	undirected	ANR
TEA009266	novel.2101	0.517760838	undirected	ANR
TEA009266	TEA023424	0.51759253	undirected	ANR
TEA009266	TEA012548	0.517528998	undirected	ANR
TEA009266	TEA007140	0.517410397	undirected	ANR
TEA009266	TEA019039	0.516997954	undirected	ANR
TEA009266	TEA008942	0.516966763	undirected	ANR
TEA009266	TEA020921	0.516552072	undirected	ANR
TEA009266	TEA024699	0.516513762	undirected	ANR
TEA009266	TEA018359	0.516361563	undirected	ANR
TEA009266	TEA013985	0.516215007	undirected	ANR
TEA009266	TEA010773	0.516081996	undirected	ANR
TEA009266	TEA029585	0.515738052	undirected	ANR
TEA009266	TEA000296	0.515504131	undirected	ANR
TEA009266	TEA030048	0.51534659	undirected	ANR
TEA009266	TEA032948	0.515344164	undirected	ANR
TEA009266	TEA024490	0.515046289	undirected	ANR
TEA009266	TEA024592	0.51473015	undirected	ANR
TEA009266	TEA019917	0.514447577	undirected	ANR
TEA009266	novel.1531	0.513926423	undirected	ANR
TEA009266	TEA011362	0.513503304	undirected	ANR
TEA009266	TEA022298	0.513393406	undirected	ANR

TEA009266	TEA029288	0.513392639	undirected	ANR
TEA009266	TEA027263	0.513118338	undirected	ANR
TEA009266	TEA004387	0.512846877	undirected	ANR
TEA009266	TEA017018	0.512668064	undirected	ANR
TEA009266	TEA027205	0.512292178	undirected	ANR
TEA009266	TEA013350	0.512289536	undirected	ANR
TEA009266	TEA031947	0.512138564	undirected	ANR
TEA009266	TEA017953	0.511933613	undirected	ANR
TEA009266	TEA028083	0.511711738	undirected	ANR
TEA009266	novel.5320	0.511671092	undirected	ANR
TEA009266	TEA005118	0.511625502	undirected	ANR
TEA009266	TEA031019	0.511620597	undirected	ANR
TEA009266	TEA023676	0.511209871	undirected	ANR
TEA009266	TEA004094	0.511114786	undirected	ANR
TEA009266	TEA008910	0.51091227	undirected	ANR
TEA009266	TEA003559	0.510650785	undirected	ANR
TEA009266	TEA016267	0.510556591	undirected	ANR
TEA009266	novel.4789	0.510551989	undirected	ANR
TEA009266	TEA028096	0.510477559	undirected	ANR
TEA009266	TEA028181	0.510312646	undirected	ANR
TEA009266	TEA010638	0.510241848	undirected	ANR
TEA009266	TEA015514	0.510007604	undirected	ANR
TEA009266	TEA033246	0.509984764	undirected	ANR
TEA009266	TEA032234	0.509934446	undirected	ANR
TEA009266	TEA024663	0.509899728	undirected	ANR
TEA009266	TEA002541	0.509882303	undirected	ANR

TEA009266	TEA019110	0.509762077	undirected	ANR
TEA009266	TEA010795	0.509761775	undirected	ANR
TEA009266	TEA027713	0.509697377	undirected	ANR
TEA009266	novel.4163	0.509652703	undirected	ANR
TEA009266	TEA009462	0.509601681	undirected	ANR
TEA009266	TEA030138	0.509488444	undirected	ANR
TEA009266	TEA029111	0.509480143	undirected	ANR
TEA009266	TEA024070	0.509465533	undirected	ANR
TEA009266	TEA018165	0.509443794	undirected	ANR
TEA009266	TEA001321	0.509436384	undirected	ANR
TEA009266	novel.6349	0.509425368	undirected	ANR
TEA009266	TEA019489	0.509260155	undirected	ANR
TEA009266	novel.1474	0.509048016	undirected	ANR
TEA009266	TEA032448	0.509037537	undirected	ANR
TEA009266	TEA008737	0.508923657	undirected	ANR
TEA009266	TEA029060	0.508793601	undirected	ANR
TEA009266	TEA022591	0.508185884	undirected	ANR
TEA009266	TEA033176	0.508173947	undirected	ANR
TEA009266	TEA008682	0.508131426	undirected	ANR
TEA009266	TEA001160	0.508086183	undirected	ANR
TEA009266	TEA014056	0.508025995	undirected	ANR
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TEA034012	TEA017349	0.560086985	undirected	4CL
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TEA034012	TEA033076	0.557222592	undirected	4CL
TEA034012	TEA000319	0.557162196	undirected	4CL
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TEA034012	novel.2317	0.556375276	undirected	4CL
TEA034012	TEA009462	0.556301347	undirected	4CL
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TEA034012	TEA013126	0.555893943	undirected	4CL

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TEA014864	TEA029957	0.553860051	undirected	C4H
TEA014864	TEA014001	0.553499585	undirected	C4H

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TEA014864	TEA022720	0.551740933	undirected	C4H
TEA014864	TEA008910	0.551688502	undirected	C4H
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