

Supplementary Table 4: False Discovery Rate (FDR)-Based Confidence Assessment for Compounds Identified in LC–HRMS Analysis of Black Tea Samples

Name	f.value	p.value	(-LOG10(p))	FDR
9-HpODE	1012.6	1.89E-18	17.723	2.97E-18
Malic acid	1073.6	1.19E-18	17.925	1.92E-18
(1S)-1,5-Anhydro-2-O-(6-deoxy- α -L-mannopyranosyl)-1-[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-6-yl]-D-glucitol	11364	7.83E-27	26.106	9.98E-26
(1 ξ)-1,5-Anhydro-1-[(2R,3R)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro-2H-chromen-6-yl]-D-glucitol	4384.7	1.58E-23	22.8	5.30E-23
1-(5,8-Dimethoxy-2,2-dimethyl-2H-chromen-6-yl)ethanone	33683	1.32E-30	29.88	4.48E-29
1,3,6-Trigalloyl glucose	7754.5	1.66E-25	24.779	8.69E-25
1,6-Bis-O-(3,4,5-trihydroxybenzoyl)hexopyranose	9618.5	2.97E-26	25.527	2.33E-25
1-[(3-Carboxypropyl)amino]-1-deoxy-beta-D-fructofuranose	1763.8	2.27E-20	19.643	4.38E-20
13(S)-HpOTrE	1264.8	3.22E-19	18.492	5.52E-19
13-HOTrE	408.23	2.54E-15	14.595	3.32E-15
1-Oxo-1,2,4-butanetricarboxylic acid	1020.3	1.78E-18	17.749	2.82E-18
1-Vinyl-2-pyrrolidone	10509	1.46E-26	25.835	1.57E-25
2-(2-phenylethoxy)-6-[[[(3,4,5-trihydroxyoxan-2-yl)oxy]methyl]oxane-3,4,5-triol	2339.6	2.39E-21	20.622	5.02E-21
2-(acetylamino)-3-(1H-indol-3-yl)propanoic acid	2316.3	2.59E-21	20.587	5.33E-21
2,4-Dihydroxybenzoic acid	1925.6	1.13E-20	19.947	2.30E-20
2,5-Furandicarboxylic acid	421.86	1.96E-15	14.708	2.60E-15
2,6-Diamino-4-hexenoic acid	48.192	3.10E-08	7.5091	3.40E-08
2-[1-(2H-1,3-benzodioxol-5-yl)propan-2-yl]-6-methoxy-4-(prop-2-en-1-yl)phenol	862.61	6.77E-18	17.17	1.02E-17
2-Coumaroylquinic acid	3280.2	1.61E-22	21.794	4.21E-22
2'-deoxymugineic acid	26.02	2.16E-06	5.6663	2.34E-06
2-Deoxypentose	460.57	9.79E-16	15.009	1.31E-15
2-monolinolenin	2525.5	1.30E-21	20.887	2.82E-21
3-(Sulfoxy)butanoic acid	4711	8.92E-24	23.05	3.09E-23
3,4,5-trihydroxycyclohex-1-ene-1-carboxylic acid	532.15	3.12E-16	15.505	4.34E-16
3,4-Dihydroxybenzaldehyde	234.33	1.99E-13	12.702	2.40E-13
3,5-Dihydroxy-4-(sulfoxy)benzoic acid	1602.6	4.88E-20	19.311	8.90E-20
3,6-Dideoxy-6-sulfohex-2-ulosonic acid	869.2	6.37E-18	17.196	9.63E-18
3-Amino-2-azepanone	5358.2	3.19E-24	23.496	1.16E-23
3-Coumaric acid	1586.9	5.28E-20	19.277	9.54E-20
3-Hydroxy-4-methoxy-5-(sulfoxy)benzoic acid	8764.3	6.25E-26	25.204	3.89E-25
3-Hydroxy-N-(2-oxotetrahydro-3-furanyl)butanamide	3069.6	2.73E-22	21.563	6.64E-22
3-Isopropylmalic acid	20572	6.80E-29	28.168	1.33E-27
3-Methylxanthine	1922.1	1.15E-20	19.941	2.31E-20
3-sulfolactic acid	86.377	4.25E-10	9.3713	4.79E-10
3-sulfopropanediol	1060.7	1.31E-18	17.884	2.10E-18
4,5-Dihydroxy-3-oxo-1-cyclohexene-1-carboxylic acid	3765.1	5.35E-23	22.272	1.56E-22
4-acetamidobutyrate	4698	9.12E-24	23.04	3.10E-23
4-Coumaric acid	1673.7	3.45E-20	19.462	6.35E-20
4-Hydroxy-8-(beta-D-talopyranosyloxy)-2-quinolinecarboxylic acid	3509.6	9.37E-23	22.028	2.58E-22
4-Hydroxybenzaldehyde	8344.5	9.25E-26	25.034	5.39E-25
4-Hydroxybenzoic acid	1491.2	8.67E-20	19.062	1.55E-19
4-Methyleneglutamic acid	1114.8	8.80E-19	18.055	1.44E-18
4-METHYLUMBELLIFERYL- α -D-GLUCOSE	1211.5	4.54E-19	18.343	7.59E-19
4-Oxoproline	3889.8	4.12E-23	22.385	1.26E-22
4-p-Coumaroylquinic acid	15.31	5.81E-05	4.2355	6.18E-05
5-(2-Carboxyethyl)-2-hydroxyphenyl beta-D-glucopyranosiduronic acid	9969.2	2.23E-26	25.652	2.09E-25
5,7-Dihydroxy-2-(4-hydroxyphenyl)-6,8-bis[3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl]-4H-chromen-4-one	567.07	1.89E-16	15.724	2.64E-16
5-[5-(methoxycarbonyl)-5,8a-dimethyl-2-methylidene-decahydronaphthalen-1-yl]-3-methylpentanoic acid	2681.3	8.04E-22	21.094	1.78E-21
5-Hydroxy-2-furoic acid	837.95	8.52E-18	17.069	1.27E-17
5-hydroxy-4-methoxy-5,6-dihydro-2H-pyran-2-one	62.39	4.76E-09	8.3221	5.31E-09
7-Hydroxycoumarine	7832	1.53E-25	24.814	8.24E-25
8-hydroxy-deoxyguanosine	329.48	1.37E-14	13.862	1.74E-14
Acetophenone	2382	2.07E-21	20.684	4.40E-21
Adenine	3.3567	0.045209	1.3448	0.047295
Adenosine	9956.7	2.25E-26	25.647	2.09E-25
Adenosine 3'5'-cyclic monophosphate	1852.9	1.54E-20	19.814	3.01E-20
Adenosine 5'-monophosphate	5211.6	3.98E-24	23.4	1.42E-23
Afzelin	396.87	3.17E-15	14.499	4.12E-15
alpha-D-Xylopyranosyl-(1->6)-beta-D-glucopyranosyl-(1->4)-beta-D-glucopyranose	20438	7.16E-29	28.145	1.33E-27
alpha-Ketoglutaric acid	212.49	4.27E-13	12.37	5.06E-13
Astragaln	137.76	1.22E-11	10.913	1.43E-11
Astringin	6774.1	4.90E-25	24.31	2.32E-24
Benzoic acid	10158	1.92E-26	25.717	1.96E-25
Betaine	188.44	1.09E-12	11.964	1.28E-12
Caffeine	213.76	4.07E-13	12.39	4.86E-13
Catechin	5565.1	2.36E-24	23.628	8.90E-24
Catechin Gallate	18.762	1.72E-05	4.7635	1.85E-05
Chlorogenic acid	4143.3	2.49E-23	22.604	8.06E-23
Choline	109.5	7.08E-11	10.15	8.16E-11
Citric acid	473.54	7.86E-16	15.104	1.06E-15
L-coprine	89.316	3.31E-10	9.4805	3.75E-10

Name	f.value	p.value	(-LOG10(p))	FDR
Corchorifatty acid F	485.1	6.50E-16	15.187	8.90E-16
corilagin	3226.3	1.84E-22	21.736	4.68E-22
Corymboside	8467.3	8.23E-26	25.085	4.94E-25
Coumarin	2735.2	6.86E-22	21.163	1.56E-21
Cyanidin	95.851	1.94E-10	9.7118	2.23E-10
Cytosine	428.13	1.74E-15	14.758	2.33E-15
D-(-)-Quinic acid	687.43	4.11E-17	16.387	5.98E-17
D-(-)-Glutamine	1738.3	2.55E-20	19.593	4.78E-20
dihomomethionine	51977	4.10E-32	31.387	2.79E-30
DL-2,6-Diaminopimelic acid	891.25	5.22E-18	17.282	7.95E-18
DL-Arginine	918.77	4.10E-18	17.387	6.29E-18
D-PANTOTHENIC ACID	3521.2	9.13E-23	22.039	2.55E-22
D-(+)-Pyroglutamic Acid	1212.7	4.50E-19	18.347	7.59E-19
D-Sucrose	3092.1	2.58E-22	21.589	6.34E-22
Ellagic acid	10964	1.04E-26	25.982	1.25E-25
Epicatechin	5590.1	2.27E-24	23.643	8.90E-24
EPIGALLOCATECHIN 3-O-(3-O-METHYL)GALLATE	59.367	6.85E-09	8.1642	7.60E-09
Epigallocatechin gallate	368.53	5.69E-15	14.245	7.30E-15
Esculetin	7550.2	2.06E-25	24.687	1.05E-24
Frovatriptan	13528	1.94E-27	26.712	2.83E-26
Fructoselysine	22062	3.89E-29	28.41	8.83E-28
Fukiic acid	236.9	1.83E-13	12.739	2.22E-13
Galactonic acid	6974.9	3.88E-25	24.412	1.93E-24
Gallic acid	8756.5	6.29E-26	25.201	3.89E-25
Gallocatechin	3654.7	6.78E-23	22.169	1.95E-22
gamma-Aminobutyric acid	3245	1.75E-22	21.756	4.53E-22
gamma-glutamyltyramine	10589	1.38E-26	25.861	1.56E-25
Glucogallin	300.61	2.82E-14	13.549	3.51E-14
Glu-Glu	2325.2	2.51E-21	20.601	5.22E-21
L-Glutamic acid	2385.7	2.04E-21	20.69	4.39E-21
Guanine	348	8.94E-15	14.049	1.14E-14
Guanosine monophosphate (GMP)	3545.3	8.65E-23	22.063	2.45E-22
Heptylbenzene	3880.6	4.20E-23	22.377	1.26E-22
Hexaric acid	2922.2	4.05E-22	21.393	9.71E-22
DL-Histidine	3998.3	3.31E-23	22.48	1.05E-22
Isocitric acid	1680.7	3.34E-20	19.476	6.20E-20
Isoleucine	40377	3.09E-31	30.51	1.26E-29
isopropylmalic acid	12553	3.53E-27	26.452	4.80E-26
Juglalin	410.67	2.42E-15	14.616	3.19E-15
Kaempferol	6914.4	4.16E-25	24.381	2.02E-24
Kaempferol-3-O-(6'''-trans-P-coumaroyl-2''-glucosyl)rhamnoside	1744.2	2.49E-20	19.604	4.70E-20
Kynurenic acid	394.42	3.33E-15	14.477	4.30E-15
Lamiide	3987.7	3.38E-23	22.471	1.06E-22
Leucine	22056	3.89E-29	28.41	8.83E-28
Leucylproline	665.35	5.32E-17	16.274	7.64E-17
DL-Glutamine	5926.8	1.42E-24	23.846	5.93E-24
L-Pyroglutamic acid	3394.3	1.22E-22	21.912	3.24E-22
Luteolin	126.11	2.41E-11	10.618	2.81E-11
Maleamic acid	300.35	2.84E-14	13.546	3.52E-14
Metharbital	962.86	2.82E-18	17.549	4.40E-18
Methyl cinnamate	2834.3	5.16E-22	21.287	1.21E-21
Methyl gallate	1292.1	2.72E-19	18.566	4.70E-19
MFCD00135810	5513.6	2.54E-24	23.595	9.41E-24
Miglitol	319.55	1.75E-14	13.758	2.20E-14
muramic acid	832.49	8.98E-18	17.047	1.33E-17
Myricetin	77824	1.62E-33	32.79	3.31E-31
myricetin 3-O-beta-D-galactopyranoside	16572	3.83E-28	27.417	6.01E-27
N-(3-Carboxypropanoyl)-5-hydroxynorvaline	34.12	3.49E-07	6.4569	3.81E-07
N-acetyl-L-2-aminoadipic acid	49.898	2.41E-08	7.6175	2.66E-08
N-Acetylneuraminic acid	3124.4	2.37E-22	21.625	5.97E-22
N-Acetylmethionine	484.51	6.56E-16	15.183	8.92E-16
Naringenin	18.058	2.18E-05	4.6622	2.33E-05
N-Benzylformamide	7840.4	1.52E-25	24.818	8.24E-25
Neochlorogenic acid	292.85	3.47E-14	13.46	4.26E-14
N-Glycosyl-L-asparagine	1806.4	1.88E-20	19.726	3.65E-20
Niacin	305.65	2.48E-14	13.606	3.10E-14
nicotianamine	6559.8	6.33E-25	24.199	2.94E-24
Nicotinamide	634.85	7.72E-17	16.113	1.10E-16
Nicotinic acid	603.71	1.15E-16	15.939	1.63E-16
Nipecotic acid	9417.3	3.52E-26	25.454	2.66E-25
Nor Leucine	685.38	4.20E-17	16.376	6.08E-17
NP-000358	69096	4.20E-33	32.376	4.29E-31
NP-000587	1425.3	1.24E-19	18.905	2.21E-19
NP-001346	3868.8	4.30E-23	22.366	1.27E-22
NP-003191	1748.4	2.44E-20	19.613	4.65E-20
NP-020139	6117.7	1.11E-24	23.956	4.70E-24
NP-020760	2585.6	1.08E-21	20.969	2.36E-21
N-Succinyl-L-diaminopimelic acid	1910.8	1.20E-20	19.92	2.40E-20
N-Vinyl-2-pyrrolidone	946.87	3.23E-18	17.491	4.98E-18
Oxypinnatanine	1168.7	6.04E-19	18.219	1.00E-18
Patuletin	7.6166	0.002199	2.6578	0.002312

Name	f.value	p.value	(-LOG10(p))	FDR
L-Phenylalanine	9639.6	2.92E-26	25.535	2.33E-25
Phloionolic acid	5008.2	5.47E-24	23.262	1.92E-23
Pipecolic acid	9691.4	2.80E-26	25.554	2.33E-25
Pirbuterol	253.47	1.08E-13	12.968	1.31E-13
Procyanidin A2	9.7134	0.000688	3.1623	0.000727
Procyanidin B2	2691	7.81E-22	21.107	1.75E-21
Prodelfinidin B1	5710.4	1.92E-24	23.717	7.82E-24
Proline	5693	1.97E-24	23.707	7.86E-24
Quercetin	694.18	3.80E-17	16.42	5.58E-17
QUERCETIN 3,7-DIGLUCOSIDE	1142.6	7.23E-19	18.141	1.19E-18
Quercetin 3-O-caffeyl-glucoside	21.872	6.62E-06	5.1793	7.14E-06
Quercetin-3-O- α -pentoside	8850.4	5.78E-26	25.238	3.80E-25
Quercetin-3 β -D-glucoside	3115.1	2.43E-22	21.614	6.04E-22
Robinin	22055	3.90E-29	28.409	8.83E-28
Rutin	6516.4	6.68E-25	24.175	3.03E-24
saccharopine	1864	1.46E-20	19.835	2.90E-20
D-Serine	1368.8	1.72E-19	18.766	2.99E-19
Spermidine	3480.5	1.00E-22	21.999	2.72E-22
Spermine	2766.9	6.26E-22	21.203	1.43E-21
DL-Stachydrine	41242	2.61E-31	30.584	1.26E-29
Suberic acid	1414.4	1.32E-19	18.879	2.33E-19
Succinic acid	1044.7	1.48E-18	17.831	2.35E-18
Syringetin	9293.8	3.91E-26	25.408	2.85E-25
Theobromine	2801.6	5.67E-22	21.247	1.31E-21
Theogallin	4243.5	2.06E-23	22.687	6.77E-23
Threonine	2908.5	4.20E-22	21.377	9.97E-22
Tiliroside	86.251	4.30E-10	9.3666	4.82E-10
trans-3-Indoleacrylic acid	17009	3.11E-28	27.507	5.29E-27
Traumatic Acid	8028.2	1.26E-25	24.9	7.14E-25
Trifolin	9841.3	2.47E-26	25.607	2.19E-25
Tryptophan	1241.4	3.74E-19	18.427	6.35E-19
Tyrosine	8980.3	5.14E-26	25.289	3.62E-25
tyr-thr	123.72	2.79E-11	10.555	3.23E-11
Uracil	518.74	3.82E-16	15.418	5.27E-16
Uridine 5'-diphosphogalactose	6261.3	9.19E-25	24.037	4.07E-24
Uridine monophosphate (UMP)	214.04	4.03E-13	12.395	4.84E-13
Valine	91.591	2.74E-10	9.5628	3.12E-10
Vanillyl mandelic acid	582.85	1.52E-16	15.818	2.14E-16
Vitexin	3394.6	1.22E-22	21.913	3.24E-22
Xanthine	5570.2	2.34E-24	23.631	8.90E-24
Xanthosine	6177.3	1.02E-24	23.99	4.44E-24
ZINGEROL	8912.8	5.46E-26	25.263	3.71E-25
α,α -Trehalose	3952.9	3.62E-23	22.441	1.12E-22