

Table S1. The information on 95 non-volatile differential metabolites in fresh tea leaves.

metabolite name	TR (min)	accurate mass	theoretica l mass	ppm	MS/MS ions	formula	Ref.
Catechins and their derivatives							
8-C-Ascorbylepi gallocatechin 3-gallate	4.57	631.0938	631.0941	-0.43	163.0037,495.0568	C ₂₈ H ₂₄ O ₁₇	
(-)-Epigallocatec hin	4.60	306.0735	305.0667	-1.36	305.0664	C ₁₅ H ₁₄ O ₇	
(-)-Gallocatechin	5.76	306.0739	305.0667	-0.25	125.0243,305.0665	C ₁₅ H ₁₄ O ₇	
Epigallocatechin gallate	5.77	457.0776	457.0776	0.01	169.0141,125.0243,305.0664	C ₂₂ H ₁₈ O ₁₁	
Epicatechin 3-glucoside	8.26	452.1319	451.1246	0.04	271.0607,169.0142,125.0244,28 9.0717	C ₂₁ H ₂₄ O ₁₁	
3,5-Digalloylepic atechin	8.26	593.0930	593.0937	-1.12	423.0721,441.0824,593.0940	C ₂₉ H ₂₂ O ₁₄	
Epicatechin-(4be ta->8)-gallocatec hin	4.41	593.1289	593.1301	-1.98	305.0663,441.0827	C ₃₀ H ₂₆ O ₁₃	
Gallocatechin-(4 alpha->8)-epicate chin	4.65	593.1288	593.1301	-2.17	407.0770,289.0714,441.0823	C ₃₀ H ₂₆ O ₁₃	
Epigallocatechin -(4beta->8)-epica techin 3-O-gallate	5.64	745.1394	745.1410	-2.23	407.0769,467.0980,593.1289	C ₃₇ H ₃₀ O ₁₇	
ent-Epicatechin-(4alpha->8)-ent-e picatechin 3'-gallate	5.66	775.1492	729.1461	-3.21	407.0768,577.0983,289.0714	C ₃₇ H ₃₀ O ₁₆	
Theasinensin A	5.81	913.1451	913.1469	-2.02	457.0774,169.0142,125.0243,30 5.0666	C ₄₄ H ₃₄ O ₂₂	
Epigallocatechin 3-O-gallate-(4bet a->6)-epicatechin 3-O-gallate	6.17	898.1615	897.1520	2.47	745.1389,897.1498,727.1283,55 9.0880	C ₄₄ H ₃₄ O ₂₁	
Flavones and flavonols/their glycoside							
5-hydroxypseud obaptigenin	2.46	343.0461	297.0405	0.68	169.0141,170.0221,177.0194	C ₁₆ H ₁₀ O ₆	
(2S)-dihydrotrice tin	3.49	304.0585	303.0510	0.57	125.0242,305.0663,137.0242,16 5.0190,167.0346	C ₁₅ H ₁₂ O ₇	
Quercetin 3-(3-p-coumaroy	3.78	609.1235	609.1250	-2.40	423.0718,305.0665,407.0774,12 5.0244	C ₃₀ H ₂₆ O ₁₄	

Iglucoside)						
Myricetin					271.0454,169.0141,313.0563,21	
7-(6"-galloylglucoside)	4.77	631.0941	631.0941	-0.00	1.0242	C ₂₈ H ₂₄ O ₁₇
Eriodictyol					124.0164,347.0778,183.0296,44	
7-(6-galloylglucoside)	4.98	601.1201	601.1199	0.41	9.0981	C ₂₈ H ₂₆ O ₁₅
Isorhamnetin					303.0511,285.0402,321.0614,47	
4'-O-glucuronide	5.36	473.0724	491.0831	-0.29	3.0742	C ₂₂ H ₂₀ O ₁₃
Eriocitrin	5.86	595.1658	595.1668	-1.80	401.0761,327.0515,473.1082,43	C ₂₇ H ₃₂ O ₁₅
					3.1350	
Safflor Yellow A	5.87	593.1501	593.1512	-1.81	593.1503,357.0862,453.1027,19	C ₂₇ H ₃₀ O ₁₅
					1.0559	
6"-O-Galloylquercimeritrin	5.91	615.1002	615.0992	1.67	559.1239,327.0514	C ₂₈ H ₂₄ O ₁₆
Quercetin						
7-glucuronide	6.09	605.1137	623.1254	-1.74	453.1029,591.1140,573.1028	C ₂₇ H ₂₈ O ₁₇
3-rhamnoside						
Prunin						
6"-O-gallate	6.14	585.1250	585.1250	-0.02	465.0670,169.0141,313.0565	C ₂₈ H ₂₆ O ₁₄
Quercetin						
3-[rhamnosyl-(1->2)-alpha-L-arabinopyranoside]	6.35	625.1400		-1.78	625.1399	C ₂₆ H ₂₈ O ₁₅
Myricetin						
3-galactoside	6.36	480.0901	479.0831	-0.66	316.0222	C ₂₁ H ₂₀ O ₁₃
Kaempferol						
3-rhamnoside	6.75	589.1193	607.1305	-1.05	413.0873	C ₂₇ H ₂₈ O ₁₆
7-galacturonide						
Hydroxysafflor yellow A	6.75	593.1503	611.1618	-1.45	593.1497,413.0873,293.0453	C ₂₇ H ₃₂ O ₁₆
Scoparin						
2"-xyloside	6.83	594.1574	593.1512	-1.77	413.0875,593.1497,293.0453	C ₂₇ H ₃₀ O ₁₅
Hibiscitrin	6.89	477.0673	495.0780	-0.42	315.0146,169.0141,125.0243,47	C ₂₁ H ₂₀ O ₁₄
					7.0673	
Kaempferol						
3-arabinofuranoside						
ide	6.92	563.1401	563.1406	-0.87	169.0141,563.1403	C ₂₆ H ₂₈ O ₁₄
7-rhamnofuranoside						
Isoengeltin	6.94	415.1027	433.1140	-1.74	125.0242,269.0457,287.0562,29	C ₂₁ H ₂₂ O ₁₀
					3.0457	
Galangin					609.1450,577.1552,413.0875,29	
3-[galactosyl-(1->	7.04	578.1628	577.1563	-1.34	3.0453	C ₂₇ H ₃₀ O ₁₄

4)-rhamnoside]						
Kaempferol					755.2026,609.1449,577.1551,41	
3-gentiobioside	7.05	756.2093	755.2040	-2.58	3.0874	C ₃₃ H ₄₀ O ₂₀
7-rhamnoside						
Plantagoside	7.09	465.1033	465.1039	-1.20	313.0918,151.0037,465.1017	C ₂₁ H ₂₂ O ₁₂
2''-O-Acetylisoorientin	7.31	471.0931	489.1039	-0.42	305.0668,161.0245,327.0518,40	C ₂₃ H ₂₂ O ₁₂
					1.0887,413.0888	
Astilbin	7.35	449.1088	449.1089	-0.36	285.0401,287.0552,286.0436,15	C ₂₁ H ₂₂ O ₁₁
					1.0038	
Limocitrin	7.35	489.1039	507.1144	0.16	285.0401,287.0552,286.0436,15	C ₂₃ H ₂₄ O ₁₃
3-glucoside					1.0038	
Isorhamnetin						
3-(2G-apiosylrutinoside)	7.35	756.2098	899.1583	-2.03	755.2021,285.0401	C ₃₃ H ₄₀ O ₂₀
Kaempferol						
3-O-alpha-L-rhamnofuranoside	7.52	477.1038	431.0984	-0.08	169.0143	C ₂₁ H ₂₀ O ₁₀
6''-(4-Carboxy-3-hydroxy-3-methylbutanoyl)hyperin	7.64	589.1192	607.1305	-1.15	300.0275,437.1089	C ₂₇ H ₂₈ O ₁₆
NICTOFLORIN	7.68	593.1498	593.1512	-3.86	593.1503,285.0399,284.0323,44	C ₂₇ H ₃₀ O ₁₅
					7.0929	
Carthamone	7.69	448.1003	447.0933	-0.58	285.0397,593.1501,284.0322,44	C ₂₁ H ₂₀ O ₁₁
					7.0933	
Astragalin	7.93	447.0931	447.0933	-0.41	284.0324,255.0294,227.0347	C ₂₁ H ₂₀ O ₁₁
Naringin	8.20	579.1719	579.1719	-0.12	579.1714,459.1144	C ₂₇ H ₃₂ O ₁₄
Isolariciresinol						
4'-O-beta-D-glucoside	8.35	522.2099	521.2028	-0.33	341.1393,279.0876	C ₂₆ H ₃₄ O ₁₁
Kaempferol						
3-(6-acetylgalactoside)	8.43	489.1031	489.1039	-1.43	284.0324,489.1038,255.0299	C ₂₃ H ₂₂ O ₁₂
2'-C-Methylmyricetin						
3-rhamnoside	8.43	629.1143	629.1148	-0.79	284.0322,285.0395,169.0147,48	C ₂₉ H ₂₆ O ₁₆
5'-gallate					9.1036,629.1141	
Kaempferol						
3-neohesperidoside-7-(2''-p-coumaryllaminaribioside)	9.37	531.1442	1063.2936	1.90	755.1829,901.2385,431.0979,14	C ₄₈ H ₅₆ O ₂₇
					5.0293	
Quercetin	9.65	917.2340	917.2357	-1.85	285.0402,885.2441,739.1860,43	C ₄₂ H ₄₆ O ₂₃
3-(6-[4-glucosyl-					1.0981,145.0294	

p-coumaryl]glucosyl)(1->2)-rhamnoside Kaempferol						
2G-coumaroylrutinoside Kaempferol	9.80	739.1859	739.1880	-2.85	285.0403,593.1306,739.1868	C ₃₆ H ₃₆ O ₁₇
3-neohesperidoside-7-(2"-p-coumarylglucoside)	10.42	901.2383	901.2408	-2.74	901.2395,635.1418	C ₄₂ H ₄₆ O ₂₂
Hordatine B	15.43	561.2918	579.3049	-4.41	487.2386,488.2390	C ₂₉ H ₄₀ N ₈ O

5

Phenolic acids

Glucinol	0.75	342.1163	341.1089	0.15	179.0558,311.0982,161.0454	C ₁₂ H ₂₂ O ₁₁
Chlorogenic acid	4.21	353.0880	353.0878	0.51	151.0559,179.0349,135.0452	C ₁₆ H ₁₈ O ₉
Sanguin H4	5.02	634.0819	633.0733	1.99	300.9986,302.0020,633.0715,463.0510	C ₂₇ H ₂₂ O ₁₈
1-O-p-Coumaroyl-beta-D-glucose	5.21	325.0933	325.0929	1.22	169.0142,145.0294	C ₁₅ H ₁₈ O ₈
3-O-p-Coumaroylquinic acid	5.96	337.0931	337.0929	0.56	173.0453	C ₁₆ H ₁₈ O ₈
Gallic acid	6.04	169.0142	169.0143	-0.51	125.0242	C ₇ H ₆ O ₅
corilagin	6.15	634.0832	633.0733	3.98	465.0669,169.0140,483.0775,313.0564,125.0243	C ₂₇ H ₂₂ O ₁₈
trans-5-O-(4-coumaroyl)-D-quinic acid	6.63	337.0934	337.0929	1.50	191.0558,192.0600	C ₁₆ H ₁₈ O ₈

Amino acids

L-Theanine	1.15	174.1004	173.0932	-0.18	173.0931	C ₇ H ₁₄ N ₂ O ₃
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Authentic standard

Organic acids

Ethyl aconitate	4.99	183.0296	201.0405	-1.38	124.0165,183.0293	C ₈ H ₁₀ O ₆
2,4,6-Trihydroxybenzoic acid	5.77	169.0141	169.0143	-0.58	169.0141,125.0243	C ₇ H ₆ O ₅

Proanthocyanidins

Prodelphinidin A1	3.79	607.1085	607.1093	-1.44	423.0718,305.0665,125.0243	C ₃₀ H ₂₄ O ₁₄
3'-Galloylprodelphinidin B2	4.67	761.1341	761.1359	-2.41	423.0718,407.0766,761.1339,609.1234,177.0191	C ₃₇ H ₃₀ O ₁₈
3,3'-Digalloylprodelphinidin B2	5.38	913.1573		3.38	761.1341,743.1233,125.0243	C ₄₄ H ₃₄ O ₂₂
(2R,3S,4S)-leucocyanidin	6.78	306.0738	305.0667	-0.39	183.0296,125.0243,161.0243,30	C ₁₅ H ₁₄ O ₇

yanidin					5.0665	
Epiafzelechin						
3-O-gallate-(4bet	7.18	881.1551	881.1571	-2.17	179.0348,287.0558,269.0455	C ₄₄ H ₃₄ O ₂₀
a->6)-epigallocat						
echin 3-O-gallate						
(-)-Epiafzelechin	8.12	426.0949	425.0878	-0.31	289.0714,183.0296,273.0762,42	C ₂₂ H ₁₈ O ₉
3-gallate					5.0874	
Theaflavins						
Theaflavin	9.54	563.1189	563.1195	-0.99	125.0244,269.0455,425.0876	C ₂₉ H ₂₄ O ₁₂
Coumarins						
Aegelinol	5.74	246.0886	245.0819	-2.35	203.0707,245.0812,187.0397,22	C ₁₄ H ₁₄ O ₄
					1.0813,159.0450	
Cleomiscosin A	6.12	431.0985	385.0929	0.38	245.0452,417.0832	C ₂₀ H ₁₈ O ₈
Saccharides and glycoside derivatives						
1-alpha-D-galact						
osyl-sn-glycerol	0.77	333.0593	333.0592	0.25	333.0593,241.0112,152.9957,96	C ₉ H ₁₉ O ₁₁ P
3-phosphate					.9665,78.9587	
3-beta-Gentiobio	0.88	504.1683	503.1618	-1.40	191.0557,	C ₁₈ H ₃₂ O ₁₆
syglucose					341.1088,473.1508,503.1609	
D-Galactopyran						
osyl-(1->3)-D-gal	0.88	519.1566	473.1512	-0.12	191.0557,341.1088	C ₁₇ H ₃₀ O ₁₅
actopyranosyl-(1						
->3)-L-arabinose						
beta-Glucogallin	2.23	331.0670	331.0671	-0.10	169.0142	C ₁₃ H ₁₆ O ₁₀
Glucogallin	2.48	331.0670	331.0671	-0.06	169.0140,125.0242,331.0678	C ₁₃ H ₁₆ O ₁₀
1,2-Digalloyl-bet						
a-D-glucopyrano	2.70	465.0674	483.0780	-0.12	169.0142	C ₂₀ H ₂₀ O ₁₄
se						
1,6-bis-O-galloyl	4.24	483.0774	483.0780	-1.26	169.0141,423.0580,271.0457,17	C ₂₀ H ₂₀ O ₁₄
-beta-D-glucose					7.0194,211.0143	
1,6-Digalloyl-bet						
a-D-glucopyrano	4.53	483.0775	483.0780	-1.02	423.0579,169.0143,271.0457,21	C ₂₀ H ₂₀ O ₁₄
se					1.0245	
1,3,4-Trigalloyl-b						
eta-D-glucopyra	6.15	636.0977	635.0890	2.31	635.0874,465.0671,169.0141,48	C ₂₇ H ₂₄ O ₁₈
nose					3.0774,125.0242	
Linalool glycosides						
Linalool oxide D						
3-[apiosyl-(1->6)-	7.47	509.2239	463.2185	-0.25	331.1765	C ₂₁ H ₃₆ O ₁₁
glucoside]						
Linalool						
3,6-oxide	8.18	464.2250	463.2185	-1.65	331.1761,463.2178,161.0456	C ₂₁ H ₃₆ O ₁₁
primeveroside						
L-Linalool	10.67	448.2304	447.2236	-0.94	315.1816,447.2241	C ₂₁ H ₃₆ O ₁₀

3-[xylosyl-(1->6)-
glucoside]

Tannins

Methyl 6-O-galloyl-beta- D-glucopyranosi de	3.65	345.0827	345.0827	-0.19	183.0297,225.0402	C ₁₄ H ₁₈ O ₁₀
Samarangenin A	4.67	759.1184	759.1203	-2.43	423.0718,609.1234,591.1130,28 9.0715	C ₃₇ H ₂₈ O ₁₈
Samarangenin B	5.83	911.1294	911.1313	-1.99	457.0773,169.0141,125.0243	C ₄₄ H ₃₂ O ₂₂
Methyl 2,3,6-tri-O-galloy 1-beta-D-glucopy ranoside	6.91	650.1148	649.1046	4.45	169.0142,477.0682,479.0801	C ₂₈ H ₂₆ O ₁₈

Lipids

Gingerglycolipid A	16.34	676.3649	675.3597	-3.09	397.1348,415.1452,277.2171	C ₃₃ H ₅₆ O ₁₄
LysoPC(18:3(9Z, 12Z,15Z))	16.59	562.3144	516.3096	-1.15	277.2169,502.2932	C ₂₆ H ₄₈ NO ₇ P
2-linoleoyl-sn-gl ycero-3-phospho choline	17.09	564.3305	518.3252	-0.35	279.2325,504.3089	C ₂₆ H ₅₀ NO ₇ P
1-pentadecanoyl -sn-glycero-3-ph osphocholine	17.49	480.3090	480.3096	-1.24	255.2323,480.3091	C ₂₃ H ₄₈ NO ₇ P
LysoPC(16:0)	17.49	540.3304	494.3252	-0.60	255.2323,480.3090	C ₂₄ H ₅₀ NO ₇ P
LysoPC(18:1(9Z))	17.71	566.3460	520.3409	-0.69	281.2482,506.3243	C ₂₆ H ₅₂ NO ₇ P

Others

4-coumaroyltriac etic acid lactone	7.16	272.0684	271.0612	-0.23	125.0243,245.0813	C ₁₅ H ₁₂ O ₅
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