

Supplementary Table S1. Control table of fungal metabolic activities (KEGG database).

Pathway	Description
PWY-3781	aerobic respiration I (cytochrome c)
PWY-7279	aerobic respiration II (cytochrome c) (yeast)
PWY-7288	fatty acid β -oxidation (peroxisome, yeast)
GLYOXYLATE-BYPASS	glyoxylate cycle
PWY-5994	palmitate biosynthesis I (animals and fungi)
NONOXIPENT-PWY	pentose phosphate pathway (non-oxidative branch)
PWY-5659	GDP-mannose biosynthesis
PWY-7007	methyl ketone biosynthesis
PWY-5690	TCA cycle II (plants and fungi)
PWY-7111	pyruvate fermentation to isobutanol (engineered)
PWY-7388	octanoyl-[acyl-carrier protein] biosynthesis (mitochondria, yeast)
VALSYN-PWY	L-valine biosynthesis
PWY-6351	D-myo-inositol (1,4,5)-trisphosphate biosynthesis
TRNA-CHARGING-PWY	tRNA charging
PWY-7219	adenosine ribonucleotides de novo biosynthesis
PWY-7118	chitin degradation to ethanol
PWY-6606	guanosine nucleotides degradation II
PANTO-PWY	phosphopantetheenate biosynthesis I

Pathway	Description
PWY-7229	superpathway of adenosine nucleotides de novo biosynthesis I
PENTOSE-P-PWY	pentose phosphate pathway
PWY-5067	glycogen biosynthesis II (from UDP-D-Glucose)
SER-GLYSYN-PWY	superpathway of L-serine and glycine biosynthesis I
PWY-6126	superpathway of adenosine nucleotides de novo biosynthesis II
PWY66-422	D-galactose degradation V (Leloir pathway)
PWY-6317	galactose degradation I (Leloir pathway)
PWY-5083	NAD/NADH phosphorylation and dephosphorylation
P221-PWY	octane oxidation
PWY-7282	4-amino-2-methyl-5-phosphomethylpyrimidine biosynthesis (yeast)
PWY-7208	superpathway of pyrimidine nucleobases salvage
PWY-7411	superpathway of phosphatidate biosynthesis (yeast)
PWY-4984	urea cycle
PWY-7184	pyrimidine deoxyribonucleotides de novo biosynthesis I
PWY-7228	superpathway of guanosine nucleotides de novo biosynthesis I
PWY-6609	adenine and adenosine salvage III
PWY-7385	1,3-propanediol biosynthesis (engineered)
PWY-4981	L-proline biosynthesis II (from arginine)
THRESYN-PWY	superpathway of L-threonine biosynthesis

Pathway	Description
ANAGLYCOLYSIS-PWY	glycolysis III (from glucose)
HEME-BIOSYNTHESIS-II	heme biosynthesis I (aerobic)
PWY-7221	guanosine ribonucleotides de novo biosynthesis
PWY-922	mevalonate pathway I
UDPNACETYLGALSYN-PWY	UDP-N-acetyl-D-glucosamine biosynthesis II
P185-PWY	formaldehyde assimilation III (dihydroxyacetone cycle)
GLUCONEO-PWY	gluconeogenesis I
PWY-6837	fatty acid beta-oxidation V (unsaturated, odd number, di-isomerase-dependent)
PWY-5920	superpathway of heme biosynthesis from glycine
PWY-5189	tetrapyrrole biosynthesis II (from glycine)
PWY-7197	pyrimidine deoxyribonucleotide phosphorylation
PWY-5667	CDP-diacylglycerol biosynthesis I
PWY-7210	pyrimidine deoxyribonucleotides biosynthesis from CTP
LEU-DEG2-PWY	L-leucine degradation I
SO4ASSIM-PWY	sulfate reduction I (assimilatory)
PWY-6121	5-aminoimidazole ribonucleotide biosynthesis I
TYRFUMCAT-PWY	L-tyrosine degradation I
PWY-621	sucrose degradation III (sucrose invertase)
PWY3O-355	stearate biosynthesis III (fungi)

Pathway	Description
PWY-7269	NAD/NADP-NADH/NADPH mitochondrial interconversion (yeast)
PWY-7268	NAD/NADP-NADH/NADPH cytosolic interconversion (yeast)
PWY4FS-7	phosphatidylglycerol biosynthesis I (plastidic)
PWY4FS-8	phosphatidylglycerol biosynthesis II (non-plastidic)
PWY-7409	phospholipid remodeling (phosphatidylethanolamine, yeast)
LIPASYN-PWY	phospholipases
PWY-2723	trehalose degradation V
GLUCOSE1PMETAB-PWY	glucose and glucose-1-phosphate degradation
PWY-7235	superpathway of ubiquinol-6 biosynthesis (eukaryotic)
PWY-7420	monoacylglycerol metabolism (yeast)
PWY-5651	L-tryptophan degradation to 2-amino-3-carboxymuconate semialdehyde
PWY-5871	ubiquinol-9 biosynthesis (eukaryotic)
PWY-5873	ubiquinol-7 biosynthesis (eukaryotic)
PWY66-409	superpathway of purine nucleotide salvage
ARGSYNBSUB-PWY	L-arginine biosynthesis II (acetyl cycle)
PWY-7196	superpathway of pyrimidine ribonucleosides salvage
HSERMETANA-PWY	L-methionine biosynthesis III
POLYAMINSYN3-PWY	superpathway of polyamine biosynthesis II

Supplementary Table S2. Total metabolomics in all Pu-erh tea samples.

no.	Rt (min)	m/z	formula	mass	tentative identification
				error (mDa)	
1	4.73	915.1619	C44H36O22	-0.7	Assamicain A
2	4.73	915.1619	C44H36O22	-0.7	Assamicain B
3	4.73	915.1619	C44H36O22	-0.7	Assamicain C
4	5.81	441.0823	C22H18O10	-0.4	(-)Epicatechin 3-O-gallate
5	5.81	441.0823	C22H18O10	-0.4	(+)-Catechin 3-O-gallate
6	4.07	305.0667	C15H14O7	0.1	(-)Epigallocatechin
7	4.07	305.0667	C15H14O7	0.1	(+)-Gallocatechin
8	4.72	457.0774	C22H18O11	-0.3	(-)Epigallocatechin-3-O-gallate
9	4.72	457.0774	C22H18O11	-0.3	Gallocatechin 3-O-gallate
10	4.14	633.073	C27H22O18	-0.4	Strictinin
11	4.8	635.0889	C27H24O18	0	1,2,6-tri-O-G- β -D-glu
12	4.8	635.0889	C27H24O18	0	1,4,6-tri-O-G- β -D-glu
13	3.46	343.0668	C14H16O10	-0.3	5-G-quinic acid
14	3.46	343.0668	C14H16O10	-0.3	Theogallin
15	4.68	289.0717	C15H14O6	-0.1	(-)Epicatechin
16	4.68	289.0717	C15H14O6	-0.1	Catechin

no.	Rt (min)	m/z	formula	mass	
				error (mDa)	tentative identification
17	6.48	593.1508	C27H30O15	-0.4	2"-O- β -D-Glu-vitexin
18	6.48	593.1508	C27H30O15	-0.4	Biorobin
19	6.48	593.1508	C27H30O15	-0.4	Kaempferol 3-O-rutinoside
20	6.48	593.1508	C27H30O15	-0.4	Nicotiflorin
21	6.48	593.1508	C27H30O15	-0.4	Vicenin 2
22	6.77	447.0927	C21H20O11	-0.6	Asiaticalin
23	6.77	447.0927	C21H20O11	-0.6	Astragalin
24	4.39	577.1345	C30H26O12	-0.7	Procyanidin B2
25	4.39	577.1345	C30H26O12	-0.7	Procyanidin B4
26	4.04	483.0778	C20H20O14	-0.2	1,2-di-O-G- β -D-glu
27	4.04	483.0778	C20H20O14	-0.2	1,6-di-O-G- β -D-glu
28	0.78	191.0559	C7H12O6	-0.2	Quinic acid
29	5.75	609.1455	C26H28O14	-0.6	Apigenin-6-C-Glu-8-arabinoside
30	5.75	609.1455	C26H28O14	-0.6	Isoschaftoside
31	5.75	609.1455	C27H30O16	-0.6	Rutin
32	4.3	353.0875	C16H18O9	-0.3	4-O-caffeooyl-quinic acid
33	4.3	353.0875	C16H18O9	-0.3	5-caffeooyl-quinic acid

no.	Rt (min)	m/z	formula	mass	
				error (mDa)	tentative identification
34	4.3	353.0875	C16H18O9	-0.3	Chlorogenic acid
35	6.03	463.0873	C21H20O12	-0.9	Isoquercitrin
36	6.03	463.0873	C21H20O12	-0.9	Myricitrin
37	4.17	321.0616	C14H12O6	0	Teadenol A
38	4.17	321.0616	C14H12O6	0	Teadenol B
39	5.24	479.0827	C21H20O13	-0.4	Myricetin 3-galactoside
40	5.24	479.0827	C21H20O13	-0.4	Myricetin 3-O- β -D-glucoside
41	5.24	479.0827	C20H18O11	-0.4	Quercetin 3-arabinopyranoside
42	5.61	755.2031	C33H40O20	-0.9	Kaempferol 7-galactoside 3-rutinoside
43	3.85	609.1247	C29H24O12	-0.3	Isotheaflavin
44	3.85	609.1247	C29H24O12	-0.3	Neotheaflavin
45	3.85	609.1247	C30H26O14	-0.3	Prodelphinidin B
46	3.85	609.1247	C30H26O14	-0.3	Prodelphinidin B-4
47	3.85	609.1247	C29H24O12	-0.3	Theaflavin
48	3.85	609.1247	C30H26O14	-0.3	Theasinensin C
49	3.85	609.1247	C30H26O14	-0.3	Theasinensin E
50	4.51	865.1973	C45H38O18	-1.3	Procyanidin C1

no.	Rt (min)	m/z	formula	mass	
				error (mDa)	tentative identification
51	3.94	353.088	C16H18O9	0.1	4-O-caffeooyl-quinic acid
52	4.8	337.093	C16H18O8	0.1	3-p-coumaroyl-quinic acid
53	4.8	337.093	C16H18O8	0.1	4-p-coumaroyl-quinic acid
54	4.8	337.093	C16H18O8	0.1	5-p-coumaroyl-quinic acid
55	4.8	337.093	C16H18O8	0.1	Coumaroylquinic acid
56	4.2	293.0666	C13H12O5	0	Fuzhuanin E
57	4.2	293.0666	C13H12O5	0	Fuzhuanin F
58	4.2	293.0666	C13H12O5	0	Xanthocerin
59	2.41	331.0668	C13H16O10	-0.2	1-O-G- β -D-glu
60	2.41	331.0668	C13H16O10	-0.2	2-O-G-D-glu
61	2.41	331.0668	C13H16O10	-0.2	6-O-G- β -D-glu
62	2.41	331.0668	C13H16O10	-0.2	β -glucogallin
63	5.5	881.1562	C44H34O20	-0.9	EA 3-O-gallate-(4 β \rightarrow 6)-EGCG
64	5.5	881.1562	C44H34O20	-0.9	Procyanidin B-2 3,3'-di-O-gallate
65	5.5	881.1562	C44H34O20	-0.9	Procyanidin B-5 3,3'-di-O-gallate
66	5.85	300.9988	C14H6O8	-0.2	Ellagic acid
67	1.13	173.093	C7H14N2O3	-0.2	Theanine

no.	Rt (min)	m/z	formula	mass	
				error (mDa)	tentative identification
68	4.9	897.1516	C44H34O21	-0.4	ECG-(4β→6)-EGCG
69	4.9	897.1516	C44H34O21	-0.4	ECG-(4β→8)-EGCG
70	4.9	897.1516	C44H34O21	-0.4	EGCG-(4β→6)-ECG
71	4.9	897.1516	C43H32O19	-0.4	Theaflavate A
72	4.9	897.1516	C44H34O21	-0.4	Theasinensin F
73	4.9	897.1516	C44H34O21	-0.4	Theasinensin G
74	6.08	865.1611	C44H34O19	-1	EA-gallate-(4β→6)-ECG
75	6.08	865.1611	C44H34O19	-1	EA-gallate-(4β→8)-ECG
76	4.45	473.072	C22H18O12	-0.5	Chicoric acid
77	4.45	473.072	C21H16O10	-0.5	Epitheaflavic acid
78	4.45	473.072	C21H16O10	-0.5	Theaflavic acid
79	4.14	761.1353	C36H28O16	-0.7	Isotheaflavin 3'-gallate
80	4.14	761.1353	C36H28O16	-0.7	Neotheaflavin 3-gallate
81	4.14	761.1353	C37H30O18	-0.7	Prodelphinidin B-2 3'-O-gallate
82	4.14	761.1353	C37H30O18	-0.7	Prodelphinidin B-4 3'-O-gallate
83	4.14	761.1353	C36H28O16	-0.7	Theaflavin-3'-gallate
84	4.14	761.1353	C36H28O16	-0.7	Theaflavin-3-gallate

no.	Rt (min)	m/z	formula	mass	
				error (mDa)	tentative identification
85	4.14	761.1353	C37H30O18	-0.7	Theasinensin B
86	4.14	761.1353	C37H30O18	-0.7	Theasinensin H
87	5.08	625.1404	C27H30O17	-0.7	Myricetin-3-O-rutinoside
88	4.4	913.1459	C44H34O22	-1	EGCG-(4 β →8)-EGCG
89	4.4	913.1459	C44H34O22	-1	Prodelphinidin B-2 3,3'-di-O-gallate
90	4.4	913.1459	C44H34O22	-1	Prodelphinidin B-5 3,3'-di-O-gallate
91	4.4	913.1459	C43H32O20	-1	Theaflavin 3,3'-digallate
92	4.4	913.1459	C44H34O22	-1	Theasinensin A
93	4.4	913.1459	C44H34O22	-1	Theasinensin D
94	10.59	285.0403	C15H10O6	-0.2	3',4',5,7-tetraOH-flavone
95	10.59	285.0403	C15H10O6	-0.2	Kaempferol
96	10.59	285.0403	C15H10O6	-0.2	Luteolin
97	9.43	593.129	C30H26O13	-1.1	Catechin-(4 α →8)-ECC
98	9.43	593.129	C30H26O13	-1.1	desG theasinensin F
99	9.43	593.129	C30H26O13	-1.1	Epigallocatechin-(4 β →8)-catechin
100	9.43	593.129	C30H26O13	-1.1	GC-(4 α →8)-EC
101	9.43	593.129	C30H26O13	-1.1	Tiliroside

no.	Rt (min)	m/z	formula	mass	
				error (mDa)	tentative identification
102	5.97	597.1821	C26H32O13	-0.4	Benzyl 2-neohesperidosyloxy-6-OH-benzoate
103	4.21	865.1982	C45H38O18	-0.3	Procyanidin C1
104	5.9	568.1454	C28H27NO12	-0.7	Ect-pyrrolidinone A
105	5.9	568.1454	C28H27NO12	-0.7	Ect-pyrrolidinone B
106	13.58	277.217	C18H30O2	-0.3	α -linolenic acid
107	5.62	609.088	C29H22O15	-0.6	(-)EGC 3,3'-di-O-gallate
108	5.62	609.088	C29H22O15	-0.6	(-)EGC 3,4-di-O-gallate
109	5.62	609.088	C29H22O15	-0.6	(-)EGC 3,5-di-O-gallate
110	5.62	609.088	C29H22O15	-0.6	(\pm)-GC-3,5-di-O-gallate
111	5.44	771.1986	C33H40O21	-0.3	Quercetin 3-O-Gal-rutinoside
112	5.44	771.1986	C33H40O21	-0.3	Quercetin 3-O-Glu-rutinoside
113	4.08	319.0457	C15H12O8	-0.2	Ampelopsin
114	4.08	319.0457	C15H12O8	-0.2	Fuzhuanin A
115	4.74	913.1463	C44H34O22	-0.6	EGCG-(4 β →8)-EGCG
116	4.74	913.1463	C44H34O22	-0.6	Prodelphinidin B-2 3,3'-di-O-gallate
117	4.74	913.1463	C44H34O22	-0.6	Prodelphinidin B-5 3,3'-di-O-gallate

no.	Rt (min)	m/z	formula	mass	
				error (mDa)	tentative identification
118	3.98	451.1244	C21H24O11	-0.2	(+)-catechin-8-C- β -D-glucoside
119	3.98	451.1244	C21H24O11	-0.2	Catechin-7-O- β -D-glucoside
120	3.98	451.1244	C21H24O11	-0.2	Epicatechin 8-C-glucoside
121	8.2	865.1612	C44H34O19	-0.9	EA-gallate-(4 β →6)-ECG
122	8.2	865.1612	C44H34O19	-0.9	EA-gallate-(4 β →8)-ECG
123	5.73	787.0996	C34H28O22	-0.4	1,2,3,4-tetra-O-G- β -D-glu
124	5.73	787.0996	C34H28O22	-0.4	1,2,4,6-tetra-O-G- β -D-glu
125	5.31	771.1984	C33H40O21	-0.5	Quercetin 3-O-Gal-rutinoside
126	5.31	771.1984	C33H40O21	-0.5	Quercetin 3-O-Glu-rutinoside
127	7.05	552.1505	C28H27NO11	-0.7	5"-R-ethylpyrrolidinonyl EC-3-O-gallate
128	7.05	552.1505	C28H27NO11	-0.7	Ect-pyrrolidinone E
129	7.05	552.1505	C28H27NO11	-0.7	Ect-pyrrolidinone F
130	7.05	552.1505	C28H27NO11	-0.7	Ect-pyrrolidinone J
131	0.66	132.03	C4H7NO4	-0.2	Aspartic acid
132	6.91	593.0933	C29H22O14	-0.3	(-)EC 3,5-di-O-gallate
133	5.68	941.1775	C45H36O20	-0.7	Talienbisflavan A
134	5.29	415.1605	C19H28O10	-0.4	Chakanoside II

no.	Rt (min)	m/z	formula	mass	
				error (mDa)	tentative identification
135	5.29	415.1605	C19H28O10	-0.4	Phenethylalcohol β -D-xylosyl (1 \rightarrow 6)- β -D-glucoside
136	4.66	416.1347	C21H23NO8	-0.4	5"-R-ethylpyrrolidinonyl EGC
137	4.66	416.1347	C21H23NO8	-0.4	5"-R-ethylpyrrolidinonyl GC
138	4.66	416.1347	C21H23NO8	-0.4	5"-S-ethylpyrrolidinonyl EGC
139	4.66	416.1347	C21H23NO8	-0.4	5"-S-ethylpyrrolidinonyl GC
140	4.66	416.1347	C21H23NO8	-0.4	Puerin V
141	4.66	416.1347	C21H23NO8	-0.4	Puerin VI
142	4.66	416.1347	C21H23NO8	-0.4	Puerin VII
143	4.66	416.1347	C21H23NO8	-0.4	Puerin VIII
144	6.92	552.1505	C28H27NO11	-0.6	5"-R-ethylpyrrolidinonyl EC-3-O-gallate
145	9.1	301.0351	C15H10O7	-0.3	Herbacetin
146	9.1	301.0351	C15H10O7	-0.3	Morin
147	9.1	301.0351	C15H10O7	-0.3	Quercetin
148	4.02	495.0774	C21H20O14	-0.6	3,4-di-O-G-quinic acid
149	4.02	495.0774	C21H20O14	-0.6	4,5-di-O-G-quinic acid
150	6.98	881.1561	C44H34O20	-0.9	EA 3-O-gallate-(4 β \rightarrow 6)-EGCG

no.	Rt (min)	m/z	formula	mass	
				error (mDa)	tentative identification
151	6.98	881.1561	C44H34O20	-0.9	Procyanidin B-2 3,3'-di-O-gallate
152	6.98	881.1561	C44H34O20	-0.9	Procyanidin B-5 3,3'-di-O-gallate
153	3.35	101.0606	C5H10O2	-0.2	Ethyl propanoate
154	4.98	771.1986	C33H40O21	-0.3	Quercetin 3-O-Gal-rutinoside
155	4.98	771.1986	C33H40O21	-0.3	Quercetin 3-O-Glu-rutinoside
156	4.61	565.1553	C26H30O14	-1	Theaflavanoside I
157	13.45	277.2171	C18H30O2	-0.2	α -linolenic acid
158	5.18	775.1508	C37H30O16	-0.8	Procyanidin B-2 3'-O-gallate
159	5.18	775.1508	C37H30O16	-0.8	Procyanidin B-4 3'-O-gallate
160	6.81	789.1662	C38H32O16	-1	Fangchengbisflavan B
161	7.24	941.1774	C45H36O20	-0.8	Talienbisflavan A
162	5.9	431.098	C21H20O10	-0.4	Afzelin
163	7.61	941.1774	C45H36O20	-0.7	Talienbisflavan A
164	9.23	715.1298	C36H28O16	-0.6	Isotheaflavin 3'-gallate
165	9.23	715.1298	C36H28O16	-0.6	Neotheaflavin 3-gallate
166	9.23	715.1298	C36H28O16	-0.6	Theaflavin-3'-gallate
167	9.23	715.1298	C36H28O16	-0.6	Theaflavin-3-gallate

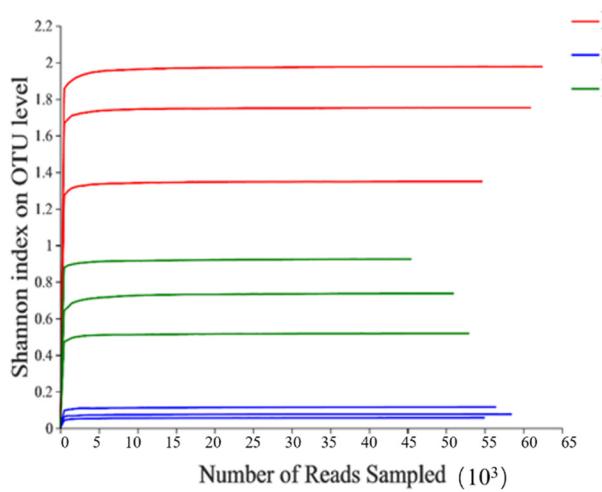
no.	Rt (min)	m/z	formula	mass	
				error (mDa)	tentative identification
168	4.04	631.094	C28H24O17	-0.1	8-C-ascorbyl (-)-EGC 3-O-gallate
169	4.04	631.094	C28H24O17	-0.1	Myricetin 3-(6"-galloylglucoside)
170	5.09	789.1667	C38H32O16	-0.5	Fangchengbisflavan B
171	7.02	911.1665	C44H34O19	-1.1	EA-gallate-(4 β →6)-ECG
172	7.02	911.1665	C44H34O19	-1.1	EA-gallate-(4 β →8)-ECG
173	6.43	789.1666	C38H32O16	-0.6	Fangchengbisflavan B
174	0.89	191.0344	C9H6O2	-0.5	Coumarin
175	7.41	467.098	C24H20O10	-0.3	(-) -EGC 3-O-caffeoate
176	3.89	347.0775	C17H16O8	0.3	6-carboxyMe-(+)-catechin
177	3.89	347.0775	C17H16O8	0.3	8-carboxyMe-(+)-catechin
178	4.48	759.1191	C37H28O18	-1.2	Dehydrotheasinensin H
179	4.48	759.1191	C37H28O18	-1.2	Prodelphinidin A2 3'-gallate
180	4.48	759.1191	C37H28O18	-1.2	Theacitrin A
181	4.48	759.1191	C37H28O18	-1.2	Theacitrin B
182	4.48	759.1191	C37H28O18	-1.2	Theacitrinin B
183	15.63	591.2608	C35H36N4O5	-0.5	Pheophorbide A
184	7.58	481.1129	C24H20O8	-1.2	(-) -EC 3-O-p-coumaroate

no.	Rt (min)	m/z	formula	mass	
				error (mDa)	tentative identification
185	7.58	481.1129	C24H20O8	-1.2	(-)EGC 3-O-cinnamate
186	7.58	481.1129	C25H22O10	-1.2	Puerin C
187	7.58	481.1129	C25H22O10	-1.2	Puerin E
188	7.58	481.1129	C25H22O10	-1.2	Puerin F
189	7.58	481.1129	C25H22O10	-1.2	PuerinD
190	4.62	135.0449	C8H8O2	-0.2	4'-Hydroxyacetophenone
191	14.99	605.2398	C35H34N4O6	-0.7	Phaeophorbide B
192	7.55	409.0924	C22H18O8	-0.5	(-)EC 3-O-p-OH-benzoate
193	4.9	387.2021	C19H32O8	-0.4	Icariside B5
194	6.54	501.1039	C23H20O10	0	(-)EC 3-O-(3-O-Me)-gallate
195	6.54	501.1039	C23H20O10	0	(-)EC 3-O-(4-O-Me)-gallate
196	1.27	85.0294	C4H6O2	-0.1	Diacetyl
197	7.21	927.1616	C45H36O22	-0.9	Oolonghomobisflavan A
198	7.21	927.1616	C45H36O22	-0.9	Oolonghomobisflavan B
199	6.15	477.1029	C21H20O10	-0.9	Afzelin
200	6.15	477.1029	C21H20O10	-0.9	Isovitexin
201	6.15	477.1029	C21H20O10	-0.9	Vitexin

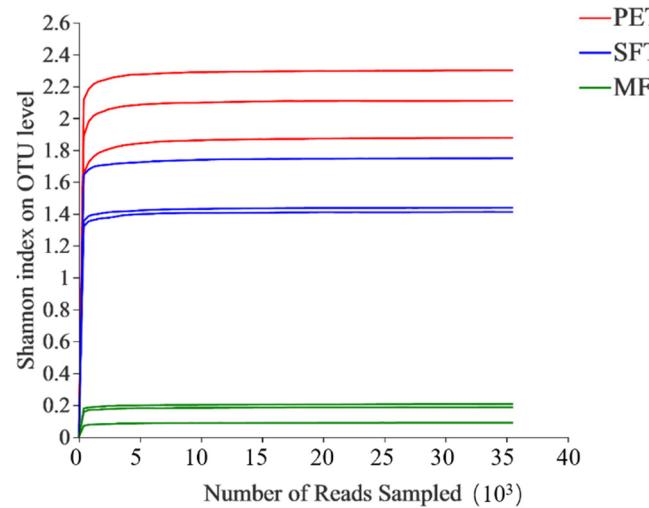
no.	Rt (min)	m/z	formula	mass	
				error (mDa)	tentative identification
202	6.63	515.1197	C25H24O12	0.2	3,5-dicaffeoyl-quinic acid
203	2.65	134.0471	C3H7NO2	1.3	Alanine
204	0.76	175.0246	C6H8O6	-0.2	Ascorbic acid
205	5.12	791.1471	C37H30O17	0.6	Catechin-(4 α →8)-EGCG
206	4.48	777.1303	C36H28O17	-0.6	Oolongtheanine
207	0.92	133.0142	C4H6O5	-0.1	Malic acid
208	3.83	799.1372	C36H32O21	0.8	Theogallinin
209	6.27	121.0658	C8H10O	-0.1	2,5-Dimethylphenol
210	6.27	121.0658	C8H10O	-0.1	3-Ethylphenol
211	6.23	513.1037	C24H20O10	-0.1	(-)EGC 3-O-caffeoate
212	7.1	515.119	C25H24O12	-0.5	3,5-dicaffeoyl-quinic acid
213	4.4	637.1553	C31H28O12	-0.9	Bis(8-epicatechiny)-methane
214	3.64	153.0191	C7H6O4	-0.2	Gentisic acid
215	3.64	153.0191	C7H6O4	-0.2	Protocatechuic acid
216	8.19	551.0831	C27H20O13	0	Epitheafagallin 3-O-gallate
217	1.43	517.0999	C23H20O11	1.2	(-)EGC 3-O-(3-O-Me)-gallate
218	1.43	517.0999	C23H20O11	1.2	(-)EGC 3-O-(4-O-Me)-gallate

no.	Rt (min)	m/z	formula	mass	
				error (mDa)	tentative identification
219	1.43	517.0999	C23H20O11	1.2	(-)EGC 3'-O-Me-gallate
220	1.43	517.0999	C23H20O11	1.2	(-)Epigallocatechin 3-(3-methyl-gallate)
221	1.43	517.0999	C23H20O11	1.2	EGCG-4"-Me
222	4.97	281.1392	C15H22O5	-0.2	Dihydrophaseic acid
223	4.97	281.1392	C15H22O5	-0.2	Epidihydrophaseic acid
224	3.99	829.1465	C36H32O20	-0.4	des-G theaflavonin
225	7.42	147.0662	C5H10O2	-0.1	Ethyl propanoate
226	8.36	579.0782	C28H20O14	0.1	Acetonyl theacitrin A
227	8.36	579.0782	C28H20O14	0.1	Epitheflavic acid 3'-gallate
228	5.7	197.0814	C9H12O2	-0.5	4-Ethyl-2-methoxyphenol
229	4.46	597.088	C27H20O13	-0.6	Epitheflagallin 3-O-gallate
230	5.34	405.1556	C20H24O6	0.1	Isolariciresinol
231	1.54	128.0716	C6H11NO2	-0.1	N-ethyl-5-OH-2-pyrrolidinone
232	6.14	195.066	C10H12O4	-0.3	3,4,5-Trimethoxybenzaldehyde
233	7.93	591.1506	C31H28O12	-0.2	Bis(8-epicatechiny)-methane
234	4.38	223.0608	C11H12O5	-0.4	Sinapic acid
235	6.37	431.1921	C19H30O8	-0.2	Roseoside

no.	Rt (min)	m/z	formula	mass	
				error (mDa)	tentative identification
236	4.8	653.1514	C31H28O13	0.2	Fangchengbisflavan A
237	2.54	174.0772	C6H11NO2	0	N-ethyl-5-OH-2-pyrrolidinone
238	1.77	152.0352	C7H7NO3	-0.1	Aminosalicylic Acid
239	1.7	175.0247	C6H8O6	-0.1	Ascorbic acid
240	15.38	171.1025	C8H14O	-0.1	(E)-2-Octenal
241	7.05	461.1454	C22H24O8	0.1	Puerin B
242	0.7	177.0405	C5H8O4	0.1	Glutaric acid
243	0.66	148.0612	C4H9NO2	-0.4	γ -Aminobutyric acid
244	15.33	313.2743	C18H36O	-0.6	6,10,14-Trimethylpentadecan-2-one
245	5.54	197.0453	C8H8O3	-0.2	4-Hydroxyphenylacetic acid
246	5.54	197.0453	C9H10O5	-0.2	Syringic acid
247	7.29	195.0661	C10H12O4	-0.2	Homoveratric acid
248	5.23	239.0924	C12H16O5	-0.1	Icariside

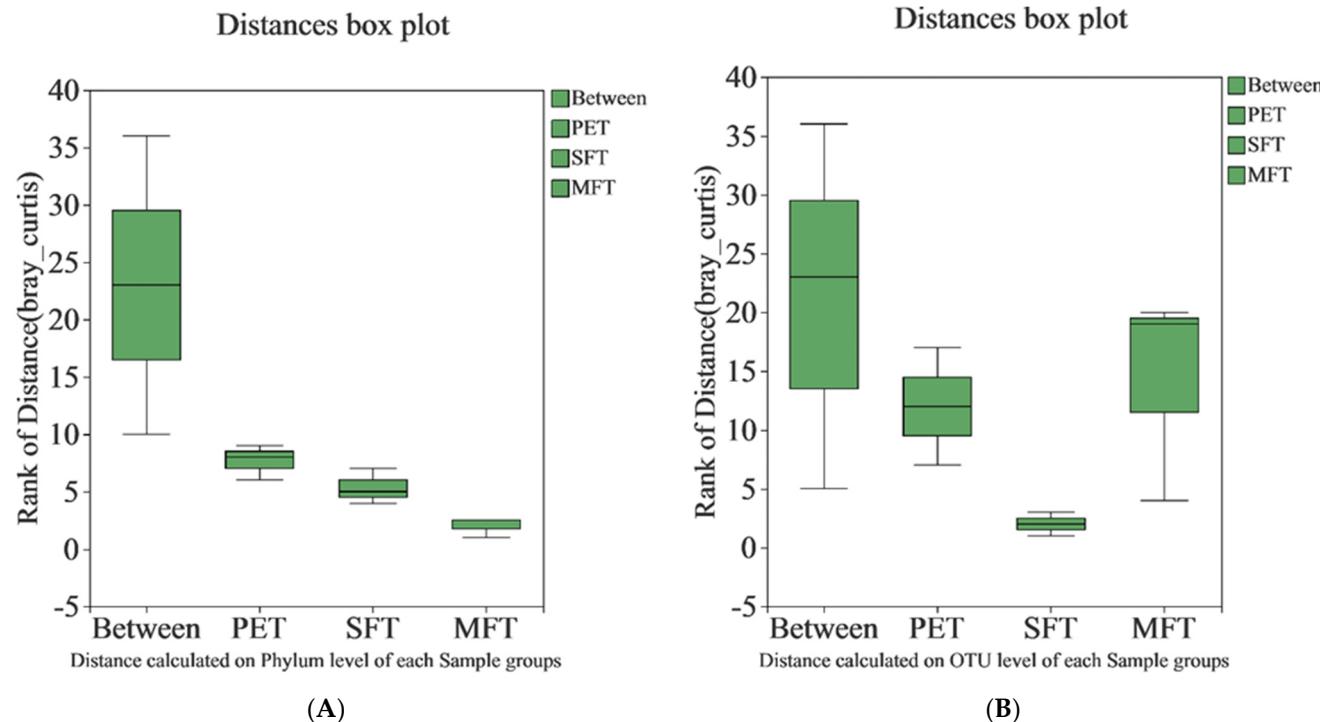


(A)

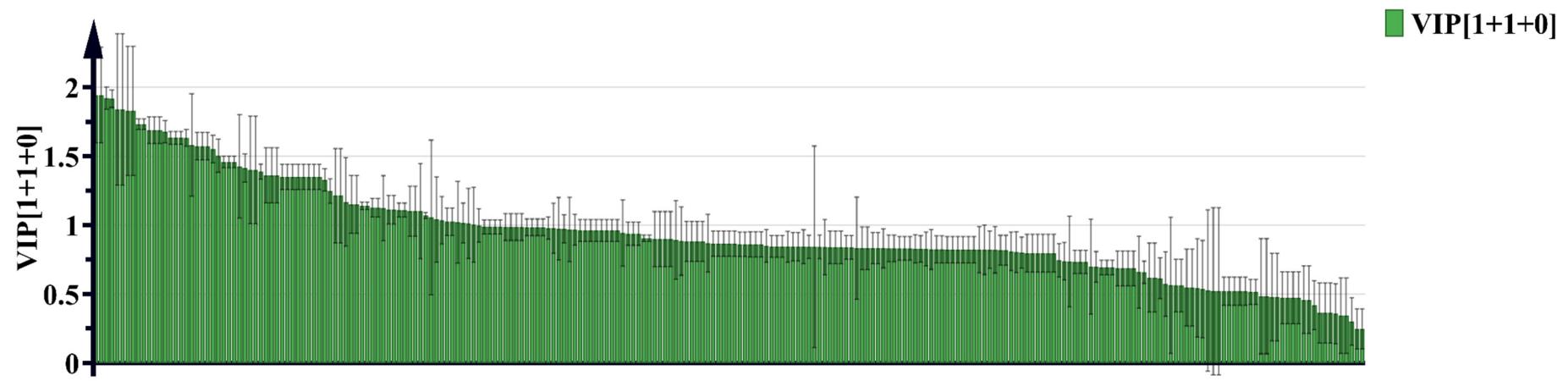


(B)

Supplementary Figure S1. High-throughput sequencing dilution Shannon curves for bacterial (A) and fungal (B).



Supplementary Figure S2. Bray-Curtis distance distribution of bacterial(A) and fungal (B) communities in different Pu-erh tea samples at the OTUs level.



Supplementary Figure S3. Variable importance of the projection (VIP>1) plots of metabolites for distinguishing different sample groups using OPLS-DA model.