

Supporting Information

Table S1 List of all identified 192 lipid species in black tea by LC-MS based tea lipid profiling approach and their RT.

Nr.	Lipid species	lipid (sub)class	RT/min
1	Cer(t18:0/22:0h)	Ceramide	9.4
2	Cer(t18:0/24:0h)	Ceramide	10.0
3	GlcCer(d18:2/h16:0)	Glucosylceramide	6.8
4	GlcCer(d18:2/h18:0)	Glucosylceramide	7.5
5	GlcCer(d18:2/h20:0)	Glucosylceramide	8.1
6	GlcCer(d18:2/h22:0)	Glucosylceramide	8.8
7	GlcCer(d18:2/h24:0)	Glucosylceramide	9.4
8	GlcCer(d18:2/h24:1)	Glucosylceramide	8.7
9	GlcCer(t18:1/h24:0)	Glucosylceramide	9.2
10	GlcCer(t18:1/h24:1)	Glucosylceramide	8.5
11	18:2-Sitosterol	Steryl ester	13.4
12	16:0-Glc-Sitosterol	Acylated steryl glycoside	10.6
13	16:0-Glc-Stigmasterol I	Acylated steryl glycoside	10.2
14	16:0-Glc-Stigmasterol II	Acylated steryl glycoside	10.4
15	18:0-Glc-Sitosterol	Acylated steryl glycoside	11.1
16	18:0-Glc-Stigmasterol	Acylated steryl glycoside	10.9
17	18:1-Glc-Sitosterol	Acylated steryl glycoside	10.6
18	18:1-Glc-Stigmasterol	Acylated steryl glycoside	10.4
19	18:2-Glc-Sitosterol	Acylated steryl glycoside	10.2
20	18:2-Glc-Stigmasterol I	Acylated steryl glycoside	9.8
21	18:2-Glc-Stigmasterol II	Acylated steryl glycoside	10.1
22	18:3-Glc-Stigmasterol I	Acylated steryl glycoside	9.3
23	18:3-Glc-Stigmasterol II	Acylated steryl glycoside	9.6
24	MGDG(16:0/18:1)	Monogalactosyldiacylglycerol	8.3
25	MGDG(16:0/18:2)	Monogalactosyldiacylglycerol	7.8
26	MGDG(16:0/18:3)	Monogalactosyldiacylglycerol	7.4
27	MGDG(16:1/18:3)	Monogalactosyldiacylglycerol	6.8
28	MGDG(16:2/18:3)	Monogalactosyldiacylglycerol	6.4
29	MGDG(16:3/18:3)	Monogalactosyldiacylglycerol	6.0
30	MGDG(17:3/18:3)	Monogalactosyldiacylglycerol	6.3
31	MGDG(18:0/18:2)	Monogalactosyldiacylglycerol	8.5
32	MGDG(18:1/18:2)	Monogalactosyldiacylglycerol	7.9
33	MGDG(18:0/18:3)	Monogalactosyldiacylglycerol	8.0
34	MGDG(18:1/18:3)	Monogalactosyldiacylglycerol	7.4
35	MGDG(18:3/18:2)	Monogalactosyldiacylglycerol	7.0
36	MGDG(18:3/18:3)	Monogalactosyldiacylglycerol	6.5
37	MGDG(20:2/18:2)	Monogalactosyldiacylglycerol	8.1
38	MGDG(20:2/18:3)	Monogalactosyldiacylglycerol	7.5
39	MGDG(20:3/18:3)	Monogalactosyldiacylglycerol	7.1
40	DGDG(16:0/18:1)	Digalactosyldiacylglycerol	7.8
41	DGDG(16:0/18:2)	Digalactosyldiacylglycerol	7.3

42	DGDG(16:0/18:3)	Digalactosyldiacylglycerol	6.8
43	DGDG(16:1/18:3)	Digalactosyldiacylglycerol	6.3
44	DGDG(16:2/18:3)	Digalactosyldiacylglycerol	5.9
45	DGDG(18:0/18:1)	Digalactosyldiacylglycerol	8.4
46	DGDG(18:0/18:2)	Digalactosyldiacylglycerol	7.9
47	DGDG(18:0/18:3)	Digalactosyldiacylglycerol	7.5
48	DGDG(18:1/18:3)	Digalactosyldiacylglycerol	6.9
49	DGDG(18:2/18:3)	Digalactosyldiacylglycerol	6.4
50	DGDG(18:3/18:3)	Digalactosyldiacylglycerol	6.0
51	DGDG(20:1/18:3)	Digalactosyldiacylglycerol	7.5
52	DGDG(20:3/18:3)	Digalactosyldiacylglycerol	6.6
53	SQDG(16:0/16:0)	Sulfoquinovosyldiacylglycerol	6.5
54	SQDG(16:0/16:1)	Sulfoquinovosyldiacylglycerol	6.1
55	SQDG(18:1/16:0)	Sulfoquinovosyldiacylglycerol	6.6
56	SQDG(18:2/16:0)	Sulfoquinovosyldiacylglycerol	6.2
57	SQDG(18:3/16:0)	Sulfoquinovosyldiacylglycerol	5.9
58	SQDG(18:3/16:1)	Sulfoquinovosyldiacylglycerol	5.5
59	SQDG(18:1/18:0)	Sulfoquinovosyldiacylglycerol	7.1
60	SQDG(18:1/18:1)	Sulfoquinovosyldiacylglycerol	6.7
61	SQDG(18:3/18:0)	Sulfoquinovosyldiacylglycerol	6.4
62	SQDG(18:2/18:2)	Sulfoquinovosyldiacylglycerol	5.9
63	SQDG(18:3/18:2)	Sulfoquinovosyldiacylglycerol	5.6
64	SQDG(18:3/18:3)	Sulfoquinovosyldiacylglycerol	5.3
65	LPC(16:0)	Lyso-phosphatidylcholine	3.0
66	LPC(18:0)	Lyso-phosphatidylcholine	4.3
67	LPC(18:1) sn-1	Lyso-phosphatidylcholine	3.3
68	LPC(18:1) sn-2	Lyso-phosphatidylcholine	3.0
69	LPC(18:2) sn-1	Lyso-phosphatidylcholine	2.5
70	LPC(18:2) sn-2	Lyso-phosphatidylcholine	2.3
71	PA(36:4)	Phosphatidic acid	6.5
72	PA(36:5)	Phosphatidic acid	6.1
73	PA(36:6)	Phosphatidic acid	5.7
74	PA(34:2)	Phosphatidic acid	6.9
75	PA(34:3)	Phosphatidic acid	6.4
76	PC(32:0)	Phosphatidylcholine	7.9
77	PC(32:1)	Phosphatidylcholine	7.3
78	PC(32:2)	Phosphatidylcholine	6.8
79	PC(32:3)	Phosphatidylcholine	6.4
80	PC(33:1)	Phosphatidylcholine	7.6
81	PC(33:2)	Phosphatidylcholine	7.1
82	PC(33:3)	Phosphatidylcholine	6.7
83	PC(34:1)	Phosphatidylcholine	7.9
84	PC(34:2)	Phosphatidylcholine	7.4
85	PC(34:3)	Phosphatidylcholine	6.9
86	PC(34:4)	Phosphatidylcholine	6.4

87	PC(34:5)	Phosphatidylcholine	6.0
88	PC(35:2)	Phosphatidylcholine	7.8
89	PC(35:3)	Phosphatidylcholine	7.4
90	PC(35:4)	Phosphatidylcholine	6.8
91	PC(36:1)	Phosphatidylcholine	8.6
92	PC(36:2)	Phosphatidylcholine	8.1
93	PC(36:3)	Phosphatidylcholine	7.6
94	PC(36:4)	Phosphatidylcholine	7.0
95	PC(36:5)	Phosphatidylcholine	6.5
96	PC(36:6)	Phosphatidylcholine	6.1
97	PC(37:3)	Phosphatidylcholine	8.0
98	PC(37:4)	Phosphatidylcholine	7.4
99	PC(37:5)	Phosphatidylcholine	7.0
100	PC(37:6)	Phosphatidylcholine	6.5
101	PC(38:2)	Phosphatidylcholine	8.8
102	PC(38:3)	Phosphatidylcholine	8.1
103	PC(38:4)	Phosphatidylcholine	7.6
104	PC(38:5)	Phosphatidylcholine	7.1
105	PC(40:2)	Phosphatidylcholine	9.4
106	PC(40:4)	Phosphatidylcholine	8.5
107	PE(34:1)	Phosphatidylethanolamine	8.0
108	PE(34:2)	Phosphatidylethanolamine	7.5
109	PE(34:3)	Phosphatidylethanolamine	7.1
110	PE(36:2)	Phosphatidylethanolamine	8.2
111	PE(36:3)	Phosphatidylethanolamine	7.6
112	PE(36:4)	Phosphatidylethanolamine	7.1
113	PE(36:5)	Phosphatidylethanolamine	6.7
114	PE(36:6)	Phosphatidylethanolamine	6.2
115	PE(38:3)	Phosphatidylethanolamine	8.2
116	PE(38:4)	Phosphatidylethanolamine	7.8
117	PE(38:5)	Phosphatidylethanolamine	7.1
118	PE(40:2)	Phosphatidylethanolamine	9.4
119	PE(40:3)	Phosphatidylethanolamine	8.8
120	PE(40:4)	Phosphatidylethanolamine	8.3
121	PE(42:2)	Phosphatidylethanolamine	10.0
122	PE(42:3)	Phosphatidylethanolamine	9.6
123	PG(34:2)	Phosphatidylglycerol	6.7
124	PG(34:3)	Phosphatidylglycerol	6.3
125	PI(34:2)	Phosphatidylinositol	6.3
126	PI(34:3)	Phosphatidylinositol	6.0
127	DG(32:0)	Diacylglycerol	9.2
128	DG(34:1)	Diacylglycerol	9.3
129	DG(34:2)	Diacylglycerol	8.8
130	DG(34:3)	Diacylglycerol	8.3
131	DG(36:2)	Diacylglycerol	9.4
132	DG(36:3)	Diacylglycerol	8.9

133	DG(36:4)	Diacylglycerol	8.4
134	DG(36:5)	Diacylglycerol	7.9
135	DG(36:6)	Diacylglycerol	7.5
136	TG(42:0)	Triacylglycerol	11.5
137	TG(43:0)	Triacylglycerol	11.7
138	TG(44:1)	Triacylglycerol	11.6
139	TG(44:2)	Triacylglycerol	11.3
140	TG(45:0)	Triacylglycerol	12.1
141	TG(46:0)	Triacylglycerol	12.3
142	TG(46:1)	Triacylglycerol	12.0
143	TG(46:2)	Triacylglycerol	11.7
144	TG(47:0)	Triacylglycerol	12.5
145	TG(47:1)	Triacylglycerol	12.2
146	TG(47:2)	Triacylglycerol	11.9
147	TG(48:0)	Triacylglycerol	12.7
148	TG(48:1)	Triacylglycerol	12.4
149	TG(48:2)	Triacylglycerol	12.1
150	TG(48:3)	Triacylglycerol	11.7
151	TG(49:0)	Triacylglycerol	12.8
152	TG(49:1)	Triacylglycerol	12.5
153	TG(49:2)	Triacylglycerol	12.3
154	TG(49:3)	Triacylglycerol	12.0
155	TG(50:0)	Triacylglycerol	13.0
156	TG(50:1)	Triacylglycerol	12.7
157	TG(50:2)	Triacylglycerol	12.4
158	TG(50:3)	Triacylglycerol	12.1
159	TG(50:4)	Triacylglycerol	11.7
160	TG(51:1)	Triacylglycerol	12.9
161	TG(51:2)	Triacylglycerol	12.6
162	TG(51:3)	Triacylglycerol	12.3
163	TG(51:4)	Triacylglycerol	11.8
164	TG(52:0)	Triacylglycerol	13.3
165	TG(52:1)	Triacylglycerol	13.0
166	TG(52:2)	Triacylglycerol	12.7
167	TG(52:3)	Triacylglycerol	12.4
168	TG(52:4)	Triacylglycerol	12.1
169	TG(52:5)	Triacylglycerol	11.8
170	TG(52:6)	Triacylglycerol	11.5
171	TG(52:7)	Triacylglycerol	11.1
172	TG(54:0)	Triacylglycerol	13.6
173	TG(54:1)	Triacylglycerol	13.3
174	TG(54:2)	Triacylglycerol	13.0
175	TG(54:3)	Triacylglycerol	12.7
176	TG(54:4)	Triacylglycerol	12.4
177	TG(54:5)	Triacylglycerol	12.1
178	TG(54:6)	Triacylglycerol	11.8

179	TG(54:7)	Triacylglycerol	11.5
180	TG(54:8)	Triacylglycerol	11.1
181	TG(54:9)	Triacylglycerol	10.8
182	TG(56:1)	Triacylglycerol	13.6
183	TG(56:5)	Triacylglycerol	12.5
184	TG(56:6)	Triacylglycerol	12.2
185	TG(56:7)	Triacylglycerol	11.9
186	TG(58:2)	Triacylglycerol	13.6
187	Co(Q10)	Ubiquinones	11.8
188	Chlorophyll a	Chlorophyll and derivatives	8.6
189	Chlorophyll b	Chlorophyll and derivatives	7.6
190	Pheophytin a	Chlorophyll and derivatives	9.9
191	Pyropheophytin a	Chlorophyll and derivatives	10.8
192	Pyropheophytin b	Chlorophyll and derivatives	9.6

Figure S1 Color changes of tea leaves during black tea manufacture. Colors are shown at different processing stages, (A) fresh leaves, (B) after withering for 20 hours, (C) after rolling, (D) after fermentation for 4 hours, (E) after drying. All tea samples shown are freeze-dried.

