SUPPLEMENTARY INFORMATION

Comparison of Potent Odorants in Raw and Ripened Pu-erh Tea Infusion Based on Odor Activity Value Calculation and Multivariate Analysis: Understanding the Role of Pile Fermentation

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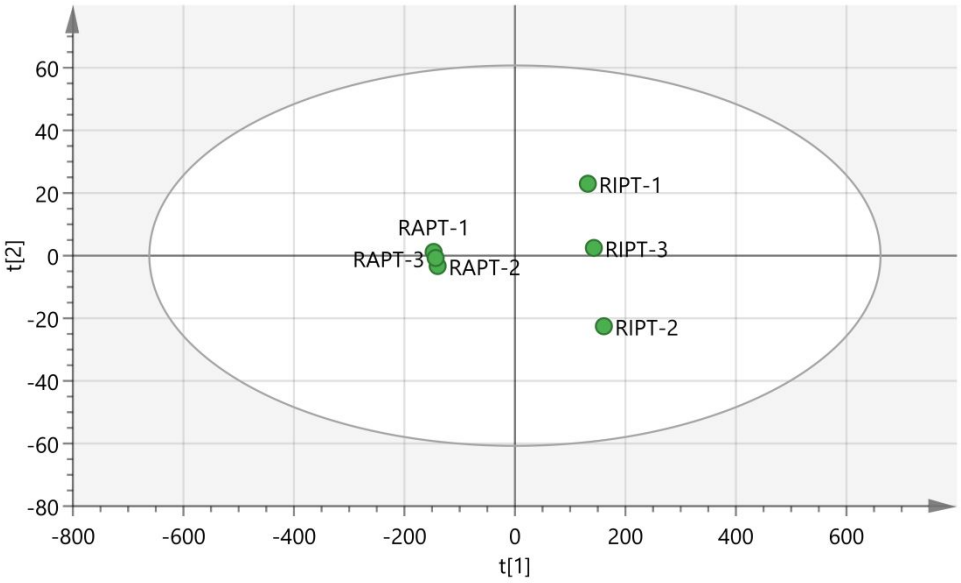
SUPPLEMENTARY FIGURE CAPTIONS

Supplemental Figure 1 The PCA scores plots of odorant contribution (OAVs) in different Pu-erh tea infusions (RAPT, raw Pu-erh tea; RIPT, ripened Pu-erh tea).

Supplemental Figure 1



Supplemental Table 1 Internal Standards, Selected Ions, and Response Factors and Isolation Efficiency Factors for Quantification

No.[a]	Compounds	Internal standard [b]	Target ion(m/z) [c]	IS ion (m/z) [d]	Rf [e] mg/kg	IEF [f]
1	2-Methylpropanal	IS1	72	128	0.294	0.29
2	2-Methylbutanal	IS1	86	128	0.432	0.47
3	3-Methylbutanal	IS1	86	128	0.576	0.39
4	Butane-2,3-dione	IS1	86	128	0.883	0.45
5	Pent-1-en-3-one	IS1	84	128	0.921	0.67
6	(*E*)-2-Methylbut-2-enal	IS1	84	128	0.633	0.65
7	Hexanal	IS1	82	128	0.605	0.78
8	4-Methylpent-3-en-2-one	IS1	98	128	0.892	0.83
9	Heptan-2-one	IS1	114	128	0.932	0.78
10	*D*-limonene	IS2	136	119	0.243	0.78
11	(*E*)-Hex-2-enal	IS1	98	128	0.567	0.89
12	(*Z*)-Hept-4-enal	IS1	84	128	0.567	0.86
13	Cyclohexanone	IS1	98	128	0.766	0.89
14	(*Z*)-Pent-2-en-1-ol	IS1	86	128	0.572	0.75
15	6-Methylhept-5-en-2-one	IS1	126	128	0.934	0.93
16	Linalool oxide (I)	IS1	111	128	0.456	0.83
17	Oct-1-en-3-ol	IS1	72	128	0.312	0.98
18	Acetic acid	IS3	60	88	1.29	1.87
19	Linalool oxide (II)	IS1	111	128	0.512	0.84
20	(2*E*,4*E*)-Hepta-2,4-dienal	IS1	110	128	0.304	0.68
21	Benzaldehyde	IS1	106	128	0.233	0.87
22	Propanoic acid	IS3	74	88	1.22	1.33
23	(*E*)-Non-2-enal	IS1	122	128	1.13	0.92
24	Linalool	IS1	136	128	0.67	0.88
25	(3*E*,5*E*)-Octa-3,5-dien-2-one	IS1	124	128	0.725	0.79
26	5-Methylfurfural	IS3	110	88	2.33	0.87
27	(2*E*,6*Z*)-Nona-2,6-dienal	IS1	70	128	0.421	0.74
29	Hotrienol	IS1	134	128	0.635	0.83
30	*β*-Cyclocitral	IS1	152	128	0.6175	0.94
31	Butyric acid	IS3	73	88	1.437	1.32
34	2-Phenylacetaldehyde	IS1	120	128	0.226	1.03
35	4-Oxoisophorone	IS1	152	128	0.728	0.94
36	α-Terpineol	IS1	136	128	0.733	0.83
38	1,2-Dimethoxybenzene	IS2	138	119	0.839	0.93
39	trans-Pyranoid linalool oxide	IS1	94	128	0.522	0.84
40	cis-Pyranoid linalool oxide	IS1	94	128	0.493	0.79
41	Nerol	IS1	121	128	0.771	0.86
42	1,2-Dimethoxy-4-methylbenzen	IS2	152	119	0.830	0.94

No.[a]	Compounds	Internal standard [b]	Target ion(m/z) [c]	IS ion (m/z) [d]	Rf [e] mg/kg	IEF [f]
	e					
43	*α*-Ionone	IS1	192	128	0.644	0.86
44	Hexanoic acid	IS3	87	88	1.228	0.97
45	2-Methoxyphenol	IS3	124	88	1.06	0.90
47	4-Ethyl-1,2-dimethoxybenzene	IS2	166	119	0.838	0.87
49	2-Phenylethanol	IS1	122	128	0.227	0.91
51	*β*-Ionone	IS1	177	128	0.518	0.85
52	2-Methoxy-4-methylphenol	IS1	138	88	1.33	0.79
53	1,2,3-Trimethoxybenzene	IS2	168	119	0.926	0.93
54	Phenol	IS1	94	128	0.249	0.35
55	4-Ethyl-2-methoxyphenol	IS1	152	128	0.233	0.78
58	*trans*-Methyl isoeugenol	IS1	178	128	0.478	0.87
59	1,2,3-Trimethoxy-5-methylbenz ene	IS2	182	119	0.791	0.79
60	Octanoic acid	IS3	115	88	1.203	1.03
61	4-Methylphenol	IS1	107	128	0.138	1.16
62	1,2,4-Trimethoxybenzene	IS2	168	119	0.733	1.21
63	3-Methylphenol	IS1	108	128	0.193	0.69
65	Nonanoic acid	IS3	129	88	1.097	0.88
66	4-Ethylphenol	IS1	107	128	0.255	0.79
67	2-Ethylphenol	IS1	107	128	0.194	0.90
68	2,6-Dimethoxyphenol	IS1	154	128	0.379	1.07
69	1,2,3,4-Tetramethoxybenzene	IS2	198	119	0.821	0.80
70	Dihydroactinidiolide	IS1	180	128	0.672	0.73
71	Vanillin	IS3	151	88	2.289	0.87
72	3,4-Dimethoxyphenol	IS1	154	128	0.304	0.94

[a] Compound numbers correspond to peak numbers in Table 1.

[b] Internal standard, IS1 refers to 2-methyl-3-heptanone, IS2 refers to tert-butylbenzene, IS3 refers to 2-ethyl butyric acid.

[c] Selected ion for target compound used for response factor and quantitation.

[d] Selected ion of internal standard.

[e] The response factor (1/slope) for a target compound determined by standard curve.

[f] IEF: isolation efficiency factor.