

Supplementary Material

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2.1 Supplementary Tables

Table S1. List all of the volatile compounds in round green tea process.

NO	Name	CAS	RT	RI ^A	RI ^B	FTL	STL	FTS	FLS	RTL	PF1	PF2	PF3	DTL	RPL	BHL
1	Dimethyl ether	115-10-6	2.15	738.79	-	7.7±0.71	6.6±0.62	7.38±0.46	7.75±0.58	8.14±0.72	7.41±0.47	8.26±0.3 7	8.49±1.2 1	7.68±0.5 4	9.03±1.5 6	8.12±0. 64
2	Butanal, 3-methyl-	590-86-3	2.30	743.00	678	2.17±0.1	5.24±0.09	3.92±0.68	3.89±0.81	4.28±0.32	4.1±0.49	4.3±0.87	3.92±1.0 1	3.65±0.0 9	2.82±0.8 2	3.34±0. 59
3	Butanal, 2-methyl-	96-17-3	2.40	745.80	682	2.78±0.1	7.09±0.07	5.49±0.99	5.05±1.01	6.14±0.06	5.35±0.48	5.73±1.4 2	5.15±1.4 4	4.95±0.0 5	3.81±0.6 9	4.63±0. 85
4	1-Penten-3-ol	616-25-1	2.61	751.73	685	10.29±0.54	11.91±1.77	19.9±2.57	19.03±0.6 5	16.16±0.9 4	16.15±1.6 6	17.28±1. 37	22.21±5	22.34±2. 5	20.41±5. 63	11.46±1 .71
5	Pentanal	110-62-3	2.80	757.13	701	2.13±0.15	2.44±0.34	2.92±0.41	2.77±0.33	2.42±0	2.87±0.15	3.45±0.5	4.52±1.4 3	5.82±0.6 8	6.03±1.1 4	5.41±1. 58
6	Dimethylphosphinic fluoride	753-70-8	2.86	758.87	-	2.69±0.14	3.85±0.04	2.05±0.5	2.27±0.3	2.02±0.09	2.13±0.13	2.39±0.5 9	2.24±0.6 1	2.56±0.0 9	2.53±0.2 9	1.37±0. 31
7	Benzoyl bromide	618-32-6	3.44	775.08	-	5.99±0.22	5.56±0.53	7.72±0.56	7.48±0.49	6.24±0.19	6.56±1.08	7.41±0.3 6	8.26±0.3	6.79±0.0 9	7.67±1.2 7	6.91±0. 99
8	1-Butanol, 3-methyl-	123-51-3	4.04	791.88	730	1.94±0.09	2.19±0.34	6.79±0.98	6.69±0.62	5.87±0.11	5.81±0.44	7.19±0.4 7	8.73±2.3 8	9.74±0.8 2	8.96±1.9	8.95±1. 92
9	1-Butanol, 2-methyl-	137-32-6	3.80	785.36	762	2.21±0.06	2.12±0.36	0.1±0.02	0.12±0.02	0.11±0.01	0.13±0.03	0.15±0.0 4	0.27±0.0 9	0.28±0.0 6	0.42±0.0 7	0.16±0. 07
10	Toluene	108-88-3	4.11	793.91	773	1.71±0.51	1.59±0.45	1.89±0.28	2.39±0.33	2.07±0.08	1.77±0.56	1.69±0.2 8	1.93±0.5 6	2.13±0.3	2.05±0.0 9	1.4±0.4
11	1-Pentanol	71-41-0	4.15	795.14	779	7.81±0.27	8.22±0.88	6.82±0.97	6.73±0.57	5.89±0.12	5.84±0.44	7.21±0.4 5	8.73±2.4 1	9.77±0.8 3	8.98±1.8 8	8.98±1. 92
12	Cyclobutanemethanol	4415-82- 1	4.24	797.56	-	3.58±0.43	4.7±0.45	11.3±1.04	11.45±0.4 4	9.18±0.89	9.42±0.87	10.66±0. 25	12.57±2. 43	11.97±1. 34	11.37±3. 15	6.71±0. 85
13	Furan, 2-methoxy-	25414- 22-6	4.90	816.20	-	3.23±0.07	3.41±0.13	5.16±0.87	4.31±0.41	3.48±0.15	3.32±0.43	4.14±0.4 4	3.69±0.8 4	3.74±0.1 1	3.39±0.7 1	10.76±1 .3
14	Hexanal	66-25-1	4.92	816.87	800	11.55±0.66	15.64±1.19	9.83±1.11	9.18±1.05	6.65±0.27	8.17±0.47	9.03±1.2 2	12.22±3. 43	14.98±2. 34	15.77±3. 22	10.71±2 .47
15	Cyclopentane, (2-methylpropyl)-	3788-32- 7	6.44	859.61	-	1.51±0.14	3.5±0.42	0.78±0.06	0.84±0.09	0.67±0.05	0.71±0.03	0.91±0.1 1	1.15±0.2 8	1.16±0.1 8	1.43±0.3 2	0.87±0. 2
16	3-Hexen-1-ol, (E)-	928-97-2	6.54	862.43	844	82.86±2.69	76.57±6.53	12.06±1.1 6	10.52±0.4 1	8.91±0.96	6.5±0.54	6.86±0.3	9.03±1.7 5	8.49±1.1 7	7.73±2.1 4	6.68±0. 72
17	1-Hexanol	111-27-3	6.96	874.16	879	58.49±0.86	62.18±5.67	10.83±1.5 8	8.78±0.51	7.32±0.52	6.39±0.53	7.75±0.5 4	8.53±1.7 7	8.35±0.9 5	7.07±1.9 1	5.43±0. 63
18	1,3-Cyclohexadiene, 5-ethyl-	40085- 08-3	7.22	881.60	-	3.05±0.2	3.94±0.17	0.81±0.15	1.24±0.16	1.43±0.16	1.31±0.13	1.72±0.5 1	1.01±0.2 9	0.94±0.0 3	0.91±0.1	0.62±0. 16
19	Styrene	100-42-5	7.55	890.82	890	5.43±2.76	4.14±2.41	2.51±0.28	1.91±0.23	1.89±0.14	3.61±3.77	1.99±0.4 4	2.37±0.6 7	3.03±0.8 7	1.88±0.2 6	0.78±0. 09
20	2-Heptanone	110-43-0	7.61	892.58	895	2.92±0.19	3.49±0.18	2.5±0.43	2.27±0.2	1.9±0.07	1.99±0.18	2.22±0.3 7	2.36±0.6	2.4±0.16	2.06±0.4 3	1.63±0. 3
21	Heptanal	111-71-7	7.93	901.59	901	8.89±0.6	11.21±0.6	14.78±1.6 8	16.24±1.4 2	12.23±0.6 6	12.87±0.5 1	15.29±1. 57	18.77±4. 74	21.58±2. 74	20.37±4. 88	11.93±1 .86
22	Oxime-, methoxy-phenyl-_	1000222 -86-6	8.33	912.72	-	13.9±3.01	16.6±7.87	24.44±2.7 2	24.42±0.4 3	23.56±2.6 4	23.39±5.4 8	24.16±0. 42	26.79±3. 56	24.02±1. 4	25.16±3. 17	23.05±4 .16
23	Benzene, 1-methoxy-4-methyl-	104-93-8	9.00	931.78	-	1.97±0.02	2.4±0.02	1.66±0.23	1.64±0.08	1.52±0.15	1.31±0.14	1.54±0.1 4	1.16±0.2 2	0.93±0.0 2	0.65±0.2	1.01±0. 05

24	(S)-(+)-5-Methyl-1-heptanol	57803-73-3	9.70	951.30	-	1.53±0.26	1.84±0.25	3.15±0.5	3.43±0.07	3.05±0.07	3.98±0.54	6.09±1.5 3	5.67±2.0 2	5.73±0.6 7	8.27±1.0 7	9.77±2. 84
25	Benzaldehyde	100-52-7	9.78	953.53	961	281.81±9.76	260.89±16. 5	75.25±4.1	74.12±5.2 7	71.24±7.0 6	57.18±2.2 3	57.7±2.3 6	58.29±6. 59	44.57±4. 05	45.57±1 0.89	33.69±3 .35
26	1-Heptanol	111-70-6	10.18	964.81	969	37.22±2.89	38.22±2.66	4.76±0.57	3.39±0.15	2.67±0.18	2.38±0.12	2.68±0.2 4	3.05±0.5 1	2.78±0.3 5	2.49±0.6 1	2.33±0. 23
27	1-Octen-3-ol	3391-86-4	10.47	973.04	976	26±1.07	31.58±1.28	22.42±2.8	23.13±1.6 9	25.01±0.3 4	20.7±1.24	32.44±5. 37	33.57±1 2.36	29.34±0. 69	30.53±5. 83	36.04±7 .08
28	Azetidine, 3-methyl-3-phenyl-	5961-33-1	10.50	973.84	-	1.66±0.74	1.32±0.64	0.52±0.06	0.55±0.13	0.73±0.23	0.4±0.06	0.42±0.0 6	0.68±0.1 2	0.57±0.1 8	0.37±0.0 5	0.21±0. 03
29	Pentanoic acid, 2-methyl-, anhydride	63169-61-9	10.65	978.02	-	9.42±0.3	12.74±0.53	22.47±1.9 1	23.19±2.8 3	20.17±1.7 4	21.45±0.6 8	28.05±1. 94	30.97±8. 85	27.37±0. 27	25.86±2. 96	25.41±3 .4
30	Vinyl butyrate	123-20-6	10.71	979.96	-	5.52±0.43	5.13±0.2	3.13±0.28	2.93±0.22	2.72±0.05	2.55±0.07	2.96±0.1 6	3.73±1.0 3	3.36±0.2 3	3.1±0.57	2.9±0.4 1
31	5-Hepten-2-one, 6-methyl-	110-93-0	10.72	980.07	988	10.27±0.85	10.15±0.97	7.83±0.95	7.39±0.41	6.77±0.07	6.1±0.23	7.55±0.7 3	9.26±2.4 8	8.34±0.8 1	7.52±1.5 4	6.72±0. 97
32	Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-, (1S)-	18172-67-3	10.84	983.57	-	98.17±2.78	97.27±7.4	15.2±1.46	16.75±1.0 6	14.17±0.3	11.21±1.1 8	11±0.23	12.8±1.6 2	11.89±1. 78	9.98±1.7 6	9.04±0. 78
33	Hexanoic acid, ethyl ester	123-66-0	11.14	991.94	996	9.73±0.6	12.1±0.65	2.49±0.3	2.91±0.22	2.03±0.21	1.74±0.24	2.4±0.38	3.54±0.9 6	3.22±0.4 4	2.61±0.4 4	2.42±0. 12
34	cis-2-(2-Pentenyl)furan	70424-13-4	11.16	992.42	-	0.99±0.14	1.39±0.08	1.61±0.2	1.69±0.14	1.61±0.05	1.53±0.12	1.57±0.1 8	1.52±0.2 6	1.37±0.1 5	1.17±0.2 5	0.68±0. 08
35	Octanal	124-13-0	11.21	993.81	1001	1.46±0.27	1.81±0.58	1.88±0.05	1.93±0.2	1.53±0.05	1.56±0.22	1.64±0.5 5	1.87±0.3 1	1.7±0.54	1.83±0.8 7	1.11±0. 15
36	4-Hexen-1-ol, (4E)-, acetate	1000352-71-9	11.43	999.99	-	169.89±7.35	23.54±1.88	3±0.25	3.53±0.36	3.14±0.06	3.59±0.32	3.97±0.3 4	4.76±0.6 6	4.03±0.7 2	4.83±0.8 8	2.03±0. 58
37	Furan, 2-propyl-	4229-91-8	11.44	1000.31	-	11.69±0.63	20.32±2.67	33.53±1.1 6	42.63±6.6 7	39.85±2.8 9	45.48±4.7 7	52.16±4. 34	61.44±9. 14	52.1±8.9 4	64.24±1 1.61	28.44±5 .66
38	Acetic acid, hexyl ester	142-92-7	11.55	1003.56	1008	0.74±0.03	0.12±0.02	0.05±0.02	0.05±0.01	0.04±0	0.04±0.02	0.05±0.0 3	0.03±0.0 1	0.08±0.0 1	0.09±0.0 3	0.04±0. 01
39	Ethanone, 1-(3-hydroxyphenyl)-	121-71-1	11.61	1005.14	-	3.52±0.11	3.75±0.27	0.78±0.17	0.76±0.03	0.58±0	0.65±0.11	0.63±0.0 2	0.55±0.1	0.47±0.0 5	0.37±0.0 6	0.52±0. 02
40	2-Hexen-1-ol, acetate, (E)-	2497-18-9	11.29	996.03	1007	1.79±0.12	0.16±0.02	1.13±0.03	1.14±0.1	0.88±0.03	0.91±0.11	1.05±0.1 3	1.14±0.1 8	1.1±0.39	1.09±0.4 9	0.7±0.1
41	o-Cymene	527-84-4	11.87	1012.39	1020	3.09±0.1	3.28±0.22	1.37±0.24	1.22±0.08	0.94±0.05	0.84±0.09	0.82±0.1 3	0.79±0.1 4	0.8±0.12	0.69±0.0 3	0.84±0. 15
42	D-Limonene	5989-27-5	11.99	1015.85	1029	14.11±0.34	16.01±0.62	3.92±0.8	4.43±0.32	3.99±1.03	3.65±1.76	3.87±2.2 8	3.46±0.9 1	4.29±1.9 7	3.54±1.1 1	4.89±1. 24
43	1-Hexanol, 2-ethyl-	104-76-7	12.05	1017.57	1028	21.99±2.3	20.56±2.19	5.84±0.91	7.64±0.33	6.55±0.77	6±0.47	8.51±2.0 4	8.18±2.0 3	8.14±0.1 3	7±1.22	8.85±1. 08
44	Cyclohexanone, 2,2,6-trimethyl-	2408-37-9	12.13	1019.82	1023	93.33±74.88	6.33±0.4	6.44±1.11	6.55±0.62	6±0.12	5.98±0.5	6.89±0.8 4	7.37±2.0 5	7.31±0.5 7	6.74±1.5 8	4.72±0. 9
45	Benzyl alcohol	100-51-6	12.24	1022.79	1033	80.03±1.71	78.75±7.42	23.3±1.54	15.61±12. 6	20.83±3	17.48±0.9 7	21.23±2. 74	21.23±0. 03	15.92±0. 18	16.45±3. 86	15.17±1 .37
46	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	7785-70-8	12.34	1025.82	-	23.5±1.48	24.22±1.47	2.66±0.26	3.04±0.17	2.5±0.07	2.14±0.25	2.07±0.1 2	1.84±0.1 6	1.5±0.09	1.48±0.3 7	1.62±0. 22
47	3-Octen-2-one	1669-44-9	12.37	1026.58	1037	5.64±0.23	6.49±0.46	2.51±0.16	2.62±0.12	2.13±0.23	2.27±0.06	2.5±0.21	2.94±0.5 1	2.38±0.3 6	2.23±0.5 3	1.64±0. 1
48	Benzeneacetaldehyde	122-78-1	12.48	1029.57	1043	5.66±0.96	11.06±0.93	16.05±2.4 4	20.33±1.8 8	20.42±0.0 9	18.79±1.3 1	18.83±3. 48	14.2±0.7	13.4±0.4 8	15±3.59	13.73±2 .86
49	3-Carene	13466-78-9	12.66	1034.73	1018	15.1±0.52	14.63±0.68	2.97±0.24	2.86±0.16	2.42±0.01	1.98±0.11	1.74±0.0 6	1.6±0.15	1.39±0.1 1	1.34±0.3 3	2.99±0. 13

50	Isophorone	78-59-1	12.97	1043.59	1124	12.63±0.41	10.36±1.67	9.04±1.03	9.28±0.41	8.38±0.15	8.25±0.59	9.19±0.8 8	10.17±1. 96	9.82±1.5 2	9.65±2.2 9	7.09±1. 12
51	Acetophenone	98-86-2	13.19	1049.54	1065	5.03±0.44	4.75±0.5	2.54±1.14	2.86±1.11	2.35±1.23	1.34±0.16	1.43±0.1 6	1.51±0.5 2	1.33±0.5 4	1.96±0.4 7	1.13±0. 48
52	Ethanone, 1-(1-cyclohexen-1-yl)-	932-66-1	13.38	1054.98	-	51.65±1.6	57.36±2.81	22.8±0.56	26.44±2.5 8	24.46±3.5 2	23.81±0.7 7	26.34±1. 91	27.94±3. 02	22.92±3. 16	22.17±4. 92	12.14±0 .55
53	Formic acid, octyl ester	112-32-3	13.42	1056.03	1117	33.89±0.76	39.39±0.56	14.29±1.1 5	15.38±0.7	13.28±1.0 4	12.29±0.5 7	14.01±0. 67	12.67±1. 78	11.48±0. 81	10.42±2. 66	9.93±0. 83
54	Ethanone, 1-(4-methylphenyl)-	122-00-9	13.65	1062.59	1183	0.71±0.29	0.77±0.17	0.36±0.07	0.42±0.03	0.38±0	0.33±0.04	0.35±0.0 1	0.26±0.0 2	0.26±0.0 1	0.22±0.0 7	0.25±0. 03
55	Benzene, 4-ethenyl-1,2-dimethyl-	27831- 13-6	13.93	1070.36	-	1.91±0.07	2.24±0.3	1.88±0.22	1.77±0.07	1.49±0.11	1.29±0.1	1.22±0.1 2	0.91±0.0 8	0.81±0.0 2	0.66±0.2 4	0.87±0. 04
56	Ethyl 2-(5-methyl-5-vinyltetrahydrofuran-2-yl)propan-2-yl carbonate	1000373 -80-3	13.91	1070.07	-	84.51±1.74	96.87±4.38	12.5±0.81	14.26±0.5 7	11.8±1.43	8.31±0.41	8.57±0.2 9	8.34±1.1 2	8±1.05	7.14±2.0 4	6.97±0. 33
57	Benzoic acid, hydrazide	613-94-5	14.06	1074.03	-	3.17±2.08	3.23±2.11	1.1±0.14	1.14±0.13	1.09±0.18	1.06±0.09	1.05±0.0 8	1.06±0.0 7	0.7±0.04	0.67±0.2 1	0.34±0. 03
58	Linalool	78-70-6	14.51	1086.86		336.99±135. 22	433.58±15. 04	12.23±1.0 8	11.97±0.8 5	9.65±0.99	10.04±0.5 3	11.13±0. 88	12.71±1. 31	11.5±1.3 5	11.86±3. 08	7.41±0. 76
59	1,5,7-Octatrien-3-ol, 3,7-dimethyl-	29957- 43-5	14.46	1085.51	1100	17.94±3.18	23.48±0.5	31.08±2.0 6	34.83±0.9 2	27.94±3.7 2	25.54±1.8 2	27.67±0. 99	24.31±2. 78	20.87±1. 35	18.9±5.1 9	29.64±1 .4
60	Phenylethyl Alcohol	##### #	14.68	1091.56	1116	74.47±1.22	72.62±5.08	22.14±1.9 1	23.8±2.12	21.93±2.9	18.24±1.1 9	20.62±2. 42	19.26±0. 39	15.31±0. 22	14.87±3. 48	15.41±1 .58
61	(E)-4,8-Dimethylnona-1,3,7-triene	19945- 61-0	14.77	1094.02	1116.5	14.39±1.08	167.01±4.7 5	4.62±0.52	4.82±0.32	4.18±0.31	3.3±0.22	3.23±0.3 6	3.3±0.78	2.9±0.25	2.15±0.3 1	1.95±0. 08
62	1,3,8-p-Menthatriene	18368- 95-1	14.93	1098.73	1118.7	1.76±0.11	1.73±0.02	0.35±0.05	0.4±0.03	0.34±0.04	0.28±0.03	0.27±0.0 2	0.16±0.0 8	0.14±0.0 1	0.15±0.0 5	0.25±0. 01
63	2,4,6-Octatriene, 2,6-dimethyl-	673-84-7	15.14	1104.44	1113	2.58±0.35	39.76±32.0 4	0.48±0.05	0.47±0.03	0.36±0	0.31±0.02	0.28±0.0 1	0.27±0.0 2	0.24±0.0 2	0.23±0.0 5	0.24±0. 02
64	2,6-Dimethyl-1,3,5,7-octatetraene, E,E-	460-01-5	15.18	1105.76	1130	4.94±0.17	5.23±0.15	1.2±0.1	1.24±0.06	1.2±0.07	0.88±0.06	0.84±0.0 5	0.63±0.0 5	0.48±0.0 1	0.44±0.1 1	0.78±0. 02
65	n-Pentadecanol	629-76-5	15.24	1107.37	-	3.66±0.21	3.96±0.6	0.58±0.03	0.46±0.05	0.39±0.04	0.36±0.05	0.28±0.0 2	0.35±0.0 9	0.26±0.0 6	0.22±0.0 4	0.19±0. 02
66	Benzyl nitrile	140-29-4	15.44	1112.98	1143	7.65±0.2	14.87±0.06	4.76±0.51	4.64±0.45	3.64±0.53	3.3±0.26	3.28±0.3 2	2.74±0.0 1	2.16±0.0 7	2.15±0.5 8	3.57±0. 15
67	trans-3-Nonen-2-one	18402- 83-0	15.48	1114.06	-	1.42±0.04	1.47±0.02	0.77±0.06	0.96±0.07	0.87±0.11	0.85±0.05	0.85±0.0 3	0.77±0.0 9	0.58±0.0 5	0.56±0.1 5	0.38±0. 02
68	2,4,6-Octatriene, 2,6-dimethyl-, (E,Z)-	7216-56- 0	15.53	1115.45	1131	2.31±0.06	2.38±0.13	0.54±0.06	0.42±0.05	0.45±0.1	0.23±0.02	0.2±0.01	0.17±0	0.15±0.0 2	0.16±0.0 4	0.24±0. 03
69	(R,S)-5-Ethyl-6-methyl-3E-hepten-2-one	57283- 79-1	15.68	1119.87	1143.9	5.01±0.25	7.41±0.29	2.98±0.27	3.18±0.09	2.55±0.02	2.74±0.1	2.89±0.2 1	3.02±0.4 4	2.51±0.2 8	2.19±0.4 7	1.65±0. 15
70	1,12-Dodecanediol	5675-51- 4	16.28	1136.75	-	4.25±0.22	5.3±0.2	4.15±0.19	5.8±0.35	4.66±0.69	3.73±0.27	4.24±0.4 5	3.4±0.06	2.94±0.1 7	2.65±0.7 6	2.76±0. 2
71	Undecane, 3-methyl-	1002-43- 3	16.38	1139.47	1171	5.7±0.68	6.11±0.72	1.51±0.07	1.79±0.1	2.19±0.32	1.28±0.1	1.51±0.1 1	1.82±0.3 3	1.59±0.1 6	0.95±0.1 1	0.9±0.0 4
72	Benzoic acid, ethyl ester	93-89-0	16.40	1140.04	1170	2.38±0.11	2.21±0.08	0.73±0.01	0.75±0.04	3.24±2.52	1.12±0.76	0.67±0.1 2	0.43±0.1	0.46±0.0 2	0.41±0.1 9	0.36±0. 1
73	Benzaldehyde, 2,5-dimethyl-	5779-94- 2	16.50	1142.79	1208	1.49±0.07	1.72±0.1	1.63±0.22	1.97±0.18	1.85±0.15	1.96±0.27	1.9±0.14	1.4±0.02	1.13±0.0 7	1.2±0.33	0.82±0. 05
74	1-Nonanol	143-08-8	16.52	1143.40	1186	76.33±2.16	77.87±0.59	1.32±0.09	1.52±0.03	1.25±0.16	0.98±0.08	1.11±0.1 5	1.01±0.0 5	0.91±0.0 7	0.62±0.2 2	0.85±0. 05
75	Naphthalene	91-20-3	16.70	1148.61	1191	1.24±0.1	1.12±0.06	0.43±0.02	0.45±0.05	0.44±0.07	0.38±0.01	0.4±0.01	0.37±0.0 3	0.33±0.0 2	0.25±0.1 2	0.26±0. 06

76	Butanoic acid, 3-hexenyl ester, (Z)-	16491-36-4	16.97	1156.15	1186	84.47±2.52	20.34±1.5	1.64±0.25	1.92±0.08	2.02±0.51	1.72±0.54	1.8±0.51	0.97±0.1 8	0.76±0.1 1	0.56±0.1 2	0.83±0.1 17
77	Butanoic acid, 2-hexenyl ester, (Z)-	56922-77-1	17.17	1161.67	-	4.58±0.24	1.96±0.38	2.64±0.2	2.67±0.11	1.94±0.2	1.01±0.02	0.82±0.0 8	4.97±3.8 6	0.77±0.1 1	4.95±0.1 8	4±0.26
78	Methyl salicylate	119-36-8	17.11	1160.06	1187	527.58±28.9 5	559.07±11.97	58.23±11.65	52.28±5.8 4	52.72±9.0 6	32.03±1.7 4	28.02±0.97	23.29±1.53	19.17±2.18	18.15±4.48	16.54±0.34
79	Dodecane	112-40-3	17.25	1164.04	-	43.57±7.2	41.7±7.82	13.3±0.73	15.81±1.0 7	16.36±3.6 3	11.64±0.7 6	12.45±1.46	16.66±3.25	13.44±0.76	7.42±0.3 5	6.25±0.32
80	1,3-Cyclohexadiene-1-carboxaldehyde, 2,6,6-trimethyl-	116-26-7	17.24	1163.71	1197	185.13±9.03	195.97±5.6 3	4.16±0.9	4.12±0.1	3.04±0.51	3.5±0.87	3.61±0.1 8	2.52±0.1 7	1.69±0.0 3	1.62±0.4 8	1.93±0.05
81	Decanal	112-31-2	17.44	1169.34	1195	5.2±0.06	10.44±0.29	1.5±0.05	1.67±0.16	1.36±0.18	1.43±0.05	1.66±0.1 3	1.56±0.2 3	1.39±0.1 2	1.47±0.4 2	1.31±0.14
82	Formamide, N-phenyl-	103-70-8	17.65	1175.34	-	185.11±9.03	195.91±5.6	1.12±0.18	1.15±0.07	0.97±0.09	0.49±0.06	0.48±0.0 1	0.38±0.0 1	0.33±0.0 3	0.36±0.0 7	0.35±0.04
83	1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl-	432-25-7	17.86	1181.05	1214	16.71±0.52	17.85±0.56	16.57±1.3 8	17.98±0.8 5	15.17±1.0 7	15.61±0.8 2	16.72±0.77	16.7±2.4 1	14.99±1.59	14.01±3.37	10.07±0.76
84	2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)-	106-25-2	18.72	1205.35	1229	43.68±1.29	47.43±1.36	90.85±5.9 5	110.29±1.026	109.11±1.227	91.17±6.5 9	86.86±5.09	79.46±1.32	65.94±7.22	68.21±1.845	61.51±3.29
85	n-Valeric acid cis-3-hexenyl ester	35852-46-1	18.20	1190.62	1235	53.82±2.03	15.14±0.85	11.3±0.63	12.6±0.55	12.28±1.2 8	7.58±0.03	6.9±0.48	6.89±1.2 7	5.9±0.64	4.51±0.9 7	4.02±0.11
86	Valeric anhydride	2082-59-9	18.31	1193.72	-	5.54±0.22	3.24±0.16	1.39±0.16	1.63±0.1	1.38±0.13	1.06±0.05	1.05±0.0 6	1.27±0.1 7	1.12±0.1 6	0.87±0.3	0.65±0.02
87	trans-2-Hexenyl isovalerate	68698-59-9	18.37	1195.46	1244.9	3.54±0.19	2.3±0.06	1.75±0.11	2.52±0.12	1.99±0.22	1.15±0.02	1.15±0.0 4	1.13±0.1 7	0.92±0.1 1	0.73±0.1 7	0.51±0.34
88	3H-Indazol-3-one, 1,2-dihydro-1-methyl-	1006-19-5	18.38	1195.77	-	1.15±0.04	0.94±0.04	0.12±0.02	0.1±0.01	0.1±0.01	0.49±0.36	0.28±0.3 6	0.08±0.0 1	0.38±0.3 1	0.32±0.2 5	0.1±0.05
89	1-Tetradecanol	112-72-1	18.55	1200.54	-	9.64±0.33	75.29±112.03	6.51±9.54	9.16±13.8 6	10.63±9.3	13.25±10.72	6.87±10.12	1.18±0.2 2	1±0.06	13.7±3.7 1	8.55±6.89
90	Geraniol	106-24-1	18.93	1211.18	1257	552.91±26.6 3	692.45±167.79	91.11±5.9 4	110.32±1.025	109.27±1.211	91.12±6.6 1	86.96±4.99	79.6±1	66.08±7.21	44.74±4.192	61.56±3.34
91	Benzoic acid, 2-hydroxy-, ethyl ester	118-61-6	19.28	1221.29	1267	14.51±2.06	28.76±2.9	0.76±0.66	0.48±0.38	0.59±0.07	0.22±0.33	0.17±0.2 4	0.2±0.17	0.27±0.0 2	0.29±0.0 4	0.26±0.01
92	Citral	5392-40-5	19.14	1217.33	1237	31.44±0.81	316.26±493.88	5.65±0.49	6.35±0.6	63.2±58.1 8	35.22±53.06	61.29±4.924	41.44±3.726	3.46±0.2 3	3.72±0.9	61.57±3.29
93	1-Decanol	112-30-1	19.42	1225.05	1272	10.2±0.23	9.1±0.64	0.91±0.45	1.19±0.12	1.08±0.06	0.83±0.23	0.64±0.2 1	0.64±0.0 8	0.59±0.1 2	0.52±0.2 3	1.02±0.99
94	2-Aminosuccinonitrile	5615-94-1	19.85	1237.21	-	6.87±1.03	6.07±1.12	0.81±0.25	1.09±0.03	0.94±0.38	0.85±0.01	0.78±0.0 8	0.56±0.2 2	0.24±0.0 3	0.19±0.0 8	0.26±0.11
95	n-Tridecan-1-ol	112-70-9	19.85	1237.24	-	5.36±1.09	5.29±2.63	1.02±0.16	1.15±0.07	1.22±0.31	0.87±0.03	0.9±0.07	0.66±0.3 2	0.25±0	0.19±0.0 3	0.28±0.25
96	2-Undecanone	112-12-9	19.90	1238.71	1291	8.55±0.67	6.78±0.16	2.28±0.17	2.11±0.18	1.5±0.18	1.52±0.63	1.51±0.4 1	1.19±0.4 6	0.68±0.0 3	0.56±0.1 3	0.51±0.3
97	Indole	120-72-9	19.88	1238.04	1294	60.61±7.05	43.52±1.49	24.51±2.3 6	20.67±2.5 1	18.46±2.2 8	18.04±1.2 5	15.49±1.36	14.52±0.62	11.97±0.5	12.33±2.72	11.98±1.36
98	Tridecane	629-50-5	20.06	1243.01	-	50.24±2.14	40.65±0.67	8.84±0.26	10.77±0.9 2	9.09±2.06	7.11±0.12	6.81±0.7 8	11.8±2.7 1	8.32±1.4 5	4.82±1.2 3	4.18±1.69
99	Nonane, 5-butyl-	17312-63-9	20.20	1246.98	-	5.01±0.17	4.25±0.11	1±0.06	1.15±0.07	1.13±0.2	0.78±0.03	0.8±0.14	0.54±0.0 3	0.66±0.1 3	0.34±0.1 7	0.48±0.13
100	Naphthalene, 2-methyl-	91-57-6	20.31	1250.08	1315	4.36±0.27	3.86±0.21	0.99±0.14	1.26±0.14	1.16±0.2	0.99±0.07	1.02±0.1 1	1.06±0.1	0.67±0.2 4	0.71±0.1 8	0.75±0.09
101	trans-Geranic acid methyl ester	1189-09-9	20.72	1261.57	1321	13.84±0.53	7.93±0.16	1.4±0.09	1.41±0.11	1.36±0.22	0.94±0.06	0.79±0.0 3	0.78±0.0 7	0.57±0.0 7	0.48±0.1 3	0.5±0.05

102	(E)-Hex-3-enyl (E)-2-methylbut-2-enoate	1000373-74-1	20.73	1262.03	-	10.73±0.3	4.98±0.02	1.46±0.17	1.81±0.13	1.88±0.27	1.03±0.19	0.99±0.1 1	0.95±0.2 2	0.66±0.0 9	0.64±0.1 8	0.55±0. 25
103	1,2-Ethanediol, monobenzoate	94-33-7	20.80	1264.09	-	1.46±0.1	1.35±0.71	2.46±0.22	2.52±0.17	2.33±0.57	1.88±0.11	2.17±0.4 4	1.77±0.1 9	1.11±0.0 9	0.91±0.1 8	1.19±0. 28
104	Dodecane, 1,1'-oxybis-	4542-57-8	21.02	1270.02	-	10.37±1.78	9.78±1.29	2.32±0.16	2.34±0.26	2.69±0.42	1.98±0.19	1.94±0.3	2.53±0.6 5	1.87±0.0 2	1±0.28	2.15±1. 76
105	Nonadecane, 9-methyl-	13287-24-6	21.11	1272.74	-	13.46±0.52	11.49±0.79	2.61±0.16	2.77±0.2	2.97±0.5	1.94±0.23	2.17±0.2 3	2.52±0.5 3	1.83±0.1	1.1±0.31	1.33±0. 23
106	Benzoic acid, 2-methoxy-, methyl ester	606-45-1	21.15	1273.72	1295	1.92±0.12	0.81±0.06	0.45±0.06	0.47±0.06	0.52±0.06	0.45±0.05	0.39±0.0 5	0.17±0.1 6	0.25±0	0.14±0.1 3	0.17±0. 14
107	Heptylcyclohexane	5617-41-4	21.17	1274.44	-	7.49±0.65	6.97±0.43	1.87±0.12	2.04±0.11	2.02±0.38	1.49±0.02	1.69±0.1 7	1.91±0.2 9	1.41±0.1 5	0.88±0.2 3	0.98±0. 12
108	Butane, 2,2-dimethyl-	75-83-2	21.31	1278.30	-	0.98±0.17	0.8±0.31	0.18±0.01	0.25±0.08	0.2±0.05	0.16±0.06	0.18±0.0 4	0.24±0.0 8	0.15±0.0 3	0.07±0.0 2	0.17±0. 09
109	(1S,4S,4aS)-1-Isopropyl-4,7-dimethyl-1,2,3,4,4a,5-hexahydronaphthalene	267665-20-3	21.42	1281.52	-	8.53±0.35	8.14±0.36	5.3±0.51	6.04±0.45	5.37±0.49	5.32±0.77	4.79±0.3 4	4.1±0.07	3.05±0.0 8	2.84±0.8 1	2.88±0. 13
110	Tridecane, 5-methyl-	25117-31-1	21.48	1283.18	1355	5.64±0.95	5.41±0.16	1.23±0.06	1.41±0.08	1.48±0.28	0.97±0.1	1.15±0.1 2	1.33±0.2 2	0.92±0.1	0.61±0.2	0.9±0.2 4
111	1-Aminocyclopentanecarboxylic acid, N-methoxycarbonyl-, undecyl ester	1000328-90-6	21.49	1283.50	-	0.76±0.15	0.52±0.13	0.69±0.08	0.58±0.06	0.4±0.05	0.4±0.11	0.33±0.0 3	0.28±0	0.23±0.0 1	0.2±0.05	0.44±0. 02
112	Tetradecane, 4-methyl-	25117-24-2	21.93	1295.65	-	12.9±0.6	11.41±0.45	2.44±0.13	2.64±0.18	2.68±0.58	1.83±0.07	2.11±0.2 1	2.24±0.3 6	1.66±0.1 5	0.93±0.2 5	1.18±0. 19
113	2-Octenal, 2-butyl-	13019-16-4	22.03	1298.73	1372	6.83±0.47	6.7±0.41	0.51±0.03	0.42±0.03	0.29±0	0.32±0.02	0.23±0.0 1	0.31±0.0 3	0.19±0.0 2	0.15±0.0 5	0.2±0.0 2
114	.alfa.-Copaene	1000360-33-0	22.12	1301.20	1381	2.42±0.14	2.32±0.1	1.14±0.05	1.25±0.07	1.19±0.2	1.05±0.11	1.15±0.1	1.25±0.1 7	1.01±0.1 2	0.64±0.1 8	0.7±0.0 4
115	Hexanoic acid, 3-hexenyl ester, (Z)-	31501-11-8	22.30	1306.10	1381	187.51±5.19	45.37±1.68	57.92±1.6 3	62.51±3.5 8	53.99±8.2 8	42.79±2.5 4	25.44±2 0	2.16±0.1 1	1.64±0.1 7	1.29±0.3 4	1.13±0. 01
116	cis-3-Hexenyl cis-3-hexenoate	61444-38-0	22.39	1308.80	1388.8	45.04±2.9	16.49±0.92	6.44±0.26	6.02±0.47	4.34±0.79	3.32±0.27	2.26±0.4 5	2.04±0.1 3	1.55±0.0 6	1.26±0.4 4	1.19±0. 1
117	5-Isoxazolecarboxylic acid, 4,5-dihydro-3,5-dimethyl-, methyl ester, (R)-	64018-41-3	22.71	1317.63	-	6.79±0.35	8.1±2.66	1.12±0.19	2.84±3.09	3.85±2.34	4.57±3.06	2.86±3.0 4	1.09±0.2 6	0.91±0.0 9	0.46±0.0 8	0.56±0. 06
118	Tetradecane	629-59-4	22.74	1318.68	-	65.88±2.95	66.28±3.66	15.87±0.7 5	15.64±0.8 8	15.7±3.9	13.6±0.77	14.64±1. 65	8.38±4.5 8	11.69±1. 11	1.08±0.3 2	4.13±3. 83
119	2-Cyclopenten-1-one, 3-methyl-2-(2-pentenyl)-, (Z)-	488-10-8	22.72	1318.01	1378	14.98±0.69	12.41±0.1	4.95±0.5	6.33±0.85	5.32±0.5	4.52±0.39	4.28±0.4 3	3.51±0.0 9	2.97±0.2 2	3.03±0.8 1	2.79±0. 32
120	1H-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)]-	469-61-4	23.08	1328.20	1386	11.71±1.1	9.99±0.15	3.78±0.42	4.06±0.21	4.43±0.79	3.76±0.25	3.99±0.5 8	4.02±0.5 1	2.94±0.3 3	2.35±0.9	3.56±0. 39
121	Naphthalene, 1,2-dimethyl-	573-98-8	23.18	1331.09	-	1.89±0.24	1.68±0.06	0.66±0.05	0.63±0.12	0.72±0.18	0.61±0.06	0.63±0.0 6	0.43±0.0 6	0.37±0.0 3	0.35±0.0 4	0.33±0. 01
122	D-Alanine, N-(4-butylbenzoyl)-, isohexyl ester	1000354-10-0	23.29	1334.20	-	4.58±0.2	4.16±0.1	1.77±0.12	1.89±0.14	1.97±0.43	1.64±0.12	1.89±0.0 5	1.69±0.1 8	1.28±0.1 2	1±0.34	1.42±0. 08
123	.alpha.-Ionone	127-41-3	23.45	1338.56	1421	13.27±0.45	13.06±0.3	10.37±0.5 9	13.03±1.4 4	10.96±1.1 5	10.88±0.8 1	11.14±0. 67	9.77±0.2 2	8.1±0.84	7.79±2.0 8	4.83±0. 29
124	1,2-Benzenediol, O-(4-butylbenzoyl)-O'-(isobutoxycarbonyl)-	1000329-73-6	24.03	1354.79	-	1±0.08	0.92±0.08	0.42±0.02	0.5±0.04	0.43±0.05	0.41±0.08	0.39±0.0 2	0.28±0.0 2	0.22±0.0 2	0.22±0.0 5	0.21±0. 01
125	5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-	3796-70-1	24.05	1355.48	1454	19.2±0.54	17.74±0.83	9.99±0.53	11.97±1.1 1	10.65±1.3 4	10.3±0.94	10.25±0. 65	8.19±0.2 9	6.66±0.6 1	6.2±1.75	5.45±0. 18
126	2,6,10-Trimethyltridecane	3891-99-4	24.26	1361.33	1465.1	22.41±3.95	21.23±2.42	4.79±0.12	5.84±0.71	5.66±1.11	4.89±0.35	5.26±0.6 2	4.89±0.9 7	3.49±0.1 3	2.27±0.7 9	2.28±1. 36

127	1-Isopropyl-4,7-dimethyl-1,2,3,4,5,6-hexahydronaphthalene	16729-00-3	24.61	1371.35	1481.3	2.1±0.18	1.87±0.16	0.7±0.1	0.8±0.06	0.61±0.09	0.7±0.15	0.57±0.08	0.42±0.04	0.32±0.02	0.26±0.09	0.28±0.08
128	Acenaphthene	83-32-9	24.76	1375.55	1472	1.14±0.22	1.07±0.09	0.42±0.03	0.38±0.05	0.51±0.12	0.4±0.06	0.45±0.01	0.33±0.01	0.27±0	0.27±0.08	0.38±0.01
129	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	14901-07-6	24.93	1380.16	1488.4	123.3±4.26	136.52±4.35	127.04±8.51	148.73±15.77	126.39±10.87	125.72±7.16	124.89±7.1	114.76±2.49	99.81±8.35	102.8±2.43	64.83±5.38
130	3-Pyridinecarbonitrile, 1,4-dihydro-1-methyl-	19424-15-8	25.10	1385.00	-	0.61±0.02	0.51±0.02	0.2±0.03	0.26±0.03	0.22±0.03	0.22±0.04	0.19±0.03	0.11±0.03	0.06±0	0.05±0.01	0.05±0
131	Nonyl tetradecyl ether	1000406-37-6	25.33	1391.64	-	7.35±6.94	5.94±3.43	0.83±0.23	1.01±0.27	0.83±0.24	0.56±0.22	1.02±0.74	2.28±1.05	0.47±0.21	0.4±0.08	0.96±0.8
132	2,4-Di-tert-butylphenol	96-76-4	25.50	1396.31	1513	41.04±3.92	33.59±6.05	13.48±0.88	10.95±0.82	24.32±0.46	21.17±5.55	17.48±0.94	27.7±0.35	19.83±2.14	18.45±4.95	11.47±1.78
133	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-7-methyl-4-methylene-1-(1-methylethyl)-, (1.alpha.,4a.beta.,8a.alpha.)-	39029-41-9	25.60	1399.22	1511	4±0.2	3.5±0.01	1.81±0.18	2.45±0.24	3.38±0.42	2.1±0.23	1.98±0.15	1.63±0.01	1.23±0.08	1.04±0.4	1.14±0.07
134	1-Decanol, 2-hexyl-	2425-77-6	25.71	1402.15	-	7.01±0.26	3.9±0.49	1±0.03	1.07±0.19	1.08±0.32	0.81±0.15	0.87±0.07	0.81±0.07	0.56±0.03	0.35±0.15	0.52±0.08
135	Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)-	483-76-1	25.84	1405.95	1519	24.69±1.01	22.2±1.04	12.27±0.89	15.07±1.11	12.14±1.42	12.87±1.91	11.34±1.08	5.39±4.48	0.73±0.07	0.57±0.15	0.73±0.02
136	Cubenene	29837-12-5	26.04	1411.39	1512	3.37±0.27	3.05±0.22	1.49±0.22	1.83±0.19	1.56±0.15	1.61±0.31	1.4±0.14	1.16±0.08	0.87±0.03	0.82±0.27	0.94±0.04
137	4-Isopropyl-6-methyl-1-methylene-1,2,3,4-tetrahydronaphthalene	50277-34-4	26.29	1418.67	1555	10.26±0.77	9.06±0.58	4.39±0.58	5.22±0.46	4.45±0.58	4.43±0.86	3.87±0.61	2.79±0.2	2.12±0.07	1.9±0.6	2.27±0.13
138	n-Nonylcyclohexane	2883-2-5	26.40	1421.72	1556	13.19±0.24	9.18±0.94	2.22±0.09	2.33±0.29	2.34±0.69	1.89±0.24	1.93±0.23	1.33±0.48	1.24±0.15	0.83±0.28	1.01±0.08
139	Oxazole	288-42-6	26.40	1421.65	-	5.96±0.5	3.81±1.18	1.28±0.28	1.17±0.14	1.21±0.37	1.18±0.39	1.25±0.3	1.05±0.01	0.8±0.16	0.26±0.1	0.69±0.14
140	Hexadecane, 2-methyl-	1560-92-5	26.73	1430.93	-	21.9±2.02	15.22±1.67	4.4±0.18	4.38±0.49	4.67±0.94	3.9±0.68	4.04±0.67	3.02±0.16	2.63±0.04	1.94±0.76	1.59±0.61
141	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-	7212-44-4	26.73	1430.99	1565.6	11.72±0.67	6.12±0.36	1.75±0.18	1.77±0.17	1.82±0.23	1.47±0.19	1.35±0.21	1.09±0.08	0.92±0.06	0.75±0.2	0.63±0.04
142	Pentadecane, 3-methyl-	2882-96-4	26.86	1434.54	1571	15.91±0.58	11.53±0.58	2.65±0.09	2.74±0.31	2.9±0.84	2.23±0.32	2.53±0.33	2.06±0.05	1.47±0.13	0.99±0.36	1.21±0.19
143	3-Hexen-1-ol, benzoate, (Z)-	25152-85-6	26.90	1435.85	1568	6.3±0.56	2.16±0.07	0.98±0.15	1.1±0.15	1.24±0.2	1±0.08	0.88±0.05	0.77±0.01	0.65±0.04	0.65±0.15	0.58±0.06
144	Pentadecane, 1-methoxy-13-methyl-	56196-09-9	27.21	1444.52	-	20.93±1.31	16.21±1.24	3.39±0.12	3.68±0.46	3.38±0.99	3.15±0.56	3.47±0.64	3±0.06	2.11±0.27	1.4±0.55	1.69±0.21
145	1-Hexadecanol	36653-82-4	27.36	1448.68	-	4.26±0.54	3.38±0.47	0.74±0.11	0.7±0.08	0.61±0.24	0.67±0.25	0.63±0.08	0.57±0.08	0.4±0.07	0.41±0.16	0.39±0.1
146	Dodecanoic acid, ethyl ester	106-33-2	27.43	1450.58	1597	5.36±0.47	6.16±0.58	0.77±0.11	1.04±0.13	0.84±0.02	0.82±0.06	0.78±0.06	0.68±0.02	0.55±0.01	0.59±0.06	0.61±0.04
147	Hexadecane	544-76-3	27.55	1454.00	-	31.48±1.38	26.48±2.84	6.78±0.34	7.38±0.65	7.25±1.54	6.65±1.42	6.56±0.39	5.87±0.22	4.53±0.36	0.86±0.39	1.39±0.28
148	5,5-Diethyltridecane	1000360-41-3	27.60	1455.58	1605	7.39±0.11	4.26±0.53	0.82±0.02	1.09±0.17	0.94±0.31	0.71±0.11	0.88±0.14	1.16±0.06	0.71±0.09	0.36±0.15	0.54±0.08
149	Cedrol	77-53-2	27.68	1457.72	1605.8	4.02±0.5	3.43±1	1.54±0.05	1.63±0.14	1.93±0.58	1.63±0.29	2.13±0.18	1.6±0.1	0.93±0.01	1.01±0.37	1.38±0.23
150	Di-epi-1,10-cubenol	73365-77-2	28.27	1474.27	1614	4.03±0.23	3.36±0.11	1.74±0.25	2.02±0.23	1.73±0.19	1.69±0.25	1.41±0.22	1.12±0.04	0.93±0.02	0.88±0.23	0.89±0.05
151	1,2-Benzenediol, O-acetoxyacetyl-O'-(4-butylbenzoyl)-	1000330-49-5	28.55	1482.06	-	1.84±0.09	1.48±0.07	0.78±0.1	1.07±0.12	0.96±0.07	0.8±0.1	0.79±0.13	0.58±0.06	0.48±0.01	0.45±0.11	0.44±0.04

152	3,3-Diethyltridecane	1000360-41-2	28.70	1486.43	1653	4.54±0.1	2.54±0.4	0.47±0.06	0.65±0.1	0.59±0.2	0.45±0.08	0.57±0.1	0.65±0	0.39±0.04	0.23±0.1	0.31±0.02
153	.alpha.-Cadinol	481-34-5	28.85	1490.73	1653	1.97±0.14	1.35±0.04	0.93±0.16	1.43±0.21	1.32±0.07	1.06±0.16	1.11±0.21	0.74±0.09	0.63±0.01	0.56±0.15	0.55±0.05
154	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	3075-84-1	29.37	1505.29	1656.5	3.09±0.1	2.52±0.52	0.88±0.11	0.97±0.14	1.29±0.33	1.04±0.19	1.48±0.05	0.91±0.03	0.55±0	0.56±0.19	0.87±0.09
155	7-Methyl-octadecane	1000192-63-3	29.90	1520.09	-	15.35±0.17	10.12±1.38	1.94±0.05	2.03±0.35	2.94±0.81	2.11±0.58	2.73±0.03	1.55±0.15	1.28±0.01	0.94±0.38	1.3±0.08
156	2-Hexyl-5-pentylpyrrolidine	73427-38-0	30.27	1530.73	-	1.23±0.08	0.77±0.14	0.17±0.01	0.15±0.02	0.21±0.09	0.15±0.03	0.2±0.02	0.12±0.01	0.07±0.01	0.06±0.02	0.06±0.01
157	Hexadecane, 1-iodo-	544-77-4	30.74	1543.79	-	8±1.02	5.37±0.1	0.9±0.46	1.29±0.17	1.43±0.4	0.72±0.37	0.99±0.47	1.11±0.1	0.64±0.01	0.44±0.17	0.43±0.04
158	Cyclohexane, undecyl-	54105-66-7	31.04	1552.31	1760	8.25±0.49	4.98±0.67	1.53±0.06	1.41±0.15	1.68±0.57	1.38±0.26	1.62±0.21	1.08±0.08	0.71±0.01	0.59±0.18	0.55±0.04
159	Heptadecane, 3-methyl-	6418-44-6	31.28	1559.18	1771	4.6±0.46	2.88±0.43	0.75±0.06	0.69±0.08	0.8±0.27	0.64±0.13	0.69±0.11	0.46±0.04	0.31±0.01	0.27±0.09	0.24±0.01
160	2,3,4-Trimethyl-1-pentanol	6570-88-3	31.62	1568.60	-	4.48±0.06	2.55±0.46	0.64±0.06	0.6±0.1	0.72±0.27	0.57±0.17	0.59±0.11	0.48±0.04	0.28±0.01	0.22±0.07	0.22±0.01
161	Cyclohexane, 1-isopropyl-1-methyl-	16580-26-0	31.75	1572.28	-	3.66±0.41	2.21±0.44	0.61±0.08	0.59±0.05	0.75±0.24	0.59±0.15	0.68±0.08	0.48±0.02	0.27±0.02	0.26±0.08	0.23±0.02
162	Tetradecanoic acid, ethyl ester	124-06-1	31.79	1573.30	1793	4.54±1.03	4.65±0.48	0.49±0.12	0.55±0.08	0.47±0.05	0.39±0.04	0.36±0.06	0.29±0.02	0.19±0	0.2±0.07	0.23±0.02
163	Octadecane	593-45-3	31.89	1576.19	-	4.5±0.46	3.01±0.03	0.81±0.18	0.96±0.08	1.09±0.26	0.92±0.19	0.81±0.27	0.42±0.04	0.35±0	0.37±0.1	0.28±0.01
164	5,5-Diethylpentadecane	1000360-41-0	31.97	1578.53	1805	2.54±0.09	1.1±0.22	0.26±0.02	0.31±0.05	0.28±0.11	0.22±0.05	0.29±0.05	0.34±0.02	0.18±0	0.11±0.03	0.13±0.01
165	Hexadecane, 2,6,10,14-tetramethyl-	638-36-8	32.09	1581.77	1811	9.5±0.66	5.94±1.31	1.27±0.11	1.46±0.12	2.06±0.57	1.58±0.49	1.89±0.48	1.12±0.13	0.81±0.03	0.66±0.21	0.88±0.12
166	Neophytadiene	504-96-1	32.70	1599.19	-	8.91±3.22	6.16±1.03	1.5±0.46	2.15±0.43	3.64±0.79	2.7±0.76	2.37±0.82	1.05±0.15	0.71±0.03	0.7±0.25	0.57±0.06
167	Phthalic acid, hept-4-yl isobutyl ester	1000356-78-3	33.32	1616.56	-	19.98±2.39	13.67±1.91	6.37±0.99	6.66±1.02	5.67±1.53	4.43±1.18	5.55±1.14	4.43±0.14	2.66±0.85	2.45±0.24	2.06±0.25
168	Hexadecanoic acid, methyl ester	112-39-0	34.44	1647.99	1920	5.34±1.1	2.58±0.15	0.94±0.17	1±0.15	1.04±0.17	0.82±0.14	0.78±0.14	0.48±0.04	0.41±0.01	0.37±0.1	0.83±0.02
169	Phthalic acid, butyl hept-4-yl ester	1000356-78-4	35.17	1668.48	-	0.83±0.06	0.56±0.07	0.95±1.13	0.45±0.12	0.36±0.12	0.3±0.05	0.27±0.06	0.18±0	0.1±0.01	0.1±0.02	0.1±0.01
170	Hexadecanoic acid, ethyl ester	628-97-7	35.76	1685.13	1993	18.62±2.73	14.72±1.06	4.06±0.72	4.35±0.61	4.7±0.66	3.6±0.52	2.92±0.56	2.07±0.18	1.38±0.07	1.35±0.38	1.7±0.16
171	Phytol	150-86-7	37.95	1877.40	2122	18.36±3.64	12.48±0.94	2.62±0.98	4.82±0.49	7.91±0.54	5.55±1.81	4.6±2.66	1.82±0.86	0.95±0.14	0.85±0.32	0.77±0.13
172	Linoleic acid ethyl ester	544-35-4	38.82	1964.04	2193	0.71±0.13	0.46±0.06	0.2±0.06	0.28±0.05	0.34±0	0.28±0.04	0.21±0.07	0.12±0.03	0.07±0.01	0.07±0.03	0.07±0
173	Ethyl 9,12,15-octadecatrienoate	1000336-77-4	38.94	1975.80	2101	3.97±0.69	3.1±0.53	0.97±0.26	1.36±0.17	1.59±0.01	1.32±0.2	1.02±0.34	0.67±0.16	0.46±0.02	0.44±0.14	0.52±0.06

RI^A: the linear retention indices calculated from a series of n-alkanes (C7-C40).

RI^B: retention indices referred to the literature value with same or equivalent chromatographic column shown on NIST Chemistry WebBook (<http://webbook.nist.gov/chemistry/>).

Table S2. List all of the volatile compounds in round green tea by different second-drying temperature.

NO	Name	CAS	RT	RI ^A	RI ^B	BHL70	BHL90	BHL110
1	Dimethyl ether	115-10-6	2.15	738.693	-	8.59±1.05	8.12±0.64	7.33±1.87
2	Butanal, 3-methyl-	590-86-3	2.17	743.0526	682	3.8±1.03	3.34±0.59	3.69±0.32
3	Butanal, 2-methyl-	96-17-3	2.16	739.0089	678	5.29±1.68	4.63±0.85	6.42±0.79
4	1-Penten-3-ol	616-25-1	2.30	751.7714	685	14.22±2.86	11.46±1.71	8.7±1.13
5	1-Penten-3-one	1629-58-9	2.61	753.3194	678	3.62±0.75	3.48±0.91	2.29±0.08
6	Pentanal	110-62-3	2.67	757.0788	701	6.88±2.01	5.41±1.58	2.59±0.07
7	Furan, 2-ethyl-	3208-16-0	2.80	758.9111	702	1.96±0.67	1.37±0.31	0.98±0.12
8	3-Penten-2-one	625-33-2	2.87	778.9078	744	1.02±0.2	1.02±0.1	0.98±0.02
9	Cyclobutaneethanol, beta-methylene-	116203-80-6	3.41	787.5318	-	0.99±0.23	0±0	0±0
10	Toluene	108-88-3	3.58	793.8816	773	3.1±0.85	1.41±0.42	2.35±0.15
11	1-Pentanol	71-41-0	3.88	795.1452	779	11.52±2.64	10.84±2.23	5.29±0.28
12	2-Penten-1-ol, (Z)-	1576-95-0	3.88	797.5144	769	7.93±1.37	6.71±0.85	4.91±0.32
13	Furan, 2-methoxy-	25414-22-6	4.11	816.1211	-	6.36±1.67	10.75±1.29	8.45±0.85
14	Hexanal	66-25-1	4.15	816.816	800	4.82±1.24	10.71±2.47	5.64±0.64
15	1H-Pyrrole, 3-ethyl-	1551-16-2	4.22	827.8411	-	1.19±0.25	2.04±0.16	9.84±1.34
16	2-Hexenal, (E)-	6728-26-3	4.24	859.5583	854	1.01±0.22	0.87±0.2	0.5±0.03
17	3-Hexen-1-ol, (E)-	928-97-2	4.89	862.1171	844	7.95±1.3	6.68±0.72	2.88±0.37
18	Ethylbenzene	100-41-4	4.90	872.1315	857	1.72±0.43	0±0	0±0
19	1-Hexanol	111-27-3	4.92	873.9084	867	7.1±1.33	1.66±0.18	2.89±0.28
20	Ethanone, 1-(1-cyclohexen-1-yl)-	932-66-1	4.92	887.9898	-	0.36±0.09	0.43±0.04	0.39±0.13
21	Styrene	100-42-5	5.31	890.7382	890	3.57±1.25	0±0	2.16±0.15
22	2-Heptanone	110-43-0	5.71	892.5071	895	2.15±0.61	0±0	1.34±0.15
23	4-Heptenal, (E)-	929-22-6	6.44	899.8678	905	1.34±0.31	0±0	0.57±0.06
24	Heptanal	111-71-7	6.53	901.4787	901	17.82±3.73	11.93±1.86	2.11±0.16
25	Oxime-, methoxy-phenyl-	1000222-86-6	6.68	910.1351	-	25.42±3.58	23.02±4.16	13.25±1.42
26	1-Butanol, 3-methyl-, nitrate	543-87-3	6.89	923.9402	-	1.73±0.59	1.15±0.4	0±0
27	Benzene, 1-methoxy-4-methyl-	104-93-8	6.95	931.68	-	1.17±0.34	1.02±0.05	1.14±0.11
28	2-Heptenal, (E)-	18829-55-5	7.21	950.9435	956	8.29±2.67	9.78±2.84	1.8±0.39
29	Benzaldehyde	100-52-7	7.22	953.1889	961	6.81±0.86	3.13±0.27	3.71±0.09
30	1-Heptanol	111-70-6	7.45	964.567	969	2.66±0.49	2.33±0.22	1.64±0.17
31	2-Hexene, 3,5,5-trimethyl-	26456-76-8	7.54	967.3559	-	2.85±1.01	9.41±1.79	5.2±0.76
32	1-Octen-3-ol	3391-86-4	7.55	972.8435	986	37.29±10.85	36.03±7.06	21.57±2.98
33	Pentanoic acid, 2-methyl-, anhydride	63169-61-9	7.61	977.835	-	29.52±5.16	25.41±3.4	18.9±1.11
34	5-Hepten-2-one, 6-methyl-	110-93-0	7.87	979.8887	988	7.74±1.88	6.74±0.99	4.92±0.25
35	.beta.-Myrcene	123-35-3	7.87	983.3215	981	10.07±1.75	9.06±0.82	12.99±1.1
36	Furan, 2-pentyl-	3777-69-3	7.93	983.4586	996	23.18±6.87	16.45±1.91	14.98±1.49
37	Hexanoic acid, ethyl ester	123-66-0	8.20	991.7675	998	3.54±0.67	18.62±15.13	1.36±0.22
38	cis-2-(2-Pentenyl)furan	70424-13-4	8.24	992.2099	-	0.9±0.22	0±0	0±0

39	Octanal	124-13-0	8.24	993.6631	1004	4.11±1.04	2.77±0.38	0±0
40	2,4-Heptadienal, (E,E)-	4313-03-5	8.35	999.9474	1008	7.28±1.56	6.36±1.27	1.09±0.08
41	o-Cymene	527-84-4	8.73	1012.177	1021	2.24±0.41	2.59±0.53	3.73±0.3
42	D-Limonene	5989-27-5	9.00	1015.678	1035	3.35±0.55	1.78±0.4	7.11±0.76
43	1-Hexanol, 2-ethyl-	104-76-7	9.68	1017.295	1029	7.85±1.25	8.85±1.09	3.7±0.07
44	5-Ethylcyclopent-1-enecarboxaldehyde	36431-60-4	9.76	1018.338	1026	0.82±0.13	0.76±0.1	0.62±0.02
45	Cyclohexanone, 2,2,6-trimethyl-	2408-37-9	9.93	1020.802	1022.9	6.49±1.84	4.72±0.91	3.28±0.3
46	Benzyl alcohol	100-51-6	10.17	1021.592	1033	16.81±1.72	17.36±1.77	16.84±0.51
47	Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	4889-83-2	10.27	1025.572	-	1.6±0.31	1.62±0.23	3.35±0.39
48	Benzeneacetaldehyde	122-78-1	10.43	1029.3	1043	14.21±1.74	12.66±2.67	16.02±0.53
49	Phenol, 4-amino-3-methyl-	2835-99-6	10.46	1034.513	-	2.92±0.58	17.94±0.59	56.94±2.59
50	3-Carene	13466-78-9	10.57	1034.513	1005	2.92±0.58	3.3±0.27	0±0
51	1-Undecene, 9-methyl-	74630-41-4	10.63	1042.66	-	4.84±1.22	0±0	0±0
52	Acetophenone	98-86-2	10.64	1049.172	1065	3.09±0.41	2.99±0.26	2.34±0.06
53	Cyclooctyl alcohol	696-71-9	10.71	1052.142	-	6.17±1.76	7.17±1.15	5.18±0.97
54	1-Octanol	111-87-5	10.83	1054.827	1068	11.74±1.97	9.92±0.83	0±0
55	Ethyl 2-(5-methyl-5-vinyltetrahydrofuran-2-yl)propan-2-yl carbonate	1000373-80-3	10.84	1069.47	-	4.68±0.69	8.59±0.43	8.36±0.68
56	3,5-Octadien-2-one	38284-27-4	11.11	1073.814	1093	2.03±0.31	1.81±0.02	2.15±0.14
57	Linalool	78-70-6	11.13	1080.196	1080	23.79±3.93	22.73±0.9	22.34±0.83
58	Nonanal	124-19-6	11.15	1084.145	1102	29.97±4.34	29.62±1.38	0±0
59	Phenylethyl Alcohol	60-12-8	11.20	1090.464	1116	15.1±1.63	9.73±0.91	26.61±1.28
60	Ethanone, 1-(4-methylphenyl)-	122-00-9	11.42	1105.345	1168	0.37±0.07	0±0	0±0
61	Benzene, 1-isocyano-3-methyl-	20600-54-8	11.60	1112.548	-	2.46±0.35	0±0	0±0
62	Decane, 2,3,5-trimethyl-	62238-11-3	11.86	1117.509	-	0.92±0.23	0±0	0±0
63	(R,S)-5-Ethyl-6-methyl-3E-hepten-2-one	57283-79-1	11.98	1119.436	1143.9	1.97±0.31	1.65±0.14	1.09±0.06
64	2-Oxo-4-phenyl-6-(4-chlorophenyl)-1,2-dihydropyrimidine	24030-13-5	12.04	1129.389	-	5.34±0.94	14.86±6.17	70.66±25.62
65	1-Nonanol	143-08-8	12.08	1140.289	1186	2.3±0.37	2.26±0.07	2.08±0.05
66	(3R,6S)-2,2,6-Trimethyl-6-vinyltetrahydro-2H-pyran-3-ol	39028-58-5	12.17	1142.595	1183	11.1±1.32	11.27±0.83	12.03±0.38
67	Benzaldehyde, 3-ethyl-	34246-54-3	12.19	1150.683	1168	0.28±0.06	0.32±0.01	0±0
68	cis-3-Hexenyl iso-butyrate	41519-23-7	12.33	1153.179	-	2±0.3	0±0	0±0
69	.alpha.-Terpineol	98-55-5	12.36	1155.991	1190	1.37±0.16	0±0	0±0
70	Methyl salicylate	119-36-8	12.47	1158.941	1187	16.03±1.95	16.54±0.34	18.62±0.76
71	Octanoic acid, ethyl ester	106-32-1	12.65	1181.045	1199	38.92±8.06	29.2±2.05	0±0
72	1,3-Cyclohexadiene-1-carboxaldehyde, 2,6,6-trimethyl-	116-26-7	12.65	1163.479	1178	2.12±0.47	1.56±0.01	2.64±0.17
73	Dodecane	112-40-3	12.94	1163.637	-	5.25±0.96	6.25±0.33	5.08±0.69
74	Decanal	112-31-2	12.94	1168.471	1200	1.9±0.28	2.79±0.23	1.64±0.03
75	Formamide, N-phenyl-	103-70-8	12.95	1175.8	-	0.33±0.07	0.34±0.05	0.44±0.03

76	1-Cyclohexene-1-carboxaldehyde, 2,6,6-trimethyl-	432-25-7	12.96	1180.54	1214	10.97±1.72	9.82±0.75	8.64±0.44
77	2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)-	106-25-2	13.04	1208.091	1229	65.7±7.9	0±0	67.55±2.86
78	n-Valeric acid cis-3-hexenyl ester	35852-46-1	13.05	1190.271	1235.8	5.11±0.84	4.04±0.14	3.49±0.24
79	trans-2-Hexenyl isovalerate	68698-59-9	13.05	1195.105	1244.9	0.82±0.17	0±0	0±0
80	6-Undecanone	927-49-1	13.12	1198.802	1274	18.39±3.07	17.93±2.25	0±0
81	Geraniol	106-24-1	13.17	1208.091	1267	65.81±7.88	61.66±3.29	67.71±2.8
82	1-Cyclohexene-1-acetaldehyde, 2,6,6-trimethyl-	472-66-2	13.28	1210.082	1254	1.9±0.32	1.64±0.17	2.55±0.77
83	Dodecane, 4,6-dimethyl-	61141-72-8	13.37	1227.397	-	2.27±0.61	0.83±1.04	0±0
84	1-Decanol	112-30-1	13.39	1236.086	1272	0.58±0.17	0±0	0±0
85	Indole	120-72-9	13.62	1237.129	1294	0.87±0.1	11.98±1.36	5.48±0.23
86	Tridecane	629-50-5	13.80	1242.532	-	2.12±0.33	4.74±1.05	2.81±0.12
87	Nonane, 5-butyl-	17312-63-9	13.89	1245.849	-	0.98±0.16	0±0	0±0
88	Naphthalene, 2-methyl-	91-57-6	13.92	1249.609	1315.3	0.66±0.07	0.92±0	0.71±0.02
89	Heptadecane, 7-methyl-	20959-33-5	13.94	1269.642	-	1.33±0.16	0±0	0±0
90	Methyl anthranilate	134-20-3	14.05	1273.845	1338	0.42±0.05	0.46±0.05	0.78±0.06
91	Hexane, 2,2,5,5-tetramethyl-	1071-81-4	14.27	1282.438	-	0.89±0.15	0±0	0±0
92	.alpha.-Cubebene	17699-14-8	14.41	1281.175	1354	2.87±0.34	2.87±0.14	3.6±0.25
93	Naphthalene, 1,2-dihydro-4,5,7-trimethyl-	53156-11-9	14.46	1283.197	-	0.59±0.07	0±0	0±0
94	Tridecane, 3-methyl-	6418-41-3	14.51	1295.241	1371	5.64±0.6	0±0	4.93±0.65
95	Cubenene	29837-12-5	14.53	1300.891	1552	0.99±0.1	0±0	0±0
96	Hexanoic acid, 3-hexenyl ester, (Z)-	31501-11-8	14.64	1303.925	1381	22.65±1.97	20.06±0.61	21.7±0.87
97	Hexanoic acid, hexyl ester	6378-65-0	15.14	1307.384	1385	2.57±0.23	2.59±0.05	2.66±0.14
98	Hexanoic acid, 2-hexenyl ester, (E)-	53398-86-0	15.16	1309.842	1391	3.75±0.41	0±0	3.74±0.37
99	1-Dodecanol	112-53-8	15.17	1311.161	1469	1.11±0.11	0±0	0±0
100	2-Cyclopenten-1-one, 3-methyl-2-(2-pentenyl)-, (Z)-	488-10-8	15.18	1317.322	1396	2.86±0.38	2.75±0.33	3.33±0.2
101	Tetradecane	629-59-4	15.34	1317.544	-	9.28±1.13	7.84±0.68	8.04±1.13
102	1H-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)]-	469-61-4	15.42	1327.813	1408	3.34±0.28	3.56±0.39	3.57±0.22
103	D-Alanine, N-(4-butylbenzoyl)-, isohexyl ester	1000354-10-0	15.42	1333.817	-	1.41±0.11	1.42±0.08	0±0
104	.alpha.-Ionone	127-41-3	15.43	1338.115	1426	5.02±0.54	4.83±0.29	5.25±0.32
105	Pentafluoropropionic acid, tetradecyl ester	6222-06-6	15.52	1351.07	-	1.78±0.21	2.15±0.38	1.55±0.06
106	5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-	3796-70-1	15.58	1355.019	1454	5.3±0.62	5.45±0.18	6.3±0.3
107	2,6,10-Trimethyltridecane	3891-99-4	15.60	1360.896	1465.1	3.06±0.23	3.06±0.42	3.14±0.27
108	Cyclopentane, pentyl-	3741-00-2	15.60	1369.049	1033	0.39±0.06	0±0	0±0
109	Acenaphthene	83-32-9	15.67	1375.179	1472	0.29±0.05	0.39±0.01	0.54±0.04
110	trans-.beta.-Ionone	79-77-6	16.02	1379.318	1469	67.74±7.94	64.82±5.39	71.24±4.14
111	n-Pentadecanol	629-76-5	16.23	1381.625	1772	0.91±0.11	0±0	0±0
112	Pentadecane	629-62-9	16.38	1386.919	-	2.89±0.36	3.25±0.46	3.39±0.44
113	2,4-Di-tert-butylphenol	96-76-4	16.41	1395.845	1513	16.35±2.1	11.47±1.77	0±0

114	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-7-methyl-4-methylene-1-(1-methylethyl)-, (1.alpha.,4a.beta.,8a.alpha.)-	39029-41-9	16.48	1398.815	1511	0.99±0.08	1.16±0.05	1.45±0.03
115	Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)-	483-76-1	16.49	1404.818	1519	10.29±0.81	11.13±0.51	9.04±0.63
116	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	17092-92-1	16.62	1408.768	1525	2.73±0.27	2.92±0.5	3.96±0.53
117	4-Isopropyl-6-methyl-1-methylene-1,2,3,4-tetrahydronaphthalene	50277-34-4	16.69	1418.247	1561	1.91±0.15	2.27±0.14	0±0
118	n-Nonylcyclohexane	2883-02-5	16.70	1421.06	1556	2.31±0.25	2.36±0.49	2.48±0.16
119	Nerolidol 2	1000285-43-6	16.75	1430.508	-	2.77±0.18	1.75±0.17	0±0
120	Pentadecane, 3-methyl-	2882-96-4	16.78	1434.047	1570	4.61±0.5	4.73±0.64	6.41±0.38
121	3-Hexen-1-ol, benzoate, (Z)-	25152-85-6	16.86	1435.405	1568	0.55±0.05	0.59±0.05	0.9±0.08
122	Glutaric acid, butyl cis-hex-3-enyl ester	1000359-96-4	16.87	1439.766	-	4.21±0.54	0±0	0±0
123	Ethylene diacrylate	2274-11-5	16.88	1448.298	-	0.36±0.09	0±0	0±0
124	Hexadecane	544-76-3	16.97	1453.164	-	4.55±0.37	4.17±0.27	6.17±0.21
125	5,5-Diethyltridecane	1000360-41-3	16.97	1455.186	-	0.45±0.06	0.54±0.08	0.58±0.03
126	Cedrol	77-53-2	16.99	1457.24	1607.9	1.46±0.16	1.38±0.23	2.27±0.17
127	.tau.-Cadinol	5937-11-1	17.04	1481.76	1639	2.38±0.25	2.41±0.2	0±0
128	1-Hexadecanol	36653-82-4	17.07	1488.111	1879	1.32±0.16	1.06±0.06	1.51±0.09
129	.tau.-Murolol	19912-62-0	17.23	1490.355	1640	0.54±0.07	0±0	1.81±0.18
130	Adipic acid, butyl isobutyl ester	1000324-09-3	17.24	1507.702	-	1.36±0.19	1.53±0.26	4±0.64
131	3-Ethyl-3-methylheptane	17302-01-1	17.41	1519.709	-	1.11±0.12	0±0	0±0
132	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	3075-84-1	17.67	1523.564	1663.6	1.36±0.18	1.46±0.2	3.09±0.45
133	Heptadecane, 3-methyl-	6418-44-6	17.80	1558.829	1771	0.95±0.09	0±0	0.52±0.04
134	Neophytadiene	504-96-1	17.84	1598.896	1840	0.65±0.11	0.67±0.07	1.75±0.05
135	Caffeine	58-08-2	17.86	1602.435	1842	6.41±1.28	0±0	31.7±12.11
136	Phthalic acid, isobutyl 4-octyl ester	1000314-84-7	18.01	1616.307	-	2.33±0.38	2.06±0.25	0±0
137	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	82304-66-3	18.18	1645.22	1929	1.82±0.3	0±0	2.35±0.47
138	Phthalic acid, 6-ethyl-3-octyl butyl ester	1000315-17-4	18.35	1601.215	-	1.23±0.27	1.16±0.06	0.53±0.11
139	Hexadecanoic acid, ethyl ester	628-97-7	18.49	1659.326	1993	2.61±0.37	1.7±0.16	0.98±0.05
140	Phytol	150-86-7	18.66	1875.985	2122	1.59±0.33	1.78±0.3	7.14±1.75
141	9,12,15-Octadecatrienoic acid, ethyl ester, (Z,Z,Z)-	1191-41-9	18.82	1974.87	2169	0.99±0.21	0.96±0.02	1.6±0.21
142	Ethane, 1,1-diethoxy-	105-57-7	18.82	774.1991	725	0±0	0.51±0.11	0±0
143	2,6-Dimethyl-1,3,5,7-octatetraene, E,E-	460-01-5	18.84	1105.575	1134	0±0	0±0	3.1±0.23
144	Isophthalaldehyde	626-19-7	18.89	1142.249	-	0±0	0.83±0.06	1.32±0.11
145	Naphthalene	91-20-3	18.99	1148.094	1178	0±0	2.01±0.04	0±0
146	L-.alpha.-Terpineol	10482-56-1	19.32	1156.024	1187	0±0	1.31±0.03	3.72±0.25
147	1-Decen-3-one	56606-79-2	19.50	1444.136	-	0±0	1.7±0.21	0±0

148	.alpha.-Cadinol	481-34-5	19.73	1490.333	1650	0±0	0.83±0.09	0.79±0.09
149	Sulfurous acid, 2-ethylhexyl hexyl ester	1000309-20-2	19.81	1515.833	-	0±0	0.63±0.08	0±0
150	1,2-Benzenediol, o-(4-methoxybezoyl)-o'-(5-chlorovaleryl)-	1000325-98-7	19.85	1066.903	-	0±0	0±0	0.81±0.27
151	2-Pentenal, (E)-	1576-87-0	19.89	787.5302	754	0±0	0.8±0.27	0±0
152	1-Penten-3-one, 2-methyl-	25044-01-3	20.04	797.1268	-	0±0	2.56±0.72	0±0
153	2-Propenenitrile	107-13-1	20.16	815.9929	-	0±0	1.08±0.16	0±0
154	Oxetane, 3-(1-methylethyl)-	10317-17-6	20.29	838.8964	-	0±0	0.17±0.05	0±0
155	Octatriene, 1,3-trans-5-trans-	33580-04-0	20.43	881.3859	-	0±0	0.62±0.16	0±0
156	Butanedioic acid, phenyl-	635-51-8	20.50	890.642	-	0±0	2.29±0.23	0±0
157	4-Heptenal, (Z)-	6728-31-0	21.00	899.8032	904	0±0	1.14±0.31	0±0
158	3-Octen-2-one	1669-44-9	21.15	1026.203	1037	0±0	1.99±0.16	1.55±0.13
159	1-Decanol, 2-ethyl-	21078-65-9	21.27	1042.565	-	0±0	5.31±1.08	0±0
160	Ethanone, 1-(1H-pyrrol-2-yl)-	1072-83-9	21.27	1045.791	1063.2	0±0	0.95±0.1	8.54±0.39
161	Nonane, 4,5-dimethyl-	17302-23-7	21.41	1045.696	-	0±0	1.77±1.75	0±0
162	2-n-Butyl furan	4466-24-4	21.46	1087.4	-	0±0	2±0.25	0±0
163	2-Methylthiolane, S,S-dioxide	1003-46-9	21.47	1104.461	-	0±0	0.72±0.15	0±0
164	1,3,8-p-Menthatriene	18368-95-1	21.48	1105.219	1113	0±0	0.79±0.02	1.04±0.09
165	Benzene, 1-isocyano-2-methyl-	10468-64-1	21.48	1112.423	-	0±0	3.57±0.16	0±0
166	Undecane, 4,4-dimethyl-	17312-68-4	21.59	1117.415	-	0±0	0.77±0.03	0±0
167	Butanoic acid, 3-hexenyl ester, (Z)-	16491-36-4	21.91	1153.118	1186	0±0	1.53±0.09	0±0
168	(S)-(+)-6-Methyl-1-octanol	110453-78-6	21.91	1156.656	-	0±0	0.46±0.08	0±0
169	2-Nonanone, 3-(hydroxymethyl)-	67801-33-6	22.11	1158.015	1093	0±0	0.52±0.02	0±0
170	2-Decenal, (E)-	3913-81-3	22.22	1212.929	1265	0±0	1.53±0.32	1.69±0.49
171	Dodecane, 2,6,10-trimethyl-	3891-98-3	22.34	1233.909	1376	0±0	0.91±1.16	0±0
172	1-Oxaspiro[4.5]dec-6-ene, 2,6,10,10-tetramethyl-	36431-72-8	22.43	1255.427	-	0±0	1.25±0.02	0±0
173	Undecane, 3,7-dimethyl-	17301-29-0	22.48	1277.324	1221	0±0	1.76±0.68	0±0
174	Decane, 3,6-dimethyl-	17312-53-7	22.70	1282.759	-	0±0	0.91±0.23	0±0
175	1, 1, 5-Trimethyl-1, 2-dihydronaphthalene	1000357-25-8	22.70	1283.107	-	0±0	0.9±0.01	1.91±0.11
176	Tetradecane, 2-methyl-	1560-95-8	22.80	1295.146	1461	0±0	5.41±0.98	0±0
177	Tetradecane, 3-methyl-	18435-22-8	23.07	1320.14	1468	0±0	0.67±0.13	0±0
178	Carbonic acid, decyl undecyl ester	1000383-16-0	23.28	1381.948	-	0±0	1.11±0.47	0±0

179	Hexadecane, 2,6,11,15-tetramethyl-	504-44-9	23.43	1414.716	-	0±0	2±2.05	2.43±0.12
180	Glutaric acid, di(isobutyl) ester	1000358-25-0	23.89	1439.712	-	0±0	4.93±0.56	0±0
181	1,7-Dimethyl-4-(1-methylethyl)cyclodecane	645-10-3	24.03	1448.275	-	0±0	0.39±0.1	0±0
182	Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-	483-78-3	24.24	1503.131	1674	0±0	0.55±0.02	1.1±0.07
183	Pentadecane, 2,6,10,14-tetramethyl-	1921-70-6	24.53	1519.688	1707	0±0	1.34±0.05	2.24±0.22
184	1,2-Benzenediol, o-(4-methoxybenzoyl)-o'-(2,2,3,3,4,4,4-heptafluorobutyryl)-	1000325-97-9	24.54	1414.716	-	0±0	0.61±0.03	0±0
185	6-Octen-1-ol, 3,7-dimethyl-, propanoate	141-14-0	24.61	1623.302	1446	0±0	0.44±0.03	0±0
186	Hexadecanoic acid, methyl ester	112-39-0	24.75	1647.697	1920	0±0	0.83±0.02	4.5±0.39
187	1-Hepten-3-one	2918-13-0	24.90	971.8068	-	0±0	0±0	5.85±1.17
188	Decyl octyl ether	1000406-38-3	24.98	1042.955	-	0±0	0±0	3.84±0.28
189	1,5,7-Octatrien-3-ol, 3,7-dimethyl-	29957-43-5	24.99	1085.354	1107	0±0	0±0	69.78±3.35
190	Benzyl nitrile	140-29-4	25.17	1112.795	1140	0±0	0±0	9.94±0.22
191	Phenol, 4-amino-2,5-dimethyl-	3096-71-7	25.32	1149.957	-	0±0	0±0	4.82±0.24
192	Benzaldehyde, 4-methyl-	104-87-0	25.48	1179.391	1079	0±0	0±0	5±0.58
193	Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	475-03-6	25.50	1286.118	1258	0±0	0±0	0.41±0.03
194	1-Isopropyl-4,7-dimethyl-1,2,3,4,5,6-hexahydronaphthalene	16729-00-3	25.59	1371.247	1481.3	0±0	0±0	1.46±0.14
195	Di-epi-1,10-cubenol	73365-77-2	25.80	1474.231	1619	0±0	0±0	1.76±0.18
196	Phthalic acid, hept-4-yl isobutyl ester	1000356-78-3	25.94	1616.589	-	0±0	0±0	0.45±0.07
197	Linoleic acid ethyl ester	544-35-4	26.15	1963.9	2155	0±0	0±0	0.17±0.02
198	Cyclopentene, 3-methyl-	1120-62-3	26.15	739.3248	-	0±0	0±0	0.72±0.09
199	Acetic anhydride	108-24-7	26.28	816.8185	-	0±0	0±0	2.82±0.12
200	1H-Imidazole-4-methanol	822-55-9	26.29	866.2909	-	0±0	0±0	0.6±0.42
201	1,3-trans,5-cis-Octatriene	40087-61-4	26.38	881.6126	880	0±0	0±0	0.64±0.06
202	Pyrazine, 2,5-dimethyl-	123-32-0	26.71	909.2551	913	0±0	0±0	1.53±0.07
203	Ethanone, 1-(2-furanyl)-	1192-62-7	26.73	910.2027	914	0±0	0±0	2.95±0.08
204	Pyrazine, ethyl-	13925-00-3	26.84	913.3619	916	0±0	0±0	1.39±0.16
205	2-Furancarboxaldehyde, 5-methyl-	620-02-0	26.89	957.8428	966	0±0	0±0	2.67±0.15
206	Benzonitrile	100-47-0	27.04	976.0085	994	0±0	0±0	2.14±0.15
207	Phenol	108-95-2	27.04	977.4303	981	0±0	0±0	1.5±0.04
208	Pyrazine, 2-ethyl-6-methyl-	13925-03-6	27.06	991.1283	1001	0±0	0±0	4.38±0.1
209	Bicyclo[2.2.1]hept-2-ene, 1,7,7-trimethyl-	464-17-5	27.20	1005.012	-	0±0	0±0	1.07±0.15
210	.gamma.-Terpinene	99-85-4	27.35	1043.207	1062	0±0	0±0	1.67±0.06
211	Ethyl 4-(ethyloxy)-2-oxobut-3-enoate	1000305-38-2	27.35	1045.387	-	0±0	0±0	0.83±0.06
212	Octane, 2-methyl-	3221-61-2	27.36	1047.631	-	0±0	0±0	1.45±0.21
213	Cyclobutanone, 2-methyl-	1517-15-3	27.43	1055.244	-	0±0	0±0	7.29±0.14
214	Pyrazine, 3-ethyl-2,5-dimethyl-	13360-65-1	27.52	1061.827	1078	0±0	0±0	3.53±0.12

215	Benzene, 4-ethenyl-1,2-dimethyl-	27831-13-6	27.59	1070.315	-	0±0	0±0	1.99±0.09
216	1-(2,3-Dimethylphenyl)ethanone	2142-71-4	27.66	1070.915	-	0±0	0±0	0.46±0.06
217	Butane, 2-iodo-3-methyl-	18295-27-7	28.27	1086.808	-	0±0	0±0	6.54±0.39
218	2,5-Pyrrolidinedione, 1-ethyl-	2314-78-5	28.53	1110.156	-	0±0	0±0	0.71±0.05
219	2,4,6-Octatriene, 2,6-dimethyl-	673-84-7	28.76	1115.243	1113	0±0	0±0	0.85±0.04
220	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	1125-21-9	28.84	1116.981	1142	0±0	0±0	0.37±0.02
221	5-Hydroxy-7-methoxy-2-methyl-3-phenyl-4-chromenone	55927-39-4	28.84	1135.148	-	0±0	0±0	0.26±0.14
222	2-Chloroethyl benzoate	939-55-9	29.29	1139.572	-	0±0	0±0	1.5±2.24
223	Benzeneacetic acid, methyl ester	101-41-7	29.46	1146.143	1179	0±0	0±0	0.81±0.04
224	d-Proline, N-methoxycarbonyl-, heptyl ester	1000320-79-1	29.60	1148.45	-	0±0	0±0	1.96±0.14
225	Butanoic acid, 3-hexenyl ester, (E)-	53398-84-8	29.74	1153.442	1185.9	0±0	0±0	1.38±0.11
226	1-Phenyl-2-butanone	1007-32-5	29.76	1185.353	-	0±0	0±0	0.47±0.03
227	Benzeneacetic acid	103-82-2	29.88	1203.71	1254	0±0	0±0	0.63±0.18
228	Citral	5392-40-5	29.88	1208.766	-	0±0	0±0	67.68±2.83
229	Benzeneacetaldehyde, .alpha.-ethylidene-	4411-89-6	30.02	1222.29	1281	0±0	0±0	0.64±0.04
230	Sulfurous acid, 2-ethylhexyl undecyl ester	1000309-19-4	31.04	1238.468	-	0±0	0±0	2.69±0.38
231	4-Acetoxy-3-methoxystyrene	46316-15-8	31.27	1253.477	-	0±0	0±0	0.64±0.07
232	Decane, 3,8-dimethyl-	17312-55-9	31.28	1277.219	1113	0±0	0±0	2.07±0.09
233	Formic acid, decyl ester	5451-52-5	31.42	1369.414	-	0±0	0±0	0.41±0.05
234	10-Methylnonadecane	56862-62-5	32.69	1391.281	-	0±0	0±0	1.28±0.36
235	Phenol, 2,5-bis(1,1-dimethylethyl)-	5875-45-6	32.82	1396.369	1514	0±0	0±0	2.8±0.34
236	.alpha.-Calacorene	21391-99-1	32.83	1418.583	1522	0±0	0±0	4.55±0.38
237	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)-	40716-66-3	33.31	1430.876	1551	0±0	0±0	1.59±0.18
238	Glutaric acid, butyl isobutyl ester	1000358-25-1	33.32	1440.142	-	0±0	0±0	9.21±1.05
239	1-Tetradecanol	112-72-1	33.56	1448.667	1676	0±0	0±0	0.52±0.1
240	Dodecanoic acid, ethyl ester	106-33-2	34.34	1450.531	1579	0±0	0±0	0.78±0.07
241	Decyl heptyl ether	1000406-39-1	34.43	1511.898	-	0±0	0±0	1.46±0.26
242	Heptadecane	629-78-7	35.16	1516.195	-	0±0	0±0	0.97±0.11
243	Cyclohexane, undecyl-	54105-66-7	35.17	1552.283	-	0±0	0±0	1.22±0.12
244	3,5-di-tert-Butyl-4-hydroxybenzaldehyde	1620-98-0	35.75	1559.204	-	0±0	0±0	0.22±0.02
245	9H-Fluorene, 9-methylene-	4425-82-5	37.93	1562.964	-	0±0	0±0	0.69±0.03
246	2-Pentadecanone, 6,10,14-trimethyl-	502-69-2	38.82	1602.622	1838	0±0	0±0	2.14±0.24
247	Phthalic acid, butyl hept-4-yl ester	1000356-78-4	38.93	1601.815	-	0±0	0±0	3.76±0.82

RI^A: the linear retention indices calculated from a series of n-alkanes (C7-C40).

RI^B: retention indices referred to the literature value with same or equivalent chromatographic column shown on NIST Chemistry WebBook (<http://webbook.nist.gov/chemistry/>).

Table S3. List aroma characteristics and OAV values of 41 different volatile compounds in different second-drying temperature samples.

Name	OT ^A	Aroma characteristics ^B	BHL70	BHL90	BHL110
Toluene	140	Sweet	0.022±0.006	0.01±0.003	0.017±0.001
(E)-3-Hexen-1-ol	110	Mushroom-like odor	0.072±0.012	0.061±0.007	0.026±0.003
Ethylbenzene	29	Aromatic odor	0.059±0.015	0±0	0±0
1-Hexanol	0.7	Green, cut grass	10.139±1.893	2.366±0.259	4.125±0.4
Styrene	730	aromatic odour	0.005±0.002	0±0	0.003±0
2-Heptanone	1	pieplant, musty	2.15±0.614	0±0	1.34±0.145
(E)-4-Heptenal	0.02	green	67.075±15.333	0±0	28.552±2.95
Heptanal	3	Heavy, planty green odor	5.942±1.245	3.977±0.621	0.705±0.053
Benzaldehyde	3	almond-like smelle	2.269±0.288	1.043±0.091	1.237±0.03
cis-2-(2-Pentenyl)furan	6	Bean-like, fruity, green, earthy and vegetable-like smell	0.151±0.037	0±0	0±0
Octanal	0.7	Green, fatty, citruse	5.878±1.491	3.955±0.54	0±0
(E,E)-2,4-Heptadienal	56	faint sweet, faint pungent fruity	0.13±0.028	0.114±0.023	0.02±0.001
D-Limonene	10	citrus herbal terpene camphore	0.335±0.055	0.178±0.04	0.711±0.076
3-Carene	5	Leafy	0.583±0.116	0.66±0.055	0±0
1-Octanol	0.022	Green, citrus, fatty, coconut-like	533.649±89.582	450.988±37.786	0±0
Ethyl 2-(5-methyl-5-vinyltetrahydrofuran-2-yl)propan-2-yl carbonate	320	Roasted, sweet	0.015±0.002	0.027±0.001	0.026±0.002
Nonanal	1	candle-like, sweet orange-like, fatty and floral odord	29.965±4.338	29.623±1.381	0±0
Phenylethyl Alcohol	564.23	floral, sweet, rose	0.027±0.003	0.017±0.002	0.047±0.002
alpha-Terpineol	300	Citrus aromas, woody	0.005±0.001	0±0	0±0
2,6,6-trimethyl-1,3-Cyclohexadiene-1-carboxaldehyde	3	Woody, spicy, medicinal, powdery, herbal	0.707±0.156	0.519±0.003	0.881±0.058
Decanal	0.1	Aldehyde-like, candle-like, fatty and citrus-like aroma	18.955±2.782	27.893±2.264	16.438±0.336
(Z)-3,7-dimethyl-2,6-Octadien-1-ol	0.0002	Citrus, lemon-like	328487.048±39485.402	0±0	337756.081±14275.132
1-Decanol	0.023	Orange, Floral	25.13±7.387	0±0	0±0
Indole	140	animal-like	0.006±0.001	0.086±0.01	0.039±0.002
2-methyl-Naphthalene	10	piquancy	0.066±0.007	0.092±0	0.071±0.002
1-Dodecanol	5	Violet-like, oil	0.222±0.023	0±0	0±0
Nerolidol 2	0.25	Floral, green, citrus, woody, waxy	11.083±0.739	6.981±0.669	0±0
(Z)-3-Hexen-1-ol, benzoate	12.1	green, fruity, florald	0.045±0.004	0.049±0.004	0.074±0.007
Cedrol	0.5	mild cedar wood-like aroma	2.925±0.311	2.77±0.451	4.531±0.349
tau-Cadinol	0.44	Tar, camphor, and greasy	5.416±0.56	5.487±0.443	0±0
Phytol	640	Floral, balsam, powdery, waxy	0.002±0.001	0.003±0	0.011±0.003
Naphthalene	0.44	Pungent, dry, tarry odore	0±0	4.571±0.094	0±0
1-(1H-pyrrol-2-yl)-Ethanone	170000	nutty	0±0	0±0	0±0
2,6,10,10-tetramethyl-1-Oxaspiro[4.5]dec-6-ene	0.2	Fruity, woody, slightly camphor-like	0±0	6.251±0.111	0±0
3,7-dimethyl-1,5,7-Octatrien-3-ol	110	moldy	0±0	0±0	0.634±0.03
2,5-dimethyl-Pyrazine	1750	Roasted	0±0	0±0	0.001±0
ethyl-Pyrazine	4000	Nutty coffee, cocoa-like	0±0	0±0	0±0
5-methyl-2-Furancarboxaldehyde	500	Caramel, bready, coffee-like	0±0	0±0	0.005±0
2-ethyl-6-methyl-Pyrazine	40	Roasted	0±0	0±0	0.11±0.002
3-ethyl-2,5-dimethyl-Pyrazine	8.6	Roasted potato, cocoa-like, nutty	0±0	0±0	0.41±0.014
trans-beta-Ionone	0.007	Violet-like, floral, and raspberry-like	9676.937±1134.502	9260.629±769.571	10176.878±591.999

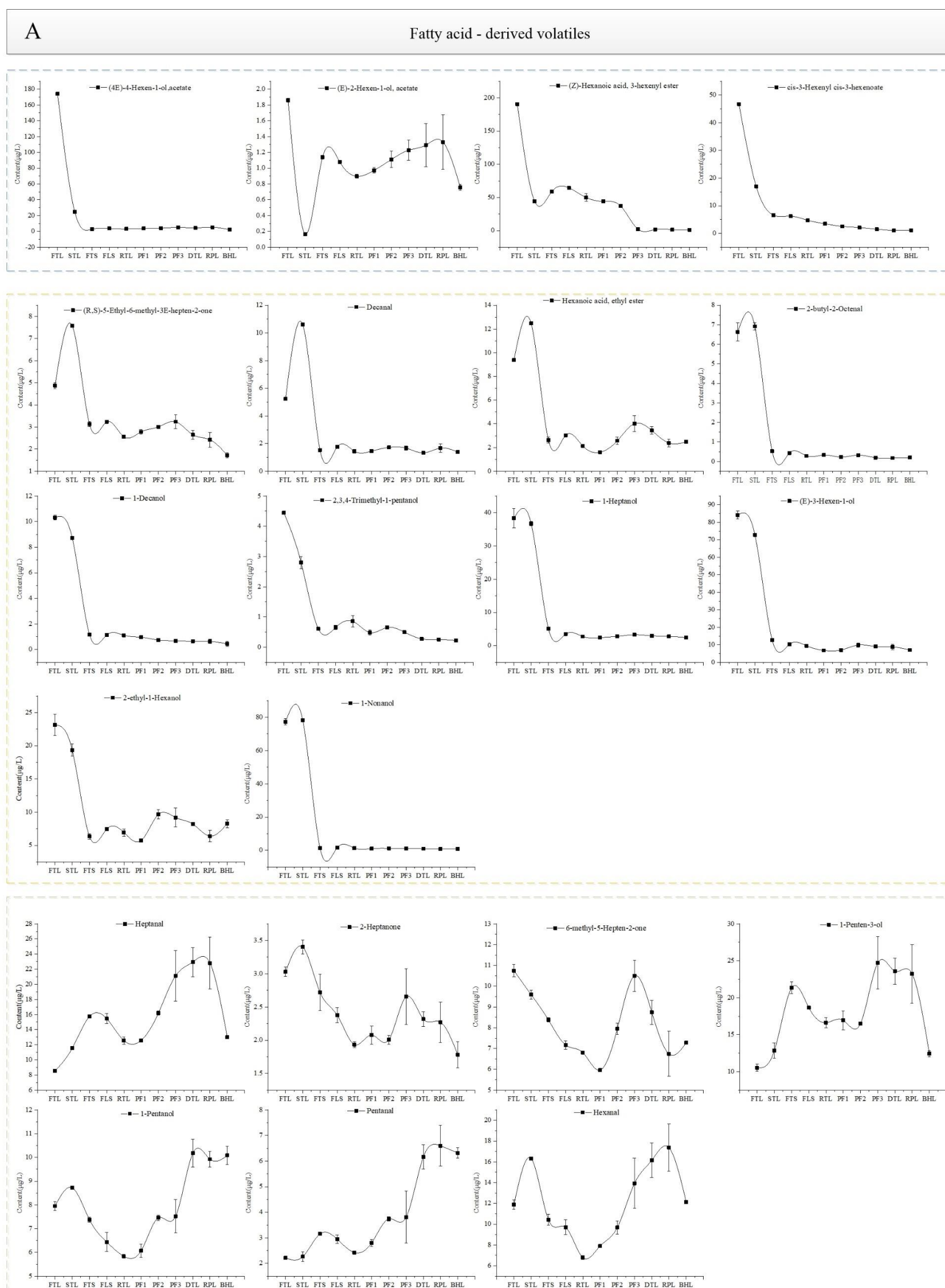
OTs: Odor thresholds in water. The values were according to the reported references.

A: (Wang et al., 2020a; Wang et al., 2020b; Guo et al., 2021a; Guo et al., 2021b); Zhu et al., 2018; Zhu et al., 2021; Zhang et al., 2019)

B: <http://www.thegoodscentcompany.com/search3.php?qOdor=20126-76-5&submit.x=9&submit.y=9>

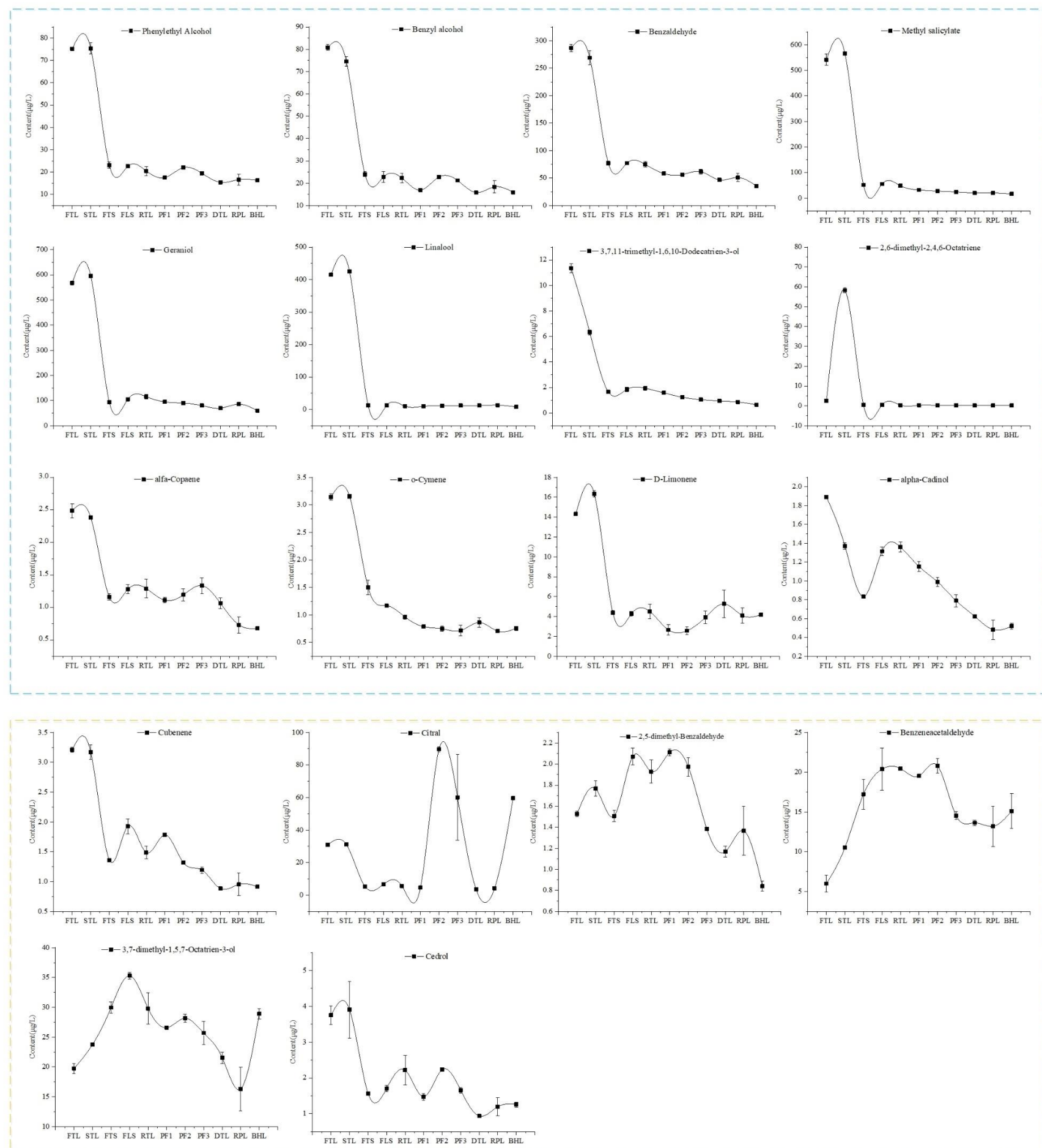
2.2 Supplementary Figures

Figure. S1 Evolution of compounds from different sources, (A) Fatty derived volatiles, (B) Glycoside-derived volatiles, (C) Amino acid-derived volatiles, (D) Carotenoid-derived volatiles

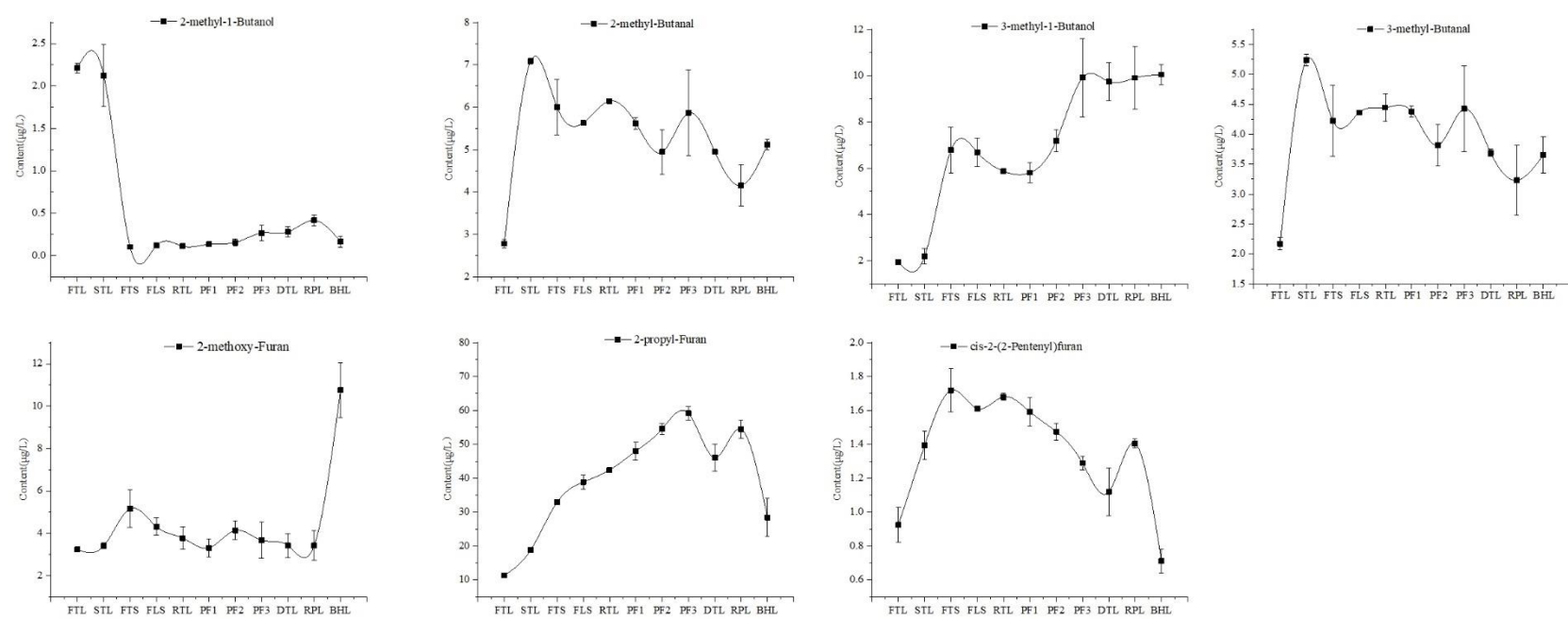


B

Glycosid - derived volatiles



C Amino acid - derived volatiles



D Carotenoid -derived volatiles

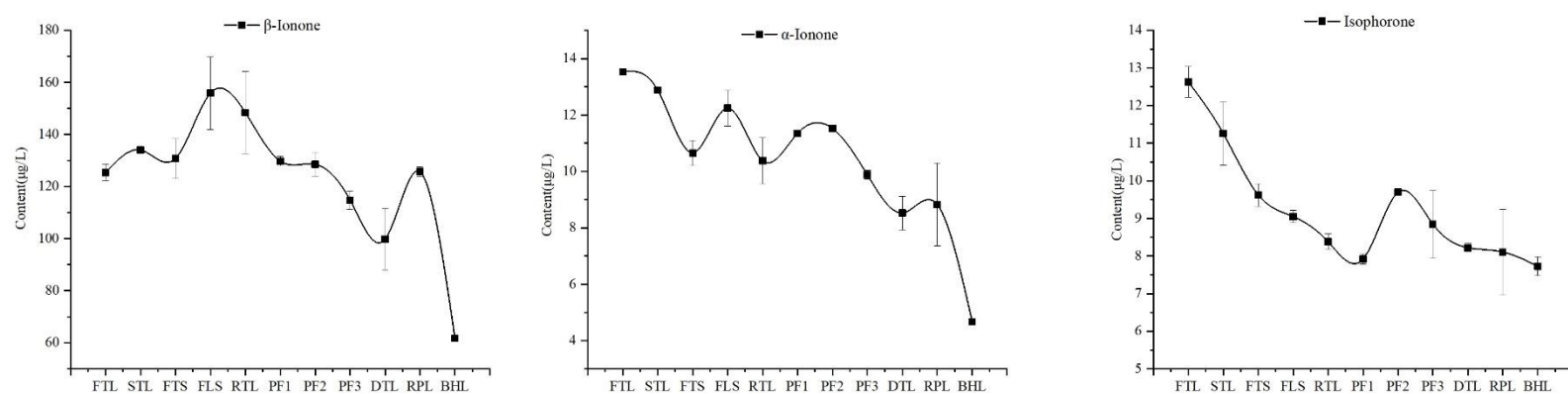


Figure. S2 Heat map of different volatile compounds screened out in different second-drying temperature

