

Supplementary Materials

Table S1. Information on the identified compounds of citrus-tea by HS-GC-IMS.

NO.	Compound	CAS#	Formula	MW ^a	RI ^b	Rt ^c (sec)	Dt ^d [RIPrel]	Comment
1	γ -Decalactone	C706149	C ₁₀ H ₁₈ O ₂	170.3	1538.1	1169.307	1.4715	
2	Decanal	C112312	C ₁₀ H ₂₀ O	156.3	1260.2	737.434	1.543	Monomer
3	Decanal	C112312	C ₁₀ H ₂₀ O	156.3	1259.4	736.205	2.056	Dimer
4	Phenylethyl acetate	C103457	C ₁₀ H ₁₂ O ₂	164.2	1318.7	828.421	1.3119	
5	Phenylacetic acid	C103822	C ₈ H ₈ O ₂	136.1	1283.9	774.321	1.3301	
6	α -Terpineol	C98555	C ₁₀ H ₁₈ O	154.3	1192.7	632.58	1.2204	
7	β -Citronellol	C106229	C ₁₀ H ₂₀ O	156.3	1229.6	689.918	1.342	
8	Linalool	C78706	C ₁₀ H ₁₈ O	154.3	1101.4	490.694	1.2217	
9	γ -Terpinene	C99854	C ₁₀ H ₁₆	136.2	1077.7	453.848	1.2194	
10	β -Ocimene	C1387791 3	C ₁₀ H ₁₆	136.2	1051.7	414.628	1.2156	Monomer
11	β -Ocimene	C1387791 3	C ₁₀ H ₁₆	136.2	1051.3	413.995	1.7034	Dimer
12	Limonene	C138863	C ₁₀ H ₁₆	136.2	1023.4	374.774	1.2979	Monomer
13	Limonene	C138863	C ₁₀ H ₁₆	136.2	1022.9	374.142	1.7148	Dimer
14	Myrcene	C123353	C ₁₀ H ₁₆	136.2	991.3	335.554	1.7186	
15	β -Pinene	C127913	C ₁₀ H ₁₆	136.2	975.0	318.474	1.2181	Monomer
16	β -Pinene	C127913	C ₁₀ H ₁₆	136.2	973.7	317.209	1.6375	Dimer
17	Camphene	C79925	C ₁₀ H ₁₆	136.2	946.2	292.538	1.2131	
18	α -Pinene	C80568	C ₁₀ H ₁₆	136.2	927.2	277.988	1.6667	
19	Octanal	C124130	C ₈ H ₁₆ O	128.2	1006.6	353.266	1.4069	Monomer
20	Octanal	C124130	C ₈ H ₁₆ O	128.2	1007.1	353.899	1.8263	Dimer
21	2-Ethyl-6-methylpyrazine	C1392503 6	C ₇ H ₁₀ N ₂	122.2	999.7	345.043	1.1776	
22	Benzaldehyde	C100527	C ₇ H ₆ O	106.1	960.9	305.189	1.1522	Monomer
23	Benzaldehyde	C100527	C ₇ H ₆ O	106.1	963.0	307.087	1.4728	Dimer
24	2-Acetylfuran	C1192627	C ₆ H ₆ O ₂	110.1	916.1	270.092	1.117	
25	Heptanal	C111717	C ₇ H ₁₄ O	114.2	903.7	261.892	1.3342	Monomer
26	Heptanal	C111717	C ₇ H ₁₄ O	114.2	902.9	261.306	1.6987	Dimer
27	Cyclohexanone	C108941	C ₆ H ₁₀ O	98.1	899.6	259.256	1.1485	Monomer

28	Cyclohexanone	C108941	C ₆ H ₁₀ O	98.1	896.8	257.499	1.4557	Dimer
29	1-Hexanol	C111273	C ₆ H ₁₄ O	102.2	875.1	244.613	1.3274	
30	(E)-2-Hexenol	C928950	C ₆ H ₁₂ O	100.2	852.2	232.02	1.1834	Monomer
31	(E)-2-Hexenol	C928950	C ₆ H ₁₂ O	100.2	853.9	232.898	1.5153	Dimer
32	Furfurol	C98011	C ₅ H ₄ O ₂	96.1	831.0	221.184	1.0855	Monomer
33	Furfurol	C98011	C ₅ H ₄ O ₂	96.1	830.4	220.891	1.3342	Dimer
34	Hexanal	C66251	C ₆ H ₁₂ O	100.2	795.6	204.49	1.2599	Monomer
35	Hexanal	C66251	C ₆ H ₁₂ O	100.2	794.4	203.905	1.5626	Dimer
36	2-Hexanone	C591786	C ₆ H ₁₂ O	100.2	784.1	199.33	1.1898	Monomer
37	2-Hexanone	C591786	C ₆ H ₁₂ O	100.2	783.4	199.017	1.5053	Dimer
38	1-Pentanol	C71410	C ₅ H ₁₂ O	88.1	765.7	191.364	1.2533	

Table S1. (continued).

NO.	Compound	CAS#	Formula	MW ^a	RI ^b	Rt ^c (sec)	Dt ^d [RIPrel]	Comment
39	Dimethyl disulfide	C624920	C ₂ H ₆ S ₂	94.2	737.6	179.961	0.9877	
40	Acetoin	C513860	C ₄ H ₈ O ₂	88.1	717.6	172.62	1.0604	Monomer
41	Acetoin	C513860	C ₄ H ₈ O ₂	88.1	713.9	171.371	1.3302	Dimer
42	2-Ethylfuran	C3208160	C ₆ H ₈ O	96.1	689.7	163.717	1.3116	
43	Pentanal	C110623	C ₅ H ₁₀ O	86.1	700.0	166.841	1.4241	
44	2-Pentanone	C107879	C ₅ H ₁₀ O	86.1	698.1	166.216	1.3666	
45	2-Methylbutanal	C96173	C ₅ H ₁₀ O	86.1	668.1	157.938	1.4013	
46	3-Methylbutanal	C590863	C ₅ H ₁₀ O	86.1	651.7	154.033	1.1991	Monomer
47	3-Methylbutanal	C590863	C ₅ H ₁₀ O	86.1	653.1	154.345	1.4063	Dimer
48	Ethyl acetate	C141786	C ₄ H ₈ O ₂	88.1	609.7	145.286	1.0977	Monomer
49	Ethyl acetate	C141786	C ₄ H ₈ O ₂	88.1	610.4	145.442	1.337	Dimer
50	Acetic acid	C64197	C ₂ H ₄ O ₂	60.1	630.0	149.347	1.0494	
51	Butanal	C123728	C ₄ H ₈ O	72.1	603.2	144.036	1.2905	
52	2-Butanone	C78933	C ₄ H ₈ O	72.1	590.2	141.537	1.2465	
53	2,3-Butanedione	C431038	C ₄ H ₆ O ₂	86.1	562.4	136.227	1.167	
54	Acetone	C67641	C ₃ H ₆ O	58.1	484.8	121.388	1.1154	
55	Ethanol	C64175	C ₂ H ₆ O	46.1	452.2	115.14	1.0469	
56	2-Furfurylthiol	C98022	C ₅ H ₆ OS	114.2	908.8	265.25	1.1008	

	Methyl						
57	N-Methyl-anthranil	C85916	C ₉ H ₁₁ NO ₂	165.2	1510.4	1126.314	1.2664
	ate						
58	Geraniol	C106241	C ₁₀ H ₁₈ O	154.3	1369.8	907.809	1.2201
59	Methylpropanal	C78842	C ₄ H ₈ O	72.1	554.4	134.703	1.2832

^aMW: molecular mass; ^bRI: retention index; ^cRt: retention time; ^dDt: drift time.

Table S2. Information on the quantitated compounds of citrus-tea by HS-SPME-GC-MS.

N o.	Compound	Concentration (µg/g)																		
		WZ M	SMQ	XQG	NFM	GC	XJ	XN	ZM	CX	HY	DD	PS	LZ	BT	JP	XC	LF	YF	NHE
Phenolic_acids																				
1	d-Alanine	-	-	-	-	1.04± 0.22	0.35± 0.01	-	-	-	-	6.53± 0.27	-	-	4.41± 0.46	-	-	-	-	-
2	Acetic acid	0.47± 0.03	0.64± 0.09	0.46± 0.01	0.76± 0.06	3.38± 0.32	0.38± 0.04	0.75± 0.06	0.64± 0.03	0.33± 0.02	0.47± 0.07	1.97± 0.04	1.08± 0.32	0.36± 0.02	0.74± 0.06	0.12± 0.01	1.13± 0.16	0.74± 0.05	1.24± 0.64	1.64±0 .13
3	dl-Alanine	-	-	-	-	0.50± 0.03	1.36± 0.27	-	-	-	-	-	-	-	-	-	-	-	-	-
4	(2,5-dioxo-1-pyridin-3-ylmethyl-4-trifluoromethylimidazolidin-4-yl)amide-Cyclopropanecarboxylic acid	-	-	-	4.76± 0.64	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
5	Tridecanoic acid	-	2.73± 0.29	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
6	n-Decanoic acid	-	-	-	-	-	-	-	1.03± 0.36	-	-	-	-	-	-	-	-	-	-	-
7	n-Hexadecanoic acid	-	-	-	-	-	-	-	0.90± 0.02	-	-	-	-	-	-	-	-	-	-	-
8	3-(2-Isopropyl-5-methylphenyl)-2-methylpropionic acid	0.48± 0.03	1.63± 0.21	0.72± 0.04	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
9	4-hydroxy-1H-Indole-3-carboxylic acid	-	-	-	-	-	-	-	-	-	2.31± 0.31	-	-	-	-	-	-	-	-	-
10	(1R,2S)-2-Acetyl-1-methylcyclobutaneacetic acid	-	-	-	-	-	-	-	-	-	-	-	-	-	-	4.93± 0.68	-	-	-	-

11	3-amino-2-methyl-Butanoic acid	-	-	-	-	-	-	-	-	-	-	-	-	-	0.69±	-	-	-	-	-
															0.04					
12	(.+/-)- α ,4-dihydroxy-Benzeneacetic acid	-	-	-	-	-	-	-	-	-	-	-	-	0.56±	-	-	-	-	-	-
														0.06						
13	3-amino-2-methyl-Acetic acid	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.37±	-	-
																		0.07		
14	i-Propyl tricosanoate	3.01±	5.51±	6.32±	2.86±	0.36±	1.42±	-	-	2.24±	-	-	-	-	-	-	-	-	-	-
		0.32	0.74	1.03	0.42	0.07	0.09			0.37										
15	Neodihydrocarveol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.68±	2.14±	-
																		0.27	0.41	
16	Thymol	-	12.95	1.79±	-	-	-	3.57±	-	-	1.84±	-	4.49±	1.99±	-	-	-	-	-	-
			±1.29	0.54				0.39			0.24		0.75	0.37						
17	Carvacrol	16.21	8.43±	27.73	162.7	42.67	5.24±	21.96	11.07	6.99±	6.56±	18.86	4.39±	2.97±	23.10	62.24	6.87±	3.05±	24.44	25.59±
		±1.32	0.98	±3.26	9±6.2	±3.29	0.98	±3.14	±0.67	1.27	0.71	±1.67	0.35	0.42	±2.09	±4.19	1.28	0.74	±3.29	2.48
	Esters																			
18	i-Propyl tricosanoate	3.01±	5.51±	6.32±	2.86±	0.36±	1.42±	-	-	2.24±	-	-	-	-	-	-	-	-	-	-
		0.65	0.42	0.68	0.37	0.02	0.13			0.14										
19	Linalyl acetate	48.52	34.71	-	-	-	-	36.95	-	-	-	239.6	-	26.23	-	-	41.16	-	44.91	-
		±4.38	±2.29					±2.28				4±9.6		±3.28			±1.68		±2.18	
												8								
20	Methyl geraniate	0.59±	-	-	0.61±	-	-	0.45±	0.43±	0.55±	0.26±	-	0.47±	0.63±	-	-	0.87±	0.65±	0.80±	1.03±0
		0.06			0.08			0.03	0.07	0.05	0.07		0.09	0.02			0.12	0.06	0.04	.13

Table S2. (continued).

N o.	Compound	Concentration ($\mu\text{g/g}$)																		
		WZ M	SMQ	XQG	NFM	GC	XJ	XN	ZM	CX	HY	DD	PS	LZ	BT	JP	XC	LF	YF	NHE
21	Pentafluoropropionic acid, octyl ester	-	-	-	-	-	-	-	-	-	-	-	3.92± 1.03	-	-	-	-	-	-	-
22	Methyl benzoate	-	-	-	-	-	22.21 ±1.36	-	-	-	-	-	-	28.78 ±2.91	-	-	-	-	-	-
23	Ethyl caprate	-	-	-	-	-	-	-	1.01± 0.02	-	-	-	-	-	-	-	-	-	-	-
24	<i>trans</i> -Carveyl acetate	-	1.17± 0.15	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
25	Bicyclogermacrene	-	-	-	-	-	0.91± 0.04	-	1.48± 0.38	-	-	-	-	-	-	14.62 ±1.38	-	-	-	-
26	Octyl acetate	6.45± 0.29	2.96± 0.24	-	4.70± 0.68	-	-	3.83±	3.09±	4.37± 0.38	3.11± 0.35	14.47 ±1.24	3.16± 0.67	-	-	-	4.63± 1.03	2.53± 0.31	4.48± 0.38	-
27	1,6-Octadien-3-ol, 3,7-dimethyl-, 2-aminobenzoate	-	-	47.43 ±3.24	47.81 ±3.68	16.35 ±1.26	36.84 ±2.57	-	27.53 ±2.19	30.94 ±2.46	45.18 ±3.67	-	35.92 ±4.26	-	99.17 ±6.38	56.23 ±4.37	-	19.71 ±2.61	14.65 ±1.38	51.06 ±2.17
28	Perillyl acetate	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.73± 0.28	-	-	-
29	Geranyl acetate (Z)	16.33 ±2.19	12.70 ±1.06	15.37 ±1.09	21.29 ±1.09	54.22 ±9.68	47.61 ±3.67	13.73 ±2.19	8.12± 1.29	21.66 ±2.18	13.12 ±0.29	70.30 ±6.26	10.70 ±1.31	14.82 ±0.76	37.13 ±2.19	12.55 ±1.65	19.30 ±1.29	17.22 ±2.91	20.40 ±1.69	29.52 ±3.67
30	Geranyl acetate (E)	17.48 ±2.31	15.16 ±2.61	19.09 ±1.26	23.09 ±2.19	61.93 ±2.94	7.16± 0.75	14.61 ±2.19	8.32± 0.98	15.01 ±1.06	13.06 ±1.06	93.77 ±4.28	10.72 ±1.03	14.10 ±1.36	40.98 ±2.97	14.68 ±0.98	15.60 ±1.09	10.04 ±0.38	19.46 ±1.59	29.20 ±2.04
31	Decyl acetate	-	4.90± 0.12	-	-	4.76± 0.39	2.39± 0.17	-	-	-	-	-	-	-	-	0.30± 0.02	-	-	-	-
32	1-Decanol acetate	-	-	-	-	-	-	-	0.71± 0.03	1.65± 0.21	0.92± 0.03	10.03 ±0.98	1.05± 0.24	-	-	-	-	-	-	-

33	3-Hydroxymandelic acid, ethyl ester, di-TMS	-	1.79± 0.25	-	-	-	-	-	-	-	-	-	-	0.18± 0.02	-	-	-	2.12± 0.12	3.93± 0.63	-
34	linalool formate	-	-	-	-	67.45 ±3.25	45.36 ±2.26	-	-	-	-	-	-	-	-	-	-	-	-	-
35	Isopropoxycarbamic acid, ethyl ester	-	-	2.09± 0.67	-	-	-	-	-	-	-	-	-	-	-	-	-	1.98± 0.19	3.53± 0.25	-
36	Myrtenyl acetate	-	-	-	-	-	-	-	-	-	-	-	-	-	-	3.45± 0.36	-	-	-	-
37	Octyl trichloroacetate	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2.61± 0.57
38	Diethyl 4,4'-methylenedioxyphthalate	-	-	-	-	-	-	0.14± 0.02	-	-	-	-	-	-	-	-	0.37± 0.02	-	-	-
39	Butanoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester	-	-	-	-	-	-	-	-	0.46± 0.03	-	-	-	-	-	-	-	-	-	-
40	Z-Methyl geranate	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.30± 0.03	0.42± 0.08	-
41	Methyl caprate	-	-	-	-	-	-	-	0.49± 0.07	-	-	-	-	-	-	-	-	-	-	-
42	1-Octyl trifluoroacetate	-	-	-	-	-	-	-	-	-	3.64± 0.36	-	-	-	-	-	-	-	-	-
43	Methyl 5-acetyl-2-methoxybenzoate	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.09± 0.000	-	-	-
44	[2-Methyl-4-(piperidine-1-sulfonyl)phenoxy]acetic acid, methyl ester	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.26± 0.01	0.72± 0.06	-

Table S2. (continued).

N o.	Compound	Concentration ($\mu\text{g/g}$)																		
		WZ M	SMQ	XQG	NFM	GC	XJ	XN	ZM	CX	HY	DD	PS	LZ	BT	JP	XC	LF	YF	NHE
45	5,6,7,7a-Tetrahydro-4,4,7a-trimethyl-2(4H)-benzofuranone	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	3.25± 0.84	1.82± 0.12	-
	Alcohols																			
46	<i>cis</i> -p-Mentha-2,8-dien-1-ol	23.27 ±1.21	-	-	-	11.65 ±0.68	8.31± 1.03	-	-	32.09 ±3.28	-	-	-	-	30.28 ±2.16	-	-	15.26 ±1.18	21.35 ±1.38	3.63± 0.15
47	Terpinen-4-ol	21.45 ±3.69	-	-	-	-	19.16 ±2.03	28.56 ±1.03	-	16.22 ±1.75	12.22 ±0.98	31.61 ±4.67	11.54 ±2.37	-	47.70 ±6.28	35.86 ±4.59	17.72 ±3.58	-	-	18.89 ±1.38
48	Carveol	13.77 ±0.27	-	3.26± 0.75	-	-	-	-	-	-	7.59± 1.05	-	-	-	53.50 ±4.68	-	-	-	-	-
49	<i>trans</i> - β -Santalol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
50	1-Octanol	-	4.43± 0.36	19.71 ±2.06	10.85 ±1.36	-	6.55± 0.46	8.15± 0.74	4.67± 0.18	-	-	-	-	-	-	-	-	4.78± 0.35	7.12± 1.06	-
51	(R)-Lavandulol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
52	<i>cis</i> - β -Terpineol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
53	Linalool	144.8 4±6.9 8	462.6 8±9.6 8	148.4 8±7.1 5	269.6 5±14. 02	184.0 6±5.1 9	187.1 0±7.6 4	171.7 2±12. 35	118.3 6±6.5 4	131.6 1±8.4 6	291.7 2±11. 21	93.86 ±3.64	107.4 8±8.4 9	108.2 4±9.5 4	174.1 5±9.3 7	91.31 ±5.37	217.3 7±17. 62	386.2 7±11. 03	289.4 5±12. 13	147.9 2±12. 32
54	<i>trans</i> -p-Mentha-2,8-dienol	-	7.61± 0.38	49.42 ±2.74	-	14.69 ±2.19	23.76 ±1.32	-	14.34 ±1.28	-	-	24.21 ±2.37	-	-	41.39 ±3.18	28.36 ±2.19	-	-	-	-
55	<i>cis</i> -p-Menth-2,8-diene-1-ol	37.68 ±3.67	4.63± 0.35	43.32 ±3.24	41.36 ±6.38	10.50 ±1.23	15.86 ±1.65	41.78 ±3.28	8.95± 1.34	17.78 ±2.19	53.05 ±4.26	32.00 ±4.25	29.78 ±3.33	41.72 ±4.11	18.52 ±2.19	54.66 ±3.27	63.43 ±5.26	20.01 ±2.18	26.81 ±2.98	62.00 ±3.28
56	2,6-Dimethyl-1,5,7-octatrien-3-ol	-	-	-	8.04± 0.32	-	3.78± 0.12	7.56± 0.64	3.88± 0.12	4.68± 0.37	8.04± 0.74	-	5.75± 0.23	8.60± 0.57	22.17 ±1.32	-	11.12 ±0.65	5.49± 0.25	9.38± 1.06	10.79 ±0.45

57	Nerolidolcistrans	-	-	-	-	-	-	-	-	-	-	-	0.57±	2.45±	-	-	-	-	-	
													0.02	0.25	-	-	-	-	-	
58	(-)-4-Terpineol	-	25.72	140.0	40.89	-	-	-	20.51	-	-	-	-	26.71	-	-	18.37	32.18	-	
			±2.64	4±21.06	±2.98				±2.75					±3.29			±1.32	±2.65		
59	Isocarveol	65.61	-	97.86	-	227.3	156.2	94.40	-	-	90.49	116.8	67.66	61.51	204.2	46.19	68.69	79.09	111.9	221.8
		±2.38		±5.64		6±32.61	8±23.24	±15.32			±6.57	2±2.19	±2.19	±4.68	5±13.26	±3.29	±6.36	±7.16	6±6.34	5±23.12
60	p-Menth-1-en-8-ol	13.83	39.78	85.64	55.20	-	22.91	31.62	27.73	14.98	9.04±	49.66	11.02	10.83	51.15	34.63	15.54	-	22.66	-
		±1.32	±2.35	±6.24	±2.03		±2.16	±3.61	±2.31	±1.67	0.68	±2.34	±1.37	±0.68	±4.22	±3.19	±2.31		±1.32	
61	cis-β-Terpineol	-	-	1.91±	-	-	-	-	-	-	-	-	-	0.62±	-	-	-	-	-	-
				0.32										0.09						
62	Nerol	-	-	-	27.82	-	-	25.81	-	17.25	-	-	13.39	-	-	-	-	25.84	32.75	-
					±3.21			±1.32		±2.01			±1.03					±2.31	±2.15	
63	2-Methyl-6-methylene-octa-1,7-dien-3-ol	-	3.64±	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
			0.35																	
64	3,6-dimethoxy-9-(2-phenylethynyl)-Fluoren-9-ol	-	1.67±	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
			0.37																	
65	(Z)-Carveol	39.77	18.24	93.75	37.26	129.6	58.01	36.91	15.52	20.09	26.52	78.74	24.52	42.79	133.6	30.31	44.48	11.43	47.13	59.00
		±2.03	±1.32	±6.24	±2.13	6±5.12	±2.17	±3.25	±0.96	±2.16	±1.38	±6.28	±3.64	±2.19	9±6.27	±2.19	±3.65	±1.32	±3.61	±3.27

77	τ -Muurolol	-	0.98± 0.21	-	-	-	-	-	-	0.38± 0.03	-	-	-	-	-	-	-	-	-
78	β -Eudesmol	-	-	-	-	-	-	-	-	0.40± 0.01	-	-	-	-	-	1.13± 0.02	-	-	-
79	1-(1-methylene-2-propenyl)-Cyclopentanol	-	-	1.38± 0.36	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
80	Phytol	-	-	-	0.29± 0.12	-	-	0.33± 0.03	0.18± 0.02	-	-	-	-	-	-	-	-	-	0.31± 0.01
81	<i>trans</i> -Nerolidol	-	-	-	-	-	-	-	-	1.93± 0.32	31.61 ±2.37	-	-	-	-	-	-	-	-
82	(+)- β -Citronellol	-	-	45.53 ±2.37	-	-	-	-	23.05 ±2.36	-	-	-	-	-	-	-	-	-	-
83	p-Mentha-1(7),8(10)-dien-9-ol	-	-	-	-	-	-	-	-	-	-	2.33± 0.35	3.18± 0.27	-	-	-	2.68± 0.16	3.84± 0.17	7.30± 0.45
84	2-Methyl-1,5-heptadien-4-ol	0.64± 0.03	-	-	-	-	-	0.71± 0.12	-	-	-	-	-	-	-	-	1.32± 0.31	1.14± 0.01	-
85	2-(4-Methylphenyl)propan-2-ol	-	8.82± 0.65	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
86	<i>L</i> - α -Terpineol netural	-	-	-	-	44.35	-	-	-	-	-	-	-	-	-	-	-	-	-
87	Nerolidol 2	-	-	-	-	-	-	-	-	-	-	0.83	0.65	-	-	-	-	-	-

Table S2. (continued).

	Compound	Concentration ($\mu\text{g/g}$)																	
		WZ M	SMQ	XQG	NFM	GC	XJ	XN	ZM	CX	HY	DD	PS	LZ	BT	JP	XC	LF	YF
88	1-(methylenecyclopropyl)-Cyclopentanol	-	19.33 ± 2.36	-	-	-	-	-	-	24.82 ± 1.12	-	-	-	-	-	-	-	-	-
89	(2Z,6E)-Farnesol	-	-	-	-	-	-	3.84 \pm 0.32	1.40 \pm 0.12	-	2.34 \pm 0.21	-	-	1.58 \pm 0.31	-	-	-	-	-
90	Coolact	-	-	4.82 \pm 0.334	-	39.99 ± 3.65	43.21 ± 3.29	-	-	-	-	-	-	-	-	-	-	-	-
91	3-Methoxybenzyl alcohol	-	-	-	-	8.11 \pm 1.31	4.36 \pm 0.31	-	-	-	-	-	-	-	-	-	-	-	-
92	1-chloro-2-Propanol	-	-	0.41 \pm 0.03	-	-	0.26 \pm 0.01	-	-	-	0.20 \pm 0.009	-	-	-	-	0.30 \pm 0.03	-	0.03 \pm 0.000	-
93	2-(2-Hydroxyethoxy)ethanol 1-nitrate	-	-	0.07 \pm 0.000	-	-	-	-	-	-	-	-	-	-	-	-	-	2.68 \pm 0.68	3.78 \pm 0.46
94	L(-)-Menthol	-	-	6.75 \pm 0.67	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
95	p-Menth-1-en-9-ol(8Cl)	-	-	11.62 ± 2.36	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
96	4-Methoxyphenyl methyl carbinol	-	-	-	-	-	-	-	-	-	-	-	-	10.93 ± 1.32	-	-	-	-	-
97	<i>trans</i> -3-methylpent-3-ene-5-ol	-	-	-	-	2.36 \pm 0.21	6.09 \pm 1.03	-	-	-	-	-	-	-	-	-	-	-	-
98	1,3-Methano-5bH-cyclobuta[cd]p entalen-5b-ol, octahydro-	-	-	-	-	4.67 \pm 0.45	9.02 \pm 0.97	-	-	-	-	-	-	-	-	-	-	-	17.19 ± 2.61

Table S2. (continued).

N o.	Compound	Concentration ($\mu\text{g/g}$)																		
		WZ M	SMQ	XQG	NFM	GC	XJ	XN	ZM	CX	HY	DD	PS	LZ	BT	JP	XC	LF	YF	NHE
11 2	$\alpha,2,6,6$ -Tetramethyl-1-cyclohexen e-1-methanol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.97 \pm 0.03	2.08 \pm 0.17	-
11 3	(+/-)-1-amino-2-Propanol	-	-	-	-	-	-	-	-	-	-	-	0.34 \pm 0.01	-	-	-	-	-	-	-
11 4	<i>cis</i> -Linaloloxide	-	-	-	-	-	-	-	-	-	-	-	2.52 \pm 0.24	-	-	-	-	-	-	-
	Aldehydes																			
11 5	Dodecanal	-	-	-	-	-	-	-	-	-	-	-	-	0.70 \pm 0.06	-	-	-	0.60 \pm 0.03	-	-
11 6	Benzeneacetaldehyde	-	-	-	-	-	4.07 \pm 0.21	-	-	-	-	-	-	-	-	-	-	-	-	-
11 7	1,3-Dioxan-5-ol	0.06 \pm 0.000 1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
11 8	(E)-3,7-dimethyl-2,6-Octadienal	-	-	-	-	-	-	-	2.40 \pm 0.29	-	-	-	2.70 \pm 0.14	-	-	-	-	6.36 \pm 0.68	7.42 \pm 0.74	-
11 9	Nonanal	-	-	-	10.16 \pm 1.02	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
12 0	Octadecanal	-	-	-	-	-	-	-	-	0.74 \pm 0.06	-	-	-	-	-	-	-	-	-	-
12 1	Citronellal	-	0.95 \pm 0.04	-	-	-	-	-	2.25 \pm 0.37	-	-	-	-	-	-	-	-	-	-	-
12 2	Citral	-	-	-	-	-	-	-	-	-	-	-	-	2.09 \pm 0.31	-	-	-	-	-	-

Table S2. (continued).

N o.	Compound	Concentration ($\mu\text{g/g}$)																		
		WZ M	SMQ	XQG	NFM	GC	XJ	XN	ZM	CX	HY	DD	PS	LZ	BT	JP	XC	LF	YF	NHE
13 4	Tridecanal	-	-	1.89± 0.24	-	9.88± 0.24	-	-	-	-	-	-	-	-	-	-	-	-	-	-
13 5	2-methyl-3-methylene-Cyclopentanecarboxaldehyde	-	16.97 ±2.31	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
13 6	4-Cyclohexylidenebutyraldehyde	-	-	124.6 2±4.2 1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
13 7	Benzaldehyde	-	-	-	-	-	-	-	-	-	-	0.39± 0.02	-	-	-	-	-	-	-	-
13 8	(+)-Citronellal	-	-	-	2.73± 0.27	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
13 9	dimethoxy-Methane	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.97± 0.04	1.25± 0.27	-
14 0	3,5-Dimethylcyclohex-1-ene-4-carboxaldehyde Ketones	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.57± 0.02	0.73± 0.03	-
14 1	(+)-Dihydrocarvone	5.92± 1.03	-	7.44± 0.68	-	-	-	-	-	2.35± 0.28	-	-	-	-	-	-	5.50± 0.45	-	-	-
14 2	Hydroxyacetone	-	-	-	-	-	-	-	0.28± 0.02	-	-	-	-	-	-	-	-	-	-	-
14 3	2-(1-methylpropyl)-Cyclopentanone	-	-	-	18.76 ±2.61	-	-	-	-	9.62± 1.24	-	-	-	20.03 ±3.17	-	-	-	-	-	-

14	2-Hydroxy-5-methyl	1.31±			0.44±															
4	acetophenone	0.21	-	-	0.01	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
14	4-Isopropenylcyclohexanone	-	-	-	-	-	-	-	2.79±	-	-	-	3.75±	-	-	-	-	-	-	
5									0.23				0.27							
14	Hydroxyacetone	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	12.37	-	-	
6																	±2.17			
14	[1,1'-Bicyclopentyl]-2-one	-	-	-	0.75±	0.57±	0.54±	-	-	-	-	-	0.45±	0.78±	-	-	-	-	1.28±	
7					0.27	0.07	0.04						0.06	0.18					0.24	
14	<i>trans</i> -Dihydrocarvone	-	2.90±	-	28.28	18.15	3.55±	-	0.90±	-	-	2.98±	18.44	1.79±	-	-	-	3.71±	-	
8			0.37		±2.31	±2.08	0.37		0.14			0.19	±2.31	0.57				0.93		
14	3-Methoxyacetophenone	-	-	-	-	-	0.54±	-	-	-	-	-	-	2.23±	-	-	-	-	-	
9							0.18							0.47						
15	3,5-Octadien-2-one	-	1.25±	-	-	-	-	0.74±	0.47±	-	-	-	-	2.18±	5.67±	-	-	-	-	
0			0.27					0.27	0.03					0.57	1.06					
15	<i>D</i> (+)-Carvone	23.01	15.57	47.23	25.31	98.32	33.30	24.08	14.52	23.17	13.12	61.32	18.72	24.48	92.50	22.81	33.44	-	31.24	29.80
1		±2.37	±0.37	±2.17	±2.57	±3.28	±3.21	±1.27	±2.34	±3.23	±2.18	±3.58	±1.27	±2.16	±0.57	±3.21	±2.31	-	±2.18	±3.57
15	Piperiton	-	-	1.16±	0.68±	-	-	0.79±	0.85±	-	-	-	-	0.50±	1.69±	-	-	-	1.29±	-
2				0.07	0.03			0.04	0.17					0.01	0.07				0.91	
15	β -Lonone	-	-	-	-	-	-	-	1.28±	-	-	-	1.63±	3.53±	1.42±	-	-	-	3.20±	-
3								0.27				0.34	0.57	0.09				0.37		
15	6,10,14-trimethyl-2-Pentadecanone	-	-	-	-	-	-	0.63±	-	-	-	-	-	0.51±	-	-	-	0.67±	0.89±	1.23±
4								0.04						0.18				0.14	0.18	0.67
15	β -Ionone	-	-	3.92±	4.01±	6.30±	-	2.79±	2.00±	-	-	-	-	1.62±	-	-	-	1.21±	-	3.74±
5				0.38	0.87	0.68		1.03	0.37					0.27				0.18		1.08
15	Jasmolin I	-	-	-	-	9.34±	7.69±	1.58±	-	2.00±	5.14±	17.54	-	0.86±	2.42±	-	-	-	-	3.05±
6						1.37	1.05	0.06		0.24	0.68	±2.27		0.29	0.37					0.37

Table S2. (continued).

N o.	Compound	Concentration ($\mu\text{g/g}$)																			
		WZ M	SMQ	XQG	NFM	GC	XJ	XN	ZM	CX	HY	DD	PS	LZ	BT	JP	XC	LF	YF	NHE	
18 1	β -Terpinene	-	-	-	0.72 \pm 0.02	-	-	-	-	-	-	-	-	-	-	-	-	0.84 \pm 0.02	0.69 \pm 0.05	-	
18 2	α -Pinene	3.05 \pm 1.02	8.79 \pm 1.07	11.36 \pm 2.03	7.80 \pm 1.27	3.94 \pm 0.36	3.32 \pm 1.03	3.19 \pm 0.75	12.83 \pm 1.45	5.80 \pm 0.57	3.59 \pm 0.37	3.32 \pm 0.74	0.87 \pm 0.18	0.98 \pm 0.05	2.23 \pm 0.43	1.23 \pm 0.36	2.36 \pm 0.27	1.36 \pm 0.45	2.77 \pm 0.14	0.67 \pm 0.34	
18 3	β -Pinene	8.92 \pm 0.87	-	-	-	-	-	-	-	4.95 \pm 0.96	-	-	-	-	-	7.78 \pm 0.37	-	-	-	-	
18 4	1,3,8-p-Menthatriene	3.79 \pm 0.27	-	50.46 \pm 2.37	4.13 \pm 1.33	47.41 \pm 3.87	31.39 \pm 2.1	-	-	6.67 \pm 0.18	1.92 \pm 0.24	-	1.93 \pm 0.27	24.05 \pm 3.57	33.03 \pm 3.14	-	4.50 \pm 0.34	3.29 \pm 0.21	4.44 \pm 0.37	38.29 \pm 1.27	
18 5	2-Isopropenyl-5-methylhex-4-enal	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	21.75 \pm 2.17	-	-	-
18 6	2,5,5-trimethyl-1,3,6-Heptatriene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.31 \pm 0.32	-	-	-
18 7	β -Myrcene	29.22 \pm 3.21	22.88 \pm 3.27	17.40 \pm 2.09	35.59 \pm 1.98	26.17 \pm 3.17	19.63 \pm 1.98	17.59 \pm 2.18	17.29 \pm 2.33	24.22 \pm 6.28	17.32 \pm 4.29	55.50 \pm 6.32	11.63 \pm 3.27	12.96 \pm 2.04	32.03 \pm 4.16	25.65 \pm 2.09	29.89 \pm 3.27	13.90 \pm 2.31	22.93 \pm 2.32	30.50 \pm 2.34	
18 8	D-Limonene	803.5 2 \pm 35.	754.9 1 \pm 24.	779.2 5 \pm 35.	901.3 4 \pm 45.	1594. 93 \pm 24	843.0 3 \pm 35.	610.8 8 \pm 17.	509.6 7 \pm 14.	674.5 2 \pm 32.	439.8 0 \pm 10.	1330. 21 \pm 35	369.7 7 \pm 17.	492.7 3 \pm 20.	2037. 63 \pm 38	948.5 9 \pm 34.	974.5 9 \pm 45.	410.5 3 \pm 17.	855.1 6 \pm 35.	1069. 29 \pm 26	
18 9	β -Ocimene	3.68 \pm 0.39	6.55 \pm 1.21	4.19 \pm 0.47	5.69 \pm 0.34	7.26 \pm 1.01	4.31 \pm 0.18	8.16 \pm 0.73	9.64 \pm 1.34	6.67 \pm 0.39	3.19 \pm 0.24	14.25 \pm 1.28	11.03 \pm 1.77	2.76 \pm 0.22	3.61 \pm 0.38	7.09 \pm 0.27	1.36 \pm 0.06	3.64 \pm 0.33	4.26 \pm 0.19	1.11 \pm 0.02	
19 0	2,5,5-trimethyl-1,5-Cyclooctadiene	-	-	-	-	-	-	-	-	-	2.33 \pm 0.27	-	-	-	-	-	-	-	-	-	
19 1	(Z)- β -Ocimene	5.57 \pm 0.68	3.17 \pm 0.38	8.94 \pm 1.06	-	7.83 \pm 2.19	-	3.39 \pm 1.06	2.90 \pm 0.37	-	3.09 \pm 0.57	16.88 \pm 2.01	1.99 \pm 0.24	-	6.34 \pm 0.39	-	4.16 \pm 0.37	4.01 \pm 0.18	3.16 \pm 0.24	1.20 \pm 0.05	

19		62.34	109.2	34.02	75.80	68.25	21.47	44.57	60.61	64.83	35.52	20.35	12.41	17.15	37.56	96.58	25.09	8.18±	28.18	27.76
2	γ -Terpinene	±5.68	6±7.68	±2.67	±6.32	±5.27	±2.07	±2.37	±3.24	±3.57	±2.18	±3.27	±2.18	±1.08	±2.27	±3.57	±3.74	1.09	±3.27	±2.19
19			6.70±							0.68±										
3	Terpinolene	-	0.67	-	-	-	-	-	-	0.06	-	-	-	-	-	-	-	-	-	-
19				1.82±		9.45±	24.80			2.76±	13.00				27.55					9.85±
4	Cosmene	-	-	0.37	-	1.32	±2.37	-	-	0.37	±3.24	-	-	-	±3.24	-	-	-	-	1.98
19	2-Methyl-3-trans-propenylpyrazi														6.12±					2.77±
5	ne	-	-	-	-	-	-	-	-	-	-	-	-	-	1.32	-	-	-	-	0.35
19						0.69±	1.77±						0.03±				0.04±			
6	4-Acetyl-1-methyl-1-cyclohexene	-	-	-	-	0.21	0.68	-	-	-	-	-	0.000	-	-	-	0.000	-	-	-
													2				1			
19		3.18±																		
7	3-Carene	1.03	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
19		4.53±											1.67±				2.63±			
8	2-methyl-6-methylene-1,7-Octadie	0.21	-	-	-	-	-	-	-	-	-	-	0.35	-	-	-	0.36	-	-	-
	n-3-one																			
19																	3.10±			
9	1,4-Pentadiene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.37	-	-	-
20			3.09±																	
0	1,Z-5,E-7-Dodecatriene	-	0.31	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
20															21.51			1.49±		
1	α -Humulene	-	-	-	-	-	-	-	-	-	-	±2.35	-	-	-	-	-	0.02	-	-
20															27.38			24.68		
2	<i>cis</i> - β -Farnesene	-	-	-	-	-	-	-	-	-	-	±4.32	-	-	-	-	-	±2.35	-	-
20								4.17±							9.37±			7.65±		
3	Cyclohexene, 2-ethenyl-1,3,3-trimethyl-	-	-	-	-	-	-	1.27	-	-	-	2.03	-	-	-	-	-	0.67	-	-

Table S2. (continued).

N o.	Compound	Concentration ($\mu\text{g/g}$)																		
		WZ M	SMQ	XQG	NFM	GC	XJ	XN	ZM	CX	HY	DD	PS	LZ	BT	JP	XC	LF	YF	NHE
20 4	Bicyclo[4.1.0]hept-2-ene, 3,7,7-trimethyl-	-	-	13.45 ± 3.27	5.28 \pm 2.03	-	-	-	-	-	1.49 \pm 0.27	-	-	-	-	10.84 ± 2.03	-	-	-	-
20 5	Longifolene-(V4)	-	-	0.60 \pm 0.01	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
20 6	α -Cubebene	2.85 \pm 0.32	5.71 \pm 1.23	2.14 \pm 0.32	3.26 \pm 1.02	15.85 ± 3.65	6.59 \pm 1.02	1.74 \pm 0.36	1.20 \pm 0.03	5.66 \pm 0.57	2.43 \pm 0.21	17.01 ± 3.21	1.86 \pm 0.23	1.97 \pm 0.21	10.10 ± 1.94	5.43 \pm 0.37	1.81 \pm 0.26	2.16 \pm 0.07	2.58 \pm 0.35	5.60 \pm 1.03
20 7	2,6-dimethyl-2,6-Octadiene	5.16 \pm 0.24	2.74 \pm 0.16	3.92 \pm 0.35	5.89 \pm 1.06	14.92 ± 1.62	2.35 \pm 0.21	3.62 \pm 1.23	2.84 \pm 0.36	4.18 \pm 1.06	2.81 \pm 0.67	13.85 ± 2.06	2.91 \pm 0.28	4.53 \pm 1.03	10.64 ± 2.06	3.73 \pm 0.67	6.54 \pm 1.06	2.43 \pm 0.24	6.24 \pm 0.26	8.19 \pm 2.14
20 8	1,6-dimethyl-1,5-Cyclooctadiene	-	-	0.75 \pm 0.01	-	-	-	-	-	-	0.65 \pm 0.06	-	-	-	-	0.51 \pm 0.02	-	-	-	-
20 9	Copaene	3.42 \pm 0.343	4.95 \pm 1.03	1.91 \pm 0.06	4.30 \pm 0.37	8.60 \pm 1.37	0.70 \pm 0.02	2.48 \pm 1.06	2.35 \pm 0.16	4.11 \pm 0.68	3.07 \pm 1.26	12.23 ± 1.26	2.50 \pm 0.24	2.41 \pm 0.35	4.37 \pm 0.34	5.71 \pm 0.39	1.87 \pm 0.34	2.68 \pm 0.16	3.64 \pm 1.03	5.81 \pm 0.37
21 0	(-)- β -Elemene	25.96 ± 5.64	63.45 ± 6.98	24.22 ± 2.15	12.85 ± 2.36	50.17 ± 6.37	29.91 ± 6.24	8.54 \pm 1.17	7.35 \pm 1.26	13.85 ± 1.35	13.26 ± 2.06	64.71 ± 6.49	8.69 \pm 0.67	9.15 \pm 1.26	16.65 ± 2.09	27.51 ± 2.18	6.58 \pm 0.36	5.22 \pm 0.29	10.38 ± 1.26	19.26 ± 1.32
21 1	β -Caryophyllene	7.08 \pm 0.79	12.99 ± 2.06	8.93 \pm 0.68	8.48 \pm 0.37	15.01 ± 1.26	2.79 \pm 0.27	5.04 \pm 1.06	4.38 \pm 0.36	11.45 ± 2.18	-	43.72 ± 5.18	7.51 \pm 0.38	4.19 \pm 0.37	14.02 ± 1.37	23.69 ± 2.19	3.26 \pm 1.02	2.69 \pm 0.35	6.45 \pm 1.36	9.45 \pm 0.26
21 2	α -Terpinene	-	-	-	-	-	-	-	-	-	0.27 \pm 0.03	-	-	-	-	0.59 \pm 0.07	-	-	-	-
21 3	(-)-Germacrene D	3.63 \pm 0.64	16.52 ± 1.37	-	8.77 \pm 1.24	8.88 \pm 0.36	6.79 \pm 1.02	-	2.54 \pm 0.12	8.59 \pm 1.36	20.63 ± 2.47	35.59 ± 3.58	1.01 \pm 0.05	4.13 \pm 0.34	5.01 \pm 1.02	8.43	0.88 \pm 0.07	0.93 \pm 0.12	5.32 \pm 1.07	4.76 \pm 0.25
21 4	γ -Elemene	2.55 \pm 0.54	8.32 \pm 1.21	4.48 \pm 1.21	4.35 \pm 0.35	10.83 ± 1.57	8.87 \pm 1.36	2.37 \pm 1.27	1.37 \pm 0.34	5.78 \pm 0.15	9.79 \pm 1.24	32.98 ± 3.54	2.36 \pm 0.12	1.55 \pm 0.07	3.80 \pm 0.58	12.80 ± 1.27	0.66 \pm 0.05	1.09 \pm 0.08	1.75 \pm 0.37	4.42 \pm 0.57
21 5	1,1,7-Trimethyl-4-methylenedeca hydro-1H-cyclopropa[e]azulene	-	1.20 \pm 0.12	0.77 \pm 0.04	-	-	-	-	-	0.96 \pm 0.12	11.63 ± 1.34	9.59 \pm 1.25	-	-	-	3.28 \pm 0.15	-	-	1.03 \pm 0.57	0.84 \pm 0.05

26	1-chloro-2-methyl-2-Butene	11.51	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
5		±2.01																		
26	2,4,4-Trimethyl-3-hydroxymethyl-5a-(3-methyl-but-2-enyl)-cyclohexene	1.09±	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
6		0.03																		
26	7,8-dehydro-8a-hydroxy-Isolongifolene	0.63±	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
7		0.02																		
26	1-methyl-5-(1-methylethenyl)-Cyclohexene	-	-	-	-	-	-	2.73±	1.49±	-	1.92±	-	-	1.84±	-	-	-	2.78±	3.16±	-
8								0.46	0.13		0.08			0.35				0.15	0.75	
26	Bicyclo[6.1.0]non-1-ene	-	-	-	-	-	-	-	2.57±	-	-	-	-	-	-	-	-	-	-	-
9									0.21											
27	1,1-dichloro-3,4-dimethyl-Germacyclopent-3-ene	-	-	-	-	-	-	-	-	-	0.77±	-	-	-	-	-	-	-	-	-
0											0.03									
27	Ledene oxide (I)	-	-	-	-	-	-	-	-	-	0.43±	-	-	-	-	-	-	-	-	-
1											0.04									
27	Cyclohexene, 1-methyl-5-(1-methylethenyl)-, (R)-	-	-	-	3.02±	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
2					0.67															
27	2-Octene, 2-methyl-6-methylene-	-	-	-	4.44±	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
3					0.45															
27	Bicyclopentyl-1,1'-diene	-	-	-	54.49	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
4					±2.36															
27	(E,E)-7,11,15-Trimethyl-3-methylene-hexadeca-1,6,10,14-tetraene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2.97±	4.36±	-
5																		0.14	0.36	

Table S2. (continued).

N o.	Compound	Concentration ($\mu\text{g/g}$)																		
		WZ M	SMQ	XQG	NFM	GC	XJ	XN	ZM	CX	HY	DD	PS	LZ	BT	JP	XC	LF	YF	NHE
27 6	1-(1,4-dimethyl-3-cyclohexen-1-yl)-Ethanone	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.98± 0.32	1.68± 0.12	-
27 7	Caryophyllene (I1)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
27 8	Tricyclo[2.2.2.0(1,4)]octane	-	-	-	0.85± 0.21	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
27 9	Alloaromadendrene oxide-(1)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.34±	-	-	-	-
28 0	Ethylene oxide	-	0.43±	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
28 1	Tricyclo[4.4.1.0(1,6)]undecane	-	0.59± 0.06	-	43.46 ±4.29	-	-	-	-	-	-	-	-	-	-	-	-	54.77 ±7.21	-	-
28 2	2,3-Epoxy-pinane	55.27 ±6.25	-	-	-	219.6 9±15.21	125.3 2±7.64	-	-	-	-	-	-	-	202.2 8±16.24	-	-	-	-	-
28 3	7-(1-methylethylidene)-Bicyclo[4.1.0]heptane	-	-	-	-	3.70± 0.23	1.02± 0.12	-	-	-	0.30± 0.01	-	-	-	-	-	-	-	-	-
28 4	8-(1-methylethylidene)-Bicyclo[5.1.0]octane	-	-	-	-	-	-	-	-	0.45± 0.08	-	-	-	-	-	-	-	-	-	-
28 5	Isoaromadendrene epoxide	0.70± 0.02	3.21± 0.23	2.28± 0.64	-	2.53± 0.12	1.36± 0.11	-	-	-	-	-	0.77± 0.31	-	-	0.91± 0.08	-	-	-	0.91± 0.02

30	7-Chloro-2,3-dihydro-3-(4-N,N-dimethylaminobenzylidene)-5-phenyl-1H-1,4-benzodiazepin-2-one	-	-	-	1.13±	-	-	1.08±	0.19±	-	-	-	-	-	-	-	-	-	-	-
9					0.02			0.32	0.001											
31	2-Chloro-4-(4-methoxyphenyl)-6-(4-nitrophenyl)pyrimidine	-	0.75±	-	-	-	-	-	-	-	-	-	-	-	-	-	0.76±	-	-	-
0			0.01														0.02			
31	3,5-Di-tert-butylcatechol	-	0.79±	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
1			0.01																	
31	4-ethyl-2-methoxy-Phenol	-	-	-	-	11.65	9.48±	-	-	-	-	-	-	-	-	-	-	-	-	-
2						±1.03	1.32													
31	3-Methyl-4-isopropylphenol	8.71±	31.91	-	-	66.93	39.90	-	-	5.75±	10.45	-	-	18.70	23.51	-	1.65±	0.78±	-	
3		1.32	±4.65			±2.31	±3.25			0.64	±2.01			±1.36	±3.26		0.35	0.08		
31	2-Methoxy-4-vinylphenol	-	-	2.23	-	193.9	65.61	-	3.07±	2.45±	-	-	1.48±	113.7	-	-	-	-	-	
4						5±7.3	±3.64		0.32	0.36			0.23	8±9.3	-	-	-	-	-	
						6								4						
31	9-Amino-7-mercapto-5,6,8,10-tetraaaza-benzo[b]fluoren-11-one	-	-	1.21±	-	-	-	0.53±	-	-	-	-	-	-	-	-	-	-	-	
5				0.03				0.01												
31	4-methyl-Benzamide	-	-	-	-	3.80±	1.36±	-	-	-	-	-	-	-	-	-	-	-	-	
6						0.12	0.26													
31	Durophenol	-	-	-	-	31.40	16.98	-	-	-	-	-	1.42±	-	-	1.54±	-	-	-	
7						±3.68	±1.32						0.05			0.01				

Table S2. (continued).

N o.	Compound	Concentration (µg/g)																		
		WZ M	SMQ	XQG	NFM	GC	XJ	XN	ZM	CX	HY	DD	PS	LZ	BT	JP	XC	LF	YF	NHE
31	(2-Nonyloxy-benzyl)-phenyl-amine	-	-	5.96±	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
8				0.32																
31	13H-Dibenzo[a,i]carbazole	-	-	-	-	-	-	-	-	-	-	-	-	-	2.15±	-	1.17±	0.68±	-	
9															0.32		0.32	0.02		

32	2-[1-(2-phenylethyl)-2-benzimidazolymethylthio]-Benzothiazole	-	-	-	-	-	-	-	-	-	-	-	-	-	1.17±	-	-	-	-
0															0.02				
32	5-ethyl-3-(3-methyl-5-phenylpyrazol-1-yl)-1,2,4-Triazol-4-amine	1.34±	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
1		0.01																	
32	2-Nitrobenzenesulfonohydrazide	-	-	-	-	-	-	-	-	-	-	-	-	3.12±	-	-	-	-	-
2														0.12					
32	1,3-dimethyl-5,6-dimethoxy-2-(3,5-dimethoxyphenyl)-1H-Indole	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.61±	1.23±	-
3																0.01	0.003		
32	N-[4-[1-(3-trifluoromethylbenzyl)-2-benzimidazolyl]-3-furazanyl]-Acetamide	-	-	-	-	-	-	-	-	-	-	-	-	3.55±	-	-	-	-	-
4														0.32					
32	2-Amino-4-hydroxy-6-phenethylpteridine	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.73±	-	-	-
5															0.03				
32	2-ethyl-4,5-dimethyl-Phenol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	4.06±	-	-	-
6															0.68				
32	2,4-dimethyl-Benzo[h]quinoline	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	10.65	12.31	-
7																	±1.32	±2.31	
32	2-(4-Methoxy-phenoxy)-6-methyl-4-phenyl-quinazoline	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2.32±	1.29±	-
8																	0.06	0.31	
32	N-[4-(1-methylethyl)benzylidene]-4-(1-pyrrolidylsulfonyl)-Benzamine	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.12±	0.67±	-
9																	0.001	0.01	
33	5-(3-aminopropyl)-5,10-dihydro-1H-Dibenzo[b,e][1,4]diazepin-11-one	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.21±	0.31±
0																	0.23	0.01	
	Others																		
33	Dimethyl ether	-	-	10.13	-	1.36±	2.54±	-	-	-	-	-	-	-	-	1.01±	-	-	-
1				±0.31		0.04	0.05									0.02			

34									1.75±											
3	N-Benzylformamide	-	-	-	-	-	-	-	0.21	-	-	-	-	-	-	-	-	-	-	-
34																				
4	5H-Naphtho[2,3-c]carbazole	-	-	3.92±	-	-	0.99±	-	-	-	-	-	-	-	-	-	-	-	-	-
				0.24			0.01													
34																				
5	1-methyl-1H-Pyrazole	-	-	-	-	-	-	-	-	-	-	-	-	-	1.47±	-	-	-	-	-
															0.01					
34																				
6	1-(5-trifluoromethyl-2-pyridyl)-4-(1H-pyrrol-1-yl)-Piperidine	-	-	-	1.40±	-	-	-	-	-	-	-	-	-	0.75±	-	-	-	-	-
					0.03										0.02					
34																				
7	(2-Aziridinyloethyl)amine	-	-	-	-	-	-	-	-	-	-	-	-	-	0.78±	-	-	-	-	-
															0.12					
34																				
8	1-ethyl-1H-Pyrrole-2-carboxaldehyde	-	-	-	-	3.45±	2.77±	-	-	-	-	-	-	-	-	-	-	-	-	-
						0.42	0.35													
34																				
9	5-methyl-1H-Indole	-	-	-	-	-	0.79±	-	-	-	-	-	-	-	-	-	-	-	-	-
							0.01													
35																				
0	2-[N-Aziridyl]methylpyrrole	-	-	-	-	0.69±	1.49±	-	-	-	-	-	-	-	-	-	-	-	-	-
						0.03	0.24													
35																				
1	2-(methylamino)-Ethanol	0.59±	-	-	-	-	-	-	1.57±	-	-	-	-	-	-	-	-	-	-	-
		0.04							0.12											
35																				
2	Betazole	0.94±	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
		0.03																		
35																				
3	9-Vinylcarbazole	-	-	-	-	-	-	2.55±	-	-	-	-	-	-	-	-	-	-	-	-
								0.34												
35																				
4	2-Propanamine	-	-	-	-	-	-	-	0.51±	-	-	-	-	-	-	-	-	-	-	-
									0.01											
35																				
5	1,2-Hydrazinedicarboxamide	-	-	-	-	-	-	-	1.39±	-	-	-	-	-	-	-	-	-	-	-
									0.12											
35																				
6	1-(1,1-Dioxo-tetrahydro-1.lambda.(6)-thiophene-3-sulfonyl)-piperidine	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	5.13±	4.21±	-	-
																	0.17	0.12		

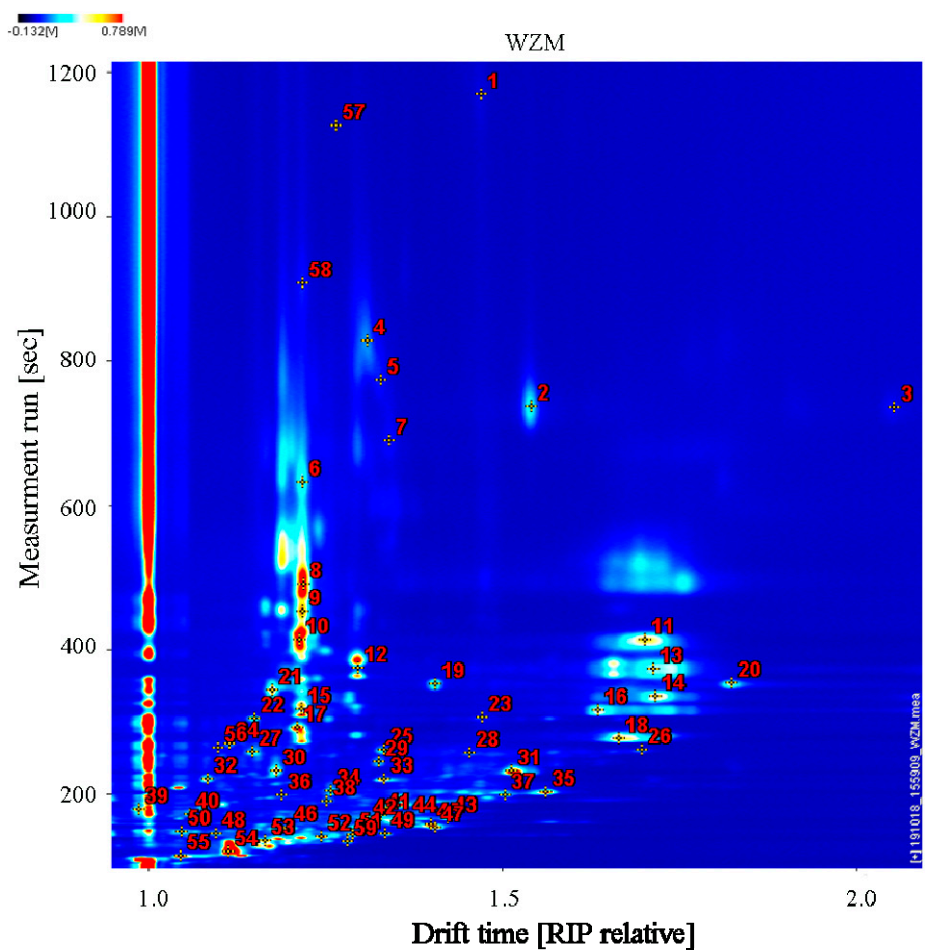


Figure S1. Ion migration spectra of WZM. The numbers are the identified volatile components.

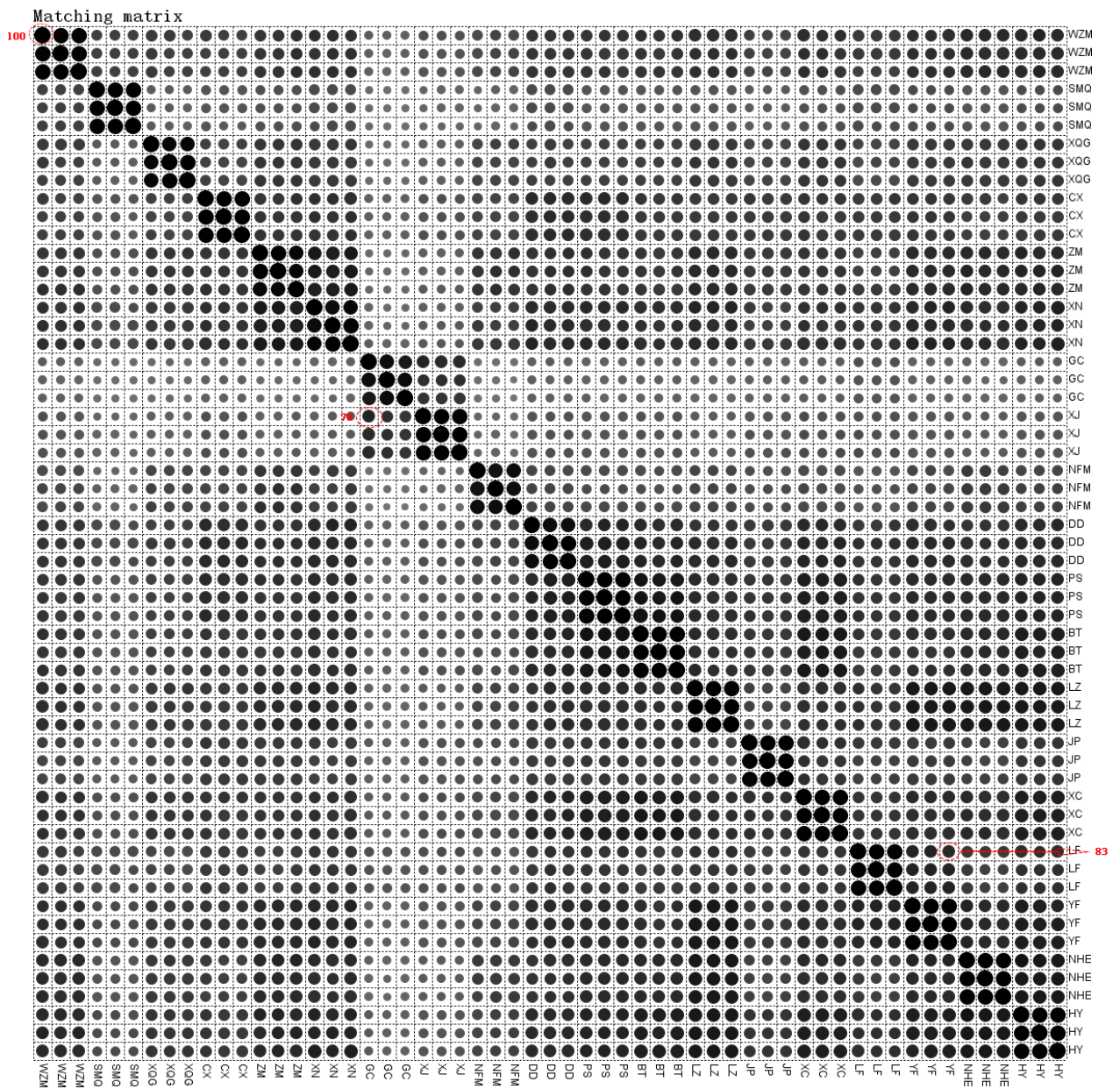
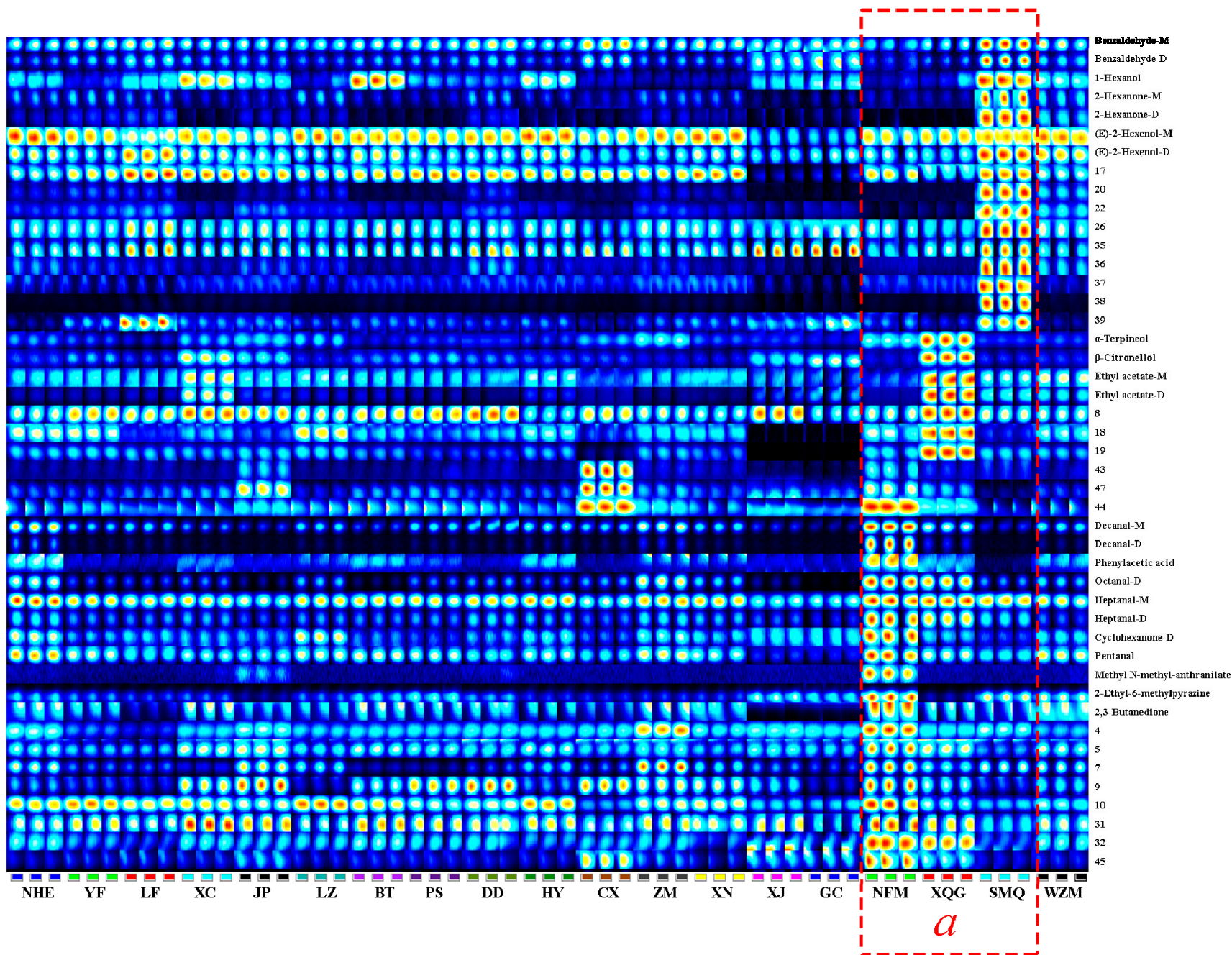
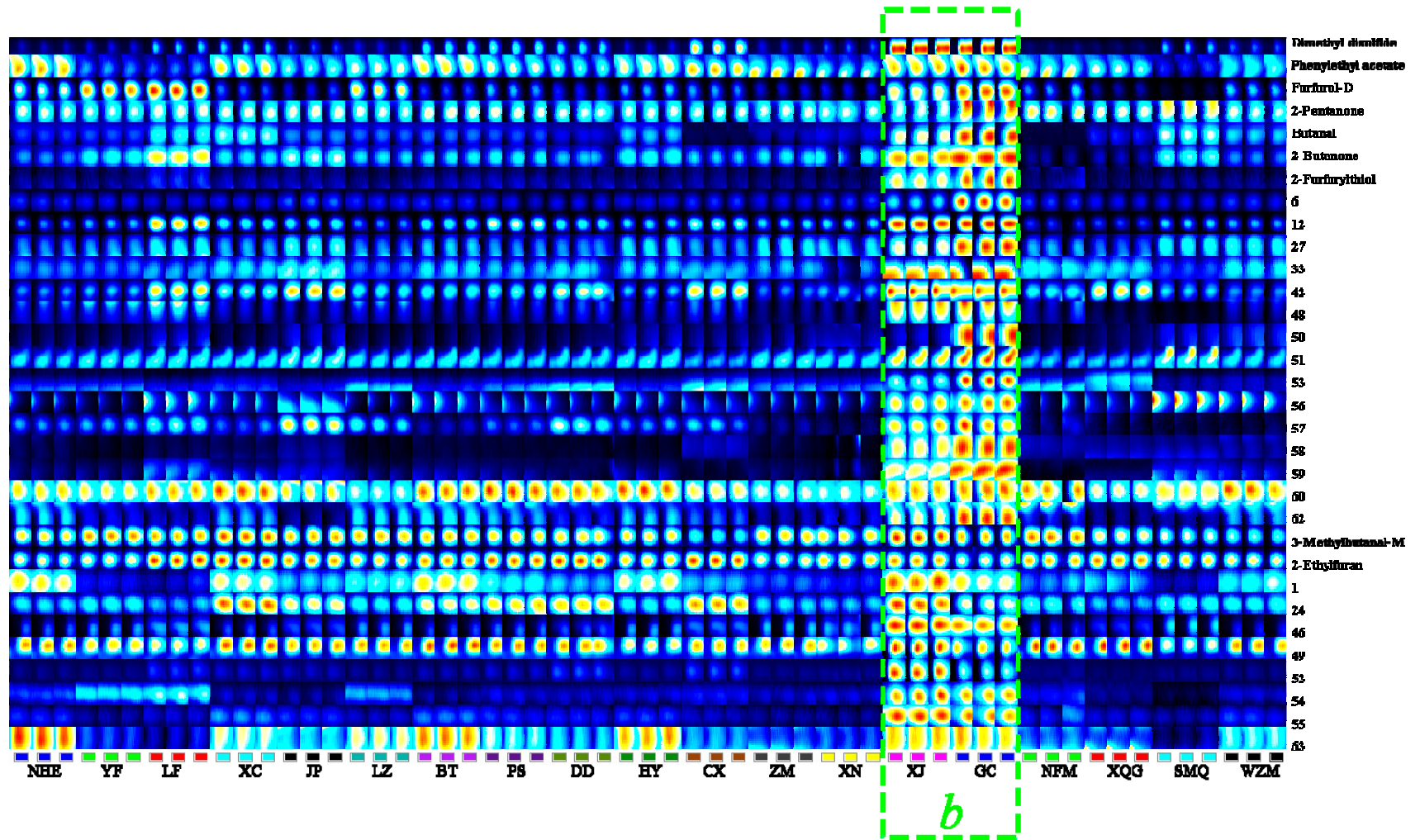


Figure S2. Similarity between samples of citrus-tea; the larger the dot, the higher the similarity.

B



C



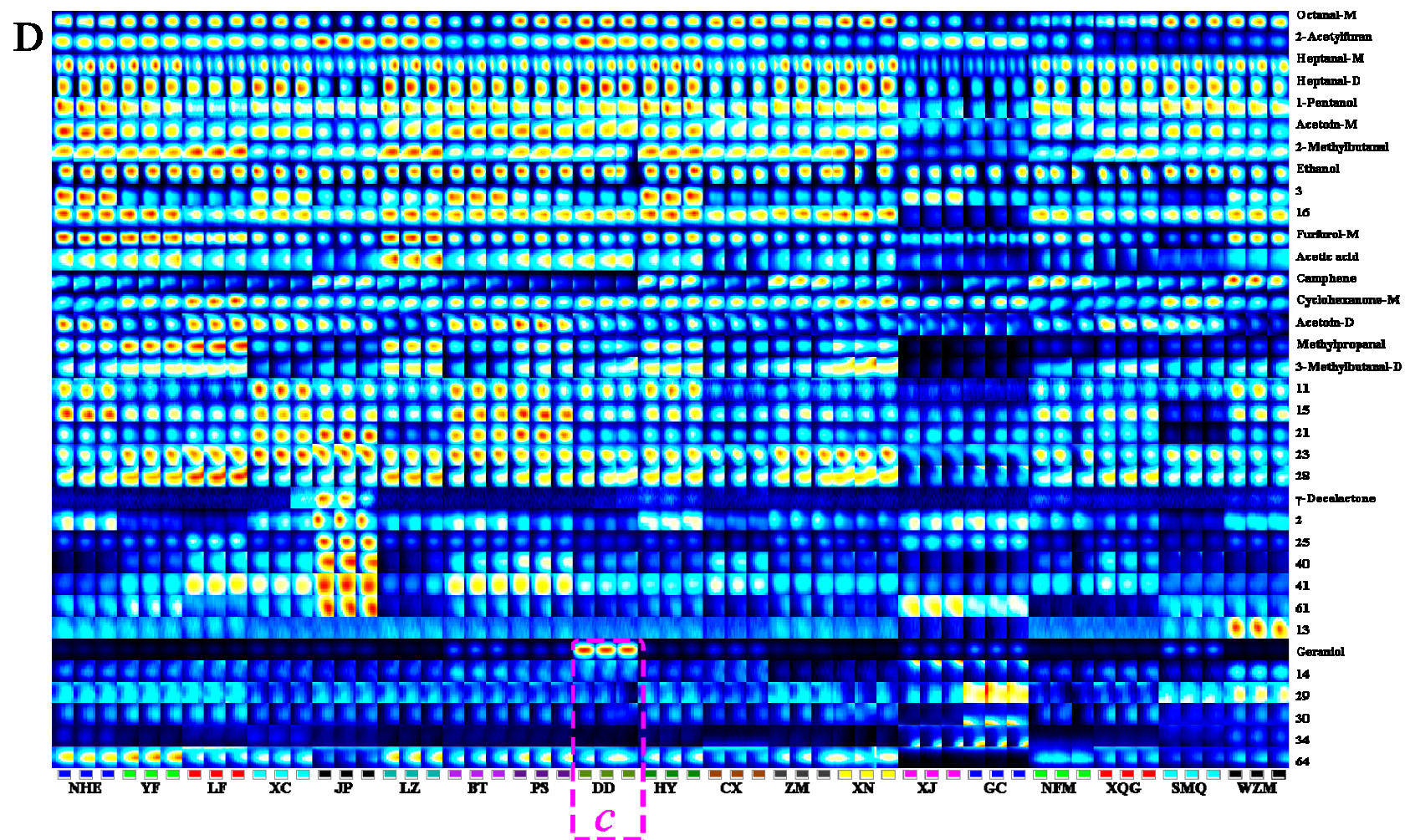


Figure S3. Four parts of the screenshots from the Gallery Plot fingerprints. Eleven kinds of identified peaks (a); 22 kinds of identified peaks (b); 9 kinds of identified peaks (c); 17 kinds of identified peaks (d).