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SUPPLEMENTARY MATERIAL TO

Chemical composition and distribution of the headspace volatiles in commercial culinary herbs and spices: Chemometric approach

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TABLE S-I. The chemical composition of the HSV of studied spices and culinary herbs

No	Compounds	Content, %[a]																			
		I[b]	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII	XVIII	XIX	XX
1.	Methyl 2-methyl butanoate	-	-	-	-	-	-	-	-	-	-	-	-	0.7	-	-	-	-	-	-	-
2.	Hexanal	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-
3.	2-Heptanone	-	-	-	-	-	-	-	1.4	-	-	-	-	-	-	-	-	-	-	-	-
4.	2-Heptanol	-	-	-	-	-	0.1	-	0.1	-	-	-	-	-	-	-	-	-	-	-	-
5.	Tricyclene	-	-	-	-	0.2	-	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-
6.	Methyl hexanoate	-	-	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-	-
7.	*α*-Thujene	2.2	1.4	-	0.1	2.5	-	-	-	-	3.1	1.7	-	0.6	0.5	-	-	-	0.2	-	-
8.	***α*-Pinene**	**11.9**	5.9	2.5	1.2	-	1.0	-	0.1	0.2	1.5	2.8	**14.5**	1.4	3.1	0.2	-	0.7	1.6	2.2	9.7
9.	Camphene	0.4	0.1	1.4	0.1	-	4.8	-	-	-	-	0.9	4.8	0.9	-	-	-	0.1	0.2	-	-
10.	Thuja-2,4(10)-diene	-	-	-	-	-	-	-	-	-	-	-	0.5	-	-	-	-	-	-	-	-
11.	Benzaldehyde	-	-	0.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
12.	**Sabinene**	6.1	7.9	-	3.1	0.1	-	-	-	0.1	**12.5**	0.4	-	0.1	0.1	-	-	0.1	1.4	-	1.0
13.	1-Octen-3-ol	-	-	-	-	-	-	-	-	-	-	0.2	0.1	0.9	-	-	-	-	-	-	-
14.	***β*-Pinene**	6.5	8.6	0.7	1.2	0.1	0.3	-	0.1	0.3	0.8	0.4	0.3	0.2	0.1	0.2	-	-	0.3	**14.7**	2.7
15.	3-Octanone	-	-	-	-	-	-	-	-	-	-	-	0.5	0.2	-	-	-	-	-	-	-
16.	6-Methyl-5-hepten-2-one	-	-	-	-	-	0.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-
17.	Dehydro-1,8-cineol	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
18.	**Myrcene**	0.3	0.9	-	-	0.6	0.6	-	-	0.1	2.4	3.4	1.9	0.6	0.4	**18.9**	-	0.2	4.0	1.0	8.9
19.	3-Octanol	-	-	-	-	-	-	-	-	-	-	-	0.1	0.1	-	-	-	-	-	-	-
20.	*E*thyl hexanoate	-	-	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-	-
21.	***α*-Phellandrene**	0.8	1.5	-	-	**56.9**	0.2	-	-	-	0.8	0.5	0.4	-	**72.4**	-	-	-	1.2	0.3	2.5
22.	*δ*-3-Carene	0.2	7.9	-	-	1.0	-	-	0.2	-	-	0.1	0.4	-	-	-	-	-	-	-	-
23.	***α*-Terpinene**	5.6	0.2	-	0.1	0.5	-	-	-	-	**10.8**	3.8	0.5	0.8	-	-	-	-	0.1	-	-
24.	***p*-Cymene**	6.6	0.6	0.4	0.7	8.3	0.3	-	-	-	3.4	**20.3**	2.5	**66.2**	**10.1**	0.4	-	4.0	0.4	0.4	3.7
25.	**Limonene**	2.0	**14.6**	0.8	-	1.7	1.2	-	0.2	0.1	2.1	0.7	1.6	1.4	-	**74.1**	**39.0**	0.8	5.5	4.8	-
26.	***β*-Phellandrene**	2.5	-	-	-	1.8	4.7	-	-	-	4.2	0.7	-	-	**12.6**	-	-	-	**38.5**	-	**42.8**
27.	**1,8-Cineole**	0.3	-	**16.0**	**88.6**	**10.0**	7.3	-	-	**11.7**	0.3	4.4	**54.3**	2.1	-	1.3	-	0.1	-	-	-
28.	(*Z*)-*β*-Ocimene	-	-	-	-	-	-	-	-	-	-	0.5	-	-	-	3.1	-	-	4.6	0.7	-
29.	2-Heptyl acetate	-	-	-	-	-	-	-	0.7	-	-	-	-	-	-	-	-	-	-	-	-
30.	(*E*)-*β*-Ocimene	-	-	-	-	-	-	-	-	-	0.1	0.1	-	-	-	-	-	-	0.1	-	-

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TABLE S-I. Continued

No	Compounds	Content, %[a]																			
		I[b]	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII	XVIII	XIX	XX
31.	***γ*-Terpinene**	6.6	0.4	-	0.2	0.8	0.1	-	-	-	**15.1**	**19.0**	0.1	3.7	-	0.3	-	1.7	0.7	-	0.4
32.	*cis*-Sabinene hydrate	0.5	-	-	0.3	-	-	-	-	-	6.1	0.1	-	0.3	-	-	-	-	-	-	-
33.	*cis*-Linalool oxide (furanoid)	-	-	-	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-
34.	**Terpinolene**	0.8	0.1	-	-	1.0	0.1	-	-	-	2.6	0.2	-	0.2	-	-	-	0.2	0.4	**70.9**	3.7
35.	*p*-Cymenene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	7.3
36.	Fenchone	-	-	-	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-
37.	2-Nonanone	-	-	-	-	-	0.1	-	0.2	-	-	-	-	-	-	-	-	-	-	-	-
38.	Rose furan	-	-	-	-	-	0.5	-	-	-	-	-	-	-	-	-	-	-	-	-	-
39.	***trans*-Sabinene hydrate**	-	-	-	-	-	-	-	-	-	**17.3**	-	-	-	-	-	-	-	-	-	-
40.	**Linalool**	1.5	0.6	0.5	1.0	-	0.8	-	0.3	**43.8**	-	**11.7**	1.0	6.5	-	-	-	**87.8**	0.1	-	-
41.	Filifolone	-	-	-	-	-	-	-	-	-	-	-	0.4	-	-	-	-	-	-	-	-
42	**1,3,8-*p*-Menthatriene**	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	**15.4**
43.	*endo*-Fenchol	-	-	-	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-
44.	*cis*-*p*-Menth-2-en--1-ol	-	-	-	-	-	-	-	-	-	0.8	-	-	-	-	-	-	-	-	-	-
45.	Chrysanthenone	-	-	-	-	-	-	-	-	-	-	-	0.2	-	-	-	-	-	-	-	-
46.	*trans*-*p*-Menth-2--en-1-ol	-	-	-	-	-	-	-	-	-	0.3	-	-	-	-	-	-	-	-	-	-
47.	Camphor	-	-	-	-	-	0.1	-	-	0.2	-	-	9.6	0.2	-	-	-	2.8	-	-	-
48.	Camphene hydrate	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-
49.	Menthone	-	-	-	-	-	-	-	-	0.5	-	-	-	0.1	-	-	-	-	0.2	-	-
50.	*trans*-Pinocamphone	-	-	-	-	-	-	-	-	-	-	-	0.4	-	-	-	-	-	-	-	-
51.	Isomenthone	-	-	-	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-
52.	*δ*-Terpineol	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
53.	Borneol	-	-	1.2	-	-	1.8	-	-	-	-	0.4	2.6	0.6	-	-	-	-	-	-	-
54.	Menthol	-	-	-	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-
55.	Rosefuran epoxide	-	-	-	-	-	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-
56.	*cis*-Pinocamphone	-	-	-	-	-	-	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-
57.	**Terpinen-4-ol**	**29.8**	0.1	1.7	1.1	-	0.1	-	-	0.1	**12.8**	0.6	0.4	0.4	-	-	-	-	-	-	-
58.	*p*-Cymen-8-ol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.6	-
59.	Dill ether	-	-	-	-	-	-	-	-	-	-	-	-	-	0.3	-	-	-	-	-	-
60.	*α*-Terpineol	2.0	-	1.5	0.6	-	0.7	-	-	0.1	1.2	-	1.0	2.1	-	-	-	0.1	0.2	-	-
61.	*cis*-Piperitol	-	-	-	-	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-
62.	Methyl salicylate	-	-	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-	-
63.	*cis*-Dihydrocarvone	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.1	-	-	-	-
64.	**Estragole**	-	-	-	-	-	-	-	-	**40.0**	-	-	-	0.1	-	-	-	-	-	-	-
65.	*trans*-Dihydrocarvone	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.3	-	-	-	-
66.	Verbenone	-	-	-	-	-	-	-	-	-	-	-	0.9	-	-	-	-	-	-	-	-
67.	neoiso-Dihydro carveol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2.2	-	-	-	-
68.	Thymol, methyl ether	-	-	-	-	-	-	-	-	-	-	-	-	1.5	-	-	-	-	-	-	-
69.	Carvacrol, methyl ether	-	-	-	-	-	-	-	-	-	-	0.3	-	0.8	-	-	-	-	-	-	-
70.	**Carvone**	-	0.9	-	-	-	-	-	-	-	-	-	-	-	-	-	**56.7**	-	-	-	-
71.	Thymoquinone	-	-	-	-	-	-	-	-	-	-	1.4	-	1.2	-	-	-	-	-	-	-
72.	Linalool acetate	-	-	-	-	-	-	-	-	-	1.1	-	-	-	-	-	-	-	-	-	-
73.	**(*E*)-Cinnamaldehyde**	-	-	**50.9**	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
74.	Isobornyl acetate	0.1	-	7.9	0.1	-	0.1	-	-	0.3	-	-	0.2	0.1	-	-	-	-	-	-	-
75.	Safrole	2.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

TABLE S-I. Continued

No	Compounds	Content, %[a]																			
		I[b]	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII	XVIII	XIX	XX
76.	Thymol	-	-	-	-	-	-	-	-	-	-	0.4	-	2.9	-	-	-	-	-	-	-
77.	Terpinen-4--ol, acetate	-	-	-	-	-	-	-	-	-	0.3	-	-	-	-	-	-	-	-	-	-
78.	**Carvacrol**	-	-	-	-	-	-	-	-	-	-	**23.5**	-	0.1	-	-	-	-	-	-	-
79.	*δ*-Terpinyl acetate	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
80.	*δ*-Elemene	-	0.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
81.	***α*-Terpinyl acetate**	-	-	-	1.3	-	-	-	-	-	-	-	-	2.4	-	-	-	-	**39.7**	-	-
82.	**Eugenol**	1.7	-	-	-	-	-	-	**68.6**	-	-	-	-	-	-	-	-	-	-	-	-
83.	*α*-Ylangene	-	-	-	-	-	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-
84.	*α*-Copaene	0.3	2.4	6.3	-	-	0.5	-	0.5	-	-	-	-	-	-	-	-	-	-	-	-
85.	Methyl (*E*)--cinnamate	-	-	-	-	-	-	-	-	0.3	-	-	-	-	-	-	-	-	-	-	-
86.	*β*-Elemene	-	0.6	-	-	-	0.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-
87.	Sesquithujene	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-
88.	Methyl eugenol	0.7	-	-	-	-	-	-	-	0.2	-	-	-	-	-	-	-	-	-	-	-
89.	α-*cis*-Bergamotene	-	-	0.7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
90.	**(*E*)-Caryophyllene**	0.1	**38.6**	2.5	-	1.1	-	-	**24.6**	-	0.5	0.4	0.1	0.2	-	0.4	0.3	-	-	-	-
91.	*α*-*trans*-Bergamotene	-	0.1	-	-	-	-	-	-	0.4	-	-	-	-	-	-	-	-	-	-	-
92.	*α*-Humulene	-	1.8	-	-	-	-	-	1.3	-	-	-	-	-	-	-	-	-	-	-	-
93.	allo-Aromadendrene	-	-	-	-	-	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-
94.	*cis*-Muurola--4(14),5--diene	-	-	-	-	-	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-
95.	**ar-Curcumene**	-	-	-	-	2.3	**12.8**	-	-	-	-	-	-	-	-	-	-	-	-	-	-
96.	Germacrene D	-	0.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
97.	***α*-Zingiberene**	-	-	-	-	3.7	**34.0**	-	-	-	-	-	-	-	-	-	-	-	-	-	-
98.	*trans*-Muurola--4(14),5-diene	-	-	-	-	-	3.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
99.	*β*-Selinene	-	1.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
100.	*α*-Selinene	-	0.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
101.	*α*-Muurolene	-	-	0.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
102.	*β*-Bisabolene	-	0.6	-	-	0.5	9.0	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-
103.	(*E*,*E*)-*α*-Farnesene	-	-	-	-	-	0.7	-	-	-	-	-	-	-	-	-	-	-	-	-	-
104.	Myristicin	5.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2.4	0.3
105.	***β*-Sesquiphellandrene**	-	-	-	-	2.1	**11.8**	-	-	-	-	-	-	-	-	-	-	-	-	-	-
106.	*δ*-Cadinene	-	-	1.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
107.	Eugenol acetate	0.2	-	-	-	-	-	-	0.6	-	-	-	-	-	-	-	-	-	-	-	-
108.	*δ*-Cadinene	-	0.5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
109.	Germacrene B	-	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
110.	ar-Turmerone	-	-	-	-	2.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
111.	**Diallyl sulfide**	-	-	-	-	-	-	**10.6**	-	-	-	-	-	-	-	-	-	-	-	-	-
112.	Methyl allyl disulfide	-	-	-	-	-	-	5.8	-	-	-	-	-	-	-	-	-	-	-	-	-
113.	(*E*)-Methyl 1-propenyl disulfide	-	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-	-	-
114.	Dimethyl trisulfide	-	-	-	-	-	-	2.4	-	-	-	-	-	-	-	-	-	-	-	-	-
115.	**Diallyl**	-	-	-	-	-	-	**18.7**	-	-	-	-	-	-	-	-	-	-	-	-	-

No	Compounds	Content, %[a]																			
		I[b]	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII	XVIII	XIX	XX
	disulfide																				
116.	**Methyl allyl trisulfide**	-	-	-	-	-	-	**17.9**	-	-	-	-	-	-	-	-	-	-	-	-	-
117.	3-Vinyl-1,2-dithia-cyclohex-4-ene	-	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-	-	-
118	3-Vinyl-1,2-dithia-cyclohex-5-ene	-	-	-	-	-	-	0.3	-	-	-	-	-	-	-	-	-	-	-	-	-
119	1,4-Dimethyl-tetrasulfide	-	-	-	-	-	-	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-
120	**Diallyl trisulfide**	-	-	-	-	-	-	**41.3**	-	-	-	-	-	-	-	-	-	-	-	-	-
	TOTAL	97.6	98.6	97.6	99.8	97.5	99.0	97.4	98.9	99.2	99.5	99.1	99.3	99.4	99.5	98.9	99.5	98.3	99.4	98.0	98.3
	MH[c]	55.8	49.9	5.8	6.5	75.4	8.5	-	0.5	44.8	58.9	55.4	27.5	76.1	99.3	97.2	39.0	7.6	59.2	95.0	98.0
	MO	30.9	1.5	28.7	93.2	10.0	11.1	-	0.3	13.5	40.1	42.9	71.0	21.1	-	1.3	60.3	90.7	40.2	0.6	-
	SH	0.4	47.1	11.6	-	9.6	73.0	-	26.3	0.4	0.5	0.5	0.1	0.2	-	0.4	0.3	-	-	-	-
	SO	-	-	-	-	2.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	PP	10.5	-	51.5	-	-	-	-	69.2	40.2	-	-	-	0.1	-	-	-	-	-	2.4	0.3
	Sulfides	-	-	-	-	-	-	97.4	-	-	-	-	-	-	-	-	-	-	-	-	-
	Others[d]	-	-	-	-	-	1.9	-	2.6	0.3	-	0.2	0.8	1.9	0.3	-	-	-	-	-	-

[a]I-nutmeg, II-black peper, III-cinnamon, IV-bay laurel, V-curcuma, VI-ginger, VII-garlic, X-clove, XI-basil, XII-marjoram, XIII-oregano, XIV-rosemary, XV-thyme, XVI-dill, XVII- celery, XVIII-caraway, XIX-coriander, XX-lovage, XXI-parsnip, XXII-parsley. [b]For all species/culinary herbs, represented with a larger number of samples, mean values are presented, except for samples assigned XVII, XX and XXI where one sample was studied per spice/culinary herb. [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. [d]Others - aliphatic alcohols, aldehydes, ketones, esters. Components represented ≥ 10 % are in boldface. Trace (<0.05 %) and not detected compounds are marked as (-). Volatiles of samples VIII and IX cannot be extracted/analyzed by described procedure.

TABLE S-II. Headspace volatiles of dill, *Anethum graveolens* samples

No	RI[a]	AI[b]	Compound	Content, %								
				s1	s2	s3	s4	s5	s6	s7	s8	Mean ± SD
1.	925	924	*α*-Thujene	0.4	0.3	0.3	0.5	0.3	0.8	0.3	0.7	0.5±0.2
2.	932	932	*α*-Pinene	2.6	2.3	2.1	3.2	2.2	5.5	2.7	4.0	3.1±1.2
3.	972	969	Sabinene	0.1	0.1	0.1	0.1	0	0.1	0	0.2	0.1±0.1
4.	975	974	*β*-Pinene	0.1	0.1	0.1	0.1	0.1	0.3	0.1	0.1	0.1±0.1
5.	989	988	Myrcene	0.4	0.4	0.5	0.3	0.3	0.5	0.3	0.5	0.4±0.1
6.	1004	1002	*α*-Phellandrene	81.7	82.7	83.4	66.8	78.6	52.1	71.6	62.2	72.4±11.3
7.	1024	1020	*p*-Cymene	3.0	3.4	2.5	15.6	5.0	22.3	12.3	16.8	10.1±7.6
8.	1028	1025	*β*-Phellandrene	10.9	10.4	10.5	13.0	12.9	17.6	11.9	13.7	12.6±2.4
9.	1186	1184	Dill ether	0.1	0.1	0.1	0.1	0.1	0.2	0.1	1.5	0.3±0.5
			MH[c]	99.2	99.7	99.5	99.6	99.4	99.2	99.2	98.2	99.3±0.5
			MO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			SH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			SO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			PP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			O	0.1	0.1	0.1	0.1	0.1	0.2	0.1	1.5	0.3±0.5
			Total:	99.3	99.8	99.6	99.7	99.5	99.4	99.3	99.7	99.5±0.2

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-III. Headspace volatiles of lovage, *Levisticum officinale*

No	RI[a]	AI[b]	Compound	Content of s9, %
1.	923	924	*α*-Thujene	0.2
2.	930	932	*α*-Pinene	1.6
3.	945	946	Camphene	0.2
4.	969	969	Sabinene	1.4
5.	973	974	*β*-Pinene	0.3
6.	987	988	Myrcene	4.0
7.	1001	1002	*α*-Phellandrene	1.2
8.	1013	1014	*α*-Terpinene	0.1
9.	1021	1020	*p*-Cymene	0.4
10.	1025	1024	Limonene	5.5
11.	1028	1025	β-Phellandrene	38.5
12.	1033	1032	(*Z*)-*β*-Ocimene	4.6
13.	1044	1044	(*E*)-*β*-Ocimene	0.1
14.	1055	1054	*γ*-Terpinene	0.7
15.	1085	1086	Terpinolene	0.4
16.	1095	1095	Linalool	0.1
17.	1151	1148	Menthone	0.2
18.	1187	1186	*α*-Terpineol	0.2
19.	1348	1346	*α*-Terpinyl acetate	39.7
			MH[c]	59.2
			MO	40.2
			SH	0.0
			SO	0.0
			PP	0.0
			O	0.0
			Total:	99.4

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-IV. Headspace volatiles of parsley, *Petroselinum crispum* samples

				Content, %							
No	RI[a]	AI[b]	Compound	s10	s11	s12	s13	s14	s15	s16	Mean±SD
1.	932	932	*α*-Pinene	5.6	3.9	16.4	7.9	5.5	13.8	14.6	9.7±5.1
2.	972	969	Sabinene	0.2	0.1	5.5	0.3	0.2	0.5	0.2	1.0±2.0
3.	975	974	*β*-Pinene	2.3	0.9	0.0	1.9	2.3	5.8	5.6	2.7±2.2
4.	989	988	Myrcene	6.4	4.5	9.1	14.8	8.5	7.6	11.7	8.9±3.4
5.	1004	1002	*α*-Phellandrene	2.3	2.8	1.2	3	3.3	2.4	2.3	2.5±0.7
6.	1024	1020	*p*-Cymene	0.7	0.8	5.2	2.5	8.9	4.2	3.3	3.7±2.8
7.	1028	1025	*β*-Phellandrene	31.1	44.3	51	54.4	38.7	39.7	40.2	42.8±7.9
8.	1055	1054	*γ*-Terpinene	0.5	0.4	0	0.4	0.5	0.6	0.4	0.4±0.2
9.	1085	1086	Terpinolene	6.2	4	0.5	0.6	6.9	4.4	3.3	3.7±2.5
10.	1087	1089	*p*-Cymenene	5.0	3.4	7.8	7.6	7.4	9.5	10.3	7.3±2.4
11.	1112	1108	1,3,8-*p*-Menthatriene	38.1	34.0	0.0	5.7	15.9	8.6	5.2	15.4±15.0
12.	1520	1517	Myristicin	0.7	0.3	0.0	0.0	0.0	1.2	0.0	0.3±0.5
			MH[c]	98.4	99.1	96.7	99.1	98.1	97.3	97.1	98.0±1.0
			MO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			SH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			SO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			PP	0.7	0.3	0.0	0.0	0.0	1.2	0.0	0.3±0.5
			O	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			Total:	99.1	99.4	96.7	99.1	98.1	98.5	97.1	98.3±1.0

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-V. Headspace volatiles of celery, *Apium graveolens*

No	RI[a]	AI[b]	Compound	Content of s17, %
1.	930	932	*α*-Pinene	0.2
2.	973	974	*β*-Pinene	0.2
3.	987	988	Myrcene	18.9
4.	1021	1020	*p*-Cymene	0.4
5.	1025	1024	Limonene	74.1
6.	1028	1026	1,8-Cineole	1.3
7.	1033	1032	(*Z*)-*β*-Ocimene	3.1
8.	1055	1054	*γ*-Terpinene	0.3
9.	1420	1417	(*E*)-Caryophyllene	0.4
			MH[c]	97.2
			MO	1.3
			SH	0.4
			SO	0.0
			PP	0.0
			O	0.0
			Total:	98.9

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-VI. Headspace volatiles of coriander, *Coriandrum sativum* samples

				Content, %		
No	RI[a]	AI[b]	Compound	s18	s19	Mean± SD
1.	931	932	*α*-Pinene	0.8	0.6	0.7±0.1
2.	945	946	Camphene	0.0	0.1	0.1±0.1
3.	973	969	Sabinene	0.0	0.1	0.1±0.1
4.	987	988	Myrcene	0.0	0.3	0.2±0.2
5.	1021	1020	*p*-Cymene	7.0	1.0	4.0±4.2
6.	1025	1024	Limonene	0.0	1.6	0.8±1.1
7.	1028	1026	1,8-Cineole	0.0	0.1	0.1±0.1
8.	1055	1054	*γ*-Terpinene	0.0	3.4	1.7±2.4
9.	1085	1086	Terpinolene	0.0	0.3	0.2±0.2
10.	1098	1095	Linalool	86.9	88.7	87.8±1.3
11.	1142	1141	Camphor	2.1	3.5	2.8±1.0
12.	1188	1186	*α*-Terpineol	0.0	0.1	0.1±0.1
			MH[c]	7.8	7.4	7.6±0.3
			MO	89	92.4	90.7±2.4
			SH	0.0	0.0	0.0±0.0
			SO	0.0	0.0	0.0±0.0
			PP	0.0	0.0	0.0±0.0
			O	0.0	0.0	0.0±0.0
			Total:	96.8	99.8	98.3±2.1

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-VII. Headspace volatiles of caraway, *Carum carvi* samples

				Content, %						
No	RI[a]	AI[b]	Compound	s20	s21	s22	s23	s24	s25	Mean±SD
1.	1028	1024	Limonene	31.1	29.4	37.0	54.4	15.6	66.2	39.0±18.3
2.	1197	1191	*cis*-Dihydrocarvone	0.2	0.0	0.2	0.1	0.0	0.1	0.1±0.1
3.	1205	1200	*trans*-Dihydrocarvone	4.3	0.3	2.5	0.1	0.6	0.2	1.3±1.7
4.	1229	1226	neoiso-Dihydro carveol	9.8	0.5	1.6	1.2	0.0	0.0	2.2±3.8
5.	1245	1239	Carvone	52.7	69.6	58.2	43.2	83.2	33.2	56.7±18.0
6.	1424	1417	(*E*)-Caryophyllene	1.5	0.0	0.1	0.0	0.0	0.0	0.3±0.6
			MH[c]	31.3	29.4	37.0	54.4	15.6	66.2	39.0±18.3
			MO	66.8	70.4	62.4	44.6	83.8	33.5	60.3±18.3
			SH	1.5	0.0	0.1	0.0	0.0	0.0	0.3±0.6
			SO	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			PP	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			O	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			Total:	99.6	99.8	99.5	99.0	99.4	99.7	99.5±0.3

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-VIII. Headspace volatiles of parsnip, *Pastinaca sativa*

No	RI[a]	AI[b]	Compound	Content of s26, %
1.	930	932	*α*-Pinene	2.2
2.	973	974	*β*-Pinene	14.7
3.	987	988	Myrcene	1.0
4.	1001	1002	*α*-Phellandrene	0.3
5.	1021	1020	*p*-Cymene	0.4
6.	1025	1024	Limonene	4.8
7.	1033	1032	(*Z*)-*β*-Ocimene	0.7
8.	1085	1086	Terpinolene	70.9
9.	1182	1179	*p*-Cymen-8-ol	0.6
10.	1520	1517	Myristicin	2.4
			MH[c]	95.0
			MO	0.6
			SH	0.0
			SO	0.0
			PP	2.4
			O	0.0
			Total:	98.0

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-IX. Headspace volatiles of basil, *Ocimum basilicum* samples

				Content, %							
No	RI[a]	AI[b]	Compound	s27	s28	s29	s30	s31	s32	s33	Mean±SD
1.	932	932	*α*-Pinene	0.3	0.4	0.3	0.3	tr	0.1	0.1	0.2±0.1
2.	848	846	Camphene	tr	0.0	tr	0.1	0.0	0.0	0.0	0.0±0.0
3.	972	969	Sabinene	0.1	0.0	0.3	0.1	tr	tr	tr	0.1±0.1
4.	975	974	*β*-Pinene	0.5	0.6	0.5	0.4	tr	0.2	0.2	0.3±0.2
5.	977	978	1-Octen-3-ol	0	0.0	0.2	0.1	tr	0	0	0.0±0.1
6.	989	988	Myrcene	0.1	0.0	0.4	0.2	0.1	tr	0.2	0.1±0.1
7.	1003	1002	*α*-Phellandrene	0.0	0.3	0.0	0.0	0.0	0.0	0.0	0.0±0.1
8.	1021	1020	*p*-Cymene	0.0	0.0	0.1	0.1	tr	tr	tr	0.0±0.0
9.	1028	1024	Limonene	0.2	0.0	tr	0.2	0.1	tr	0.1	0.1±0.1
10.	1030	1026	1,8-Cineole	8.6	14.1	22.5	20.3	1.9	9.6	4.7	11.7±7.7
11.	1044	1044	(*E*)-*β*-Ocimene	tr	0.0	0.1	0	0.1	tr	0.1	0.0±0.1
12.	1055	1054	*γ*-Terpinene	tr	0.0	0.1	0.1	tr	tr	0.0	0.0±0.0
13.	1066	1065	*cis*-Sabinene hydrate	0.0	0.0	0.2	0.0	0.0	tr	0.0	0.0±0.1
14.	1069	1067	*cis*-Linalool oxide	0.0	0.0	0.1	0.1	0.1	0	0.2	0.1±0.1
15.	1085	1083	Fenchone	0.3	0.0	0.0	0.3	0.1	0.3	0.0	0.1±0.2
16.	1088	1086	Terpinolene	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0±0.0
17.	1098	1095	Linalool	11.2	16.5	49.2	46.9	87.3	5.0	90.5	43.8±35.2
18.	1114	1114	*endo*-Fenchol	0.2	0.0	0.0	0.2	0	0.3	0	0.1±0.1
19.	1142	1141	Camphor	0.2	0.0	0.2	0.6	tr	0.2	0.5	0.2±0.2
20.	1151	1148	Menthone	0.0	0.0	0.3	0.0	2.7	0.0	0.2	0.5±1.0
21.	1161	1158	Isomenthone	0.0	0.0	0.1	0.0	0.5	0.0	0.0	0.1±0.2
22.	1169	1167	Menthol	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.1±0.4
23.	1175	1174	Terpinen-4-ol	0.1	0.0	0.2	0.2	0.0	0.1	0.1	0.1±0.1
24.	1188	1186	*α*-Terpineol	0.2	0.0	0.2	0.3	0.0	0.1	0.1	0.1±0.1
25.	1198	1195	Estragole	76.7	59.2	24.5	27.8	5.8	83.7	2.1	40.0±33.2
26.	1286	1283	Isobornyl acetate	0.1	0.7	0.1	0.7	tr	0.1	0.4	0.3±0.3
27.	1383	1376	Methyl (*E*)-cinnamate	tr	1.9	0.0	0.0	0.0	0.0	0.0	0.3±0.7
28.	1403	1403	Methyl eugenol	0.5	0.9	0.0	0.0	0.0	0.0	0.0	0.2±0.4
29.	1437	1432	*α*-*trans*-Bergamotene	0.2	2.2	0.1	0.2	0.0	tr	0.0	0.4±0.8
30.	1517	1513	*γ*-Cadinene	0.0	0.0	0.0	0.0	tr	0.0	0.0	0.0±0.0
			MH[c]	12.4	17.8	51.1	48.4	87.6	5.3	91.2	44.8±35.1
			MO	9.7	14.8	23.9	22.7	6.3	10.7	6.2	13.5±7.3
			SH	0.2	2.2	0.1	0.2	0.0	0.0	0.0	0.4±0.8
			SO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			PP	77.2	60.1	24.5	27.8	5.8	83.7	2.1	40.2±33.4
			O	0.0	1.9	0.2	0.1	0.0	0.0	0.0	0.3±0.7
			Total:	99.5	96.8	99.8	99.2	99.7	99.7	99.5	99.2±1.1

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] tr - trace (≤0.1 %). [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-X. Headspace volatiles of oregano *Origanum vulgare* samples

				Content, %						
No	RI[a]	AI[b]	Compound	s34	s35	s36	s37	s38	s39	Mean±SD
1.	925	924	*α*-Thujene	2.1	1.2	1.2	1.2	2.1	2.5	1.7±0.6
2.	932	932	*α*-Pinene	4.5	1.9	3.9	1.5	2.7	2.0	2.8±1.2
3.	947	946	Camphene	1.7	1.0	0.4	0.5	0.7	0.8	0.9±0.5
4.	970	969	Sabinene	0.3	0.0	0.0	tr	0.7	1.4	0.4±0.6
5.	974	974	1-Octen-3-ol	0	0.1	0	0	0.5	0.8	0.2±0.3
6.	975	974	*β*-Pinene	0.8	0.2	0.1	0.2	0.4	0.5	0.4±0.3
7.	989	988	Myrcene	3.9	3.2	2.1	0.9	6.6	3.6	3.4±1.9
8.	1004	1002	*α*-Phellandrene	0.6	0.4	0.3	0.2	0.8	0.4	0.5±0.2
9.	1009	1008	*δ*-3-Carene	0.0	0.2	0.0	0.0	0.3	0.1	0.1±0.1
10.	1016	1014	*α*-Terpinene	6.1	3.5	2.3	1.4	6.1	3.6	3.8±1.9
11.	1023	1020	*p*-Cymene	31.8	23.6	8.6	5.9	24.5	27.5	20.3±10.6
12.	1026	1024	Limonene	1	0.4	1.7	0.2	0.5	0.3	0.7±0.6
13.	1028	1025	*β*-Phellandrene	1.2	0.8	0	0.4	0.9	0.7	0.7±0.4
14.	1030	1026	1,8-Cineole	6.3	0.2	17.7	1.1	0.1	1.2	4.4±6.9
15.	1036	1030	(*Z*)-*β*-Ocimene	0.3	0.0	0.0	0.0	1.6	1.3	0.5±0.7
16.	1045	1044	(*E*)-*β*-Ocimene	0.0	0.0	0.0	0.0	0.4	0.4	0.1±0.2
17.	1059	1054	*γ*-Terpinene	22.4	13.4	9.4	5.6	44.6	18.6	19.0±13.9
18.	1066	1065	*cis*-Sabinene hydrate	0.0	0.2	0.0	0.0	0.4	0.0	0.1±0.2
19.	1088	1086	Terpinolene	0.3	0.3	0.1	0.0	0.4	0.2	0.2±0.1
20.	1098	1095	Linalool	1.2	16.9	41.2	7.7	0.1	3.3	11.7±15.7
21.	1166	1165	Borneol	0.0	1.2	0.0	0.9	0.1	0.4	0.4±0.5
22.	1177	1174	Terpinen-4-ol	0.7	1.2	0.3	1.0	0.1	0.5	0.6±0.4
23.	1244	1239/41	Carvacrol, methyl ether	0.0	0.4	0.0	0.3	0.5	0.8	0.3±0.3
24.	1250	1248	Thymoquinone	0.6	2.8	0.7	2.2	0.1	2.2	1.4±1.1
25.	1291	1289	Thymol	0.2	0.1	0.2	1.4	0.0	0.3	0.4±0.5
26.	1301	1298	Carvacrol	13.1	25.0	8.5	65.5	4.3	24.4	23.5±22.2
27.	1423	1417	(*E*)-Caryophyllene	0.0	0.9	0.2	0.6	0.3	0.5	0.4±0.3
28.	1507	1505	*β*-Bisabolene	0.0	0.1	0.1	0.2	tr	0.0	0.1±0.1
			MH[c]	77.0	50.1	30.1	18.0	93.3	63.9	55.4±28.4
			MO	8.2	19.7	59.2	10.7	0.8	5.4	17.3±21.5
			SH	0.0	1.0	0.3	0.8	0.3	0.5	0.5±0.4
			SO	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			PP	13.9	28.3	9.4	69.4	4.9	27.7	25.6±23.5
			O	0.0	0.1	0.0	0.0	0.5	0.8	0.2±0.3
			Total:	99.1	99.2	99.0	98.9	99.8	98.3	99.1±0.5

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] tr - trace (≤0.1 %). [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-XI. Headspace volatiles of marjoram, *Origanum majorana* samples

				Content, %		
No	RI[a]	AI[b]	Compound	s40	s41	Mean±SD
1.	923	924	*α*-Thujene	3.0	3.1	3.1±0.1
2.	930	932	*α*-Pinene	1.6	1.3	1.5±0.2
3.	945	046	Camphene	tr	tr	0.0±0.0
4.	970	969	Sabinene	11.9	13.1	12.5±0.8
5.	973	974	*β*-Pinene	0.8	0.7	0.8±0.1
6.	987	988	Myrcene	2.5	2.2	2.4±0.2
7.	1001	1002	*α*-Phellandrene	0.8	0.7	0.8±0.1
8.	1013	1014	*α*-Terpinene	11.7	9.9	10.8±1.3
9.	1021	1020	*p*-Cymene	1.9	4.9	3.4±2.1
10.	1025	1024	Limonene	2.1	2.0	2.1±0.1
11.	1028	1025	*β*-Phellandrene	4.3	4.0	4.2±0.2
12.	1028	1026	1,8-Cineole	tr	0.5	0.3±0.4
13.	1034	1032	(*Z*)-*β*-Ocimene	tr	tr	0.0±0.0
14.	1044	1044	(*E*)-*β*-Ocimene	0.1	tr	0.1±0.1
15.	1056	1054	*γ*-Terpinene	15.8	14.3	15.1±1.1
16.	1064	1065	*cis*-Sabinene hydrate	6.2	6.0	6.1±0.1
17.	1085	1086	Terpinolene	2.6	2.5	2.6±0.1
18.	1096	1098	*trans*-Sabinene hydrate	20.7	13.8	17.3±4.9
19.	1118	1118	*cis*-*p*-Menth-2-en-1-ol	0.6	0.9	0.8±0.2
20.	1136	1136	*trans*-*p*-Menth-2-en-1-ol	0.2	0.4	0.3±0.1
21.	1176	1174	Terpinen-4-ol	9.8	15.7	12.8±4.2
22.	1188	1186	*α*-Terpineol	1.0	1.4	1.2±0.3
23.	1192	1195	*cis*-Piperitol	0.1	0.1	0.1±0.0
24.	1251	1254	Linalool acetate	1.4	0.8	1.1±0.4
25.	1297	1299	Terpinen-4-ol, acetate	0.2	0.4	0.3±0.1
26.	1420	1417	(*E*)-Caryophyllene	0.4	0.6	0.5±0.1
			MH[c]	59.1	58.7	58.9±0.3
			MO	40.2	40	40.1±0.1
			SH	0.4	0.6	0.5±0.1
			SO	0.0	0.0	0.0±0.0
			PP	0.0	0.0	0.0±0.0
			O	0.0	0.0	0.0±0.0
			Total:	99.7	99.3	99.5±0.3

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] tr - trace (≤0.1 %). [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-XII. Headspace volatiles of rosemary, *Rosmarinus officinalis* samples

				Content, %					
No	RI[a]	AI[b]	Compound	s42	s43	s44	s45	s46	Mean±SD
1.	918	921	Tricyclene	0.0	0.3	0.2	0.2	tr	0.1±0.1
2.	930	932	*α*-Pinene	4.1	28.6	21.8	14.6	3.4	14.5±11.0
3.	947	946	Camphene	1.0	10.3	5.7	5.5	1.7	4.8±3.7
4.	950	953	Thuja-2,4(10)-diene	0.0	0.3	1.2	1.1	0.0	0.5±0.6
5.	974	974	1-Octen-3-ol	0.0	0.2	0.1	0.0	0.1	0.1±0.1
6.	976	974	*β*-Pinene	0.6	0.4	0.2	0.0	0.4	0.3±0.2
7.	982	979	3-Octanone	0.0	2.1	0.1	0.1	tr	0.5±0.9
8.	989	988	Myrcene	0.2	8.3	0.7	0.2	0.2	1.9±3.6
9.	991	988	3-Octanol	0.0	0.4	0.0	0.0	0.0	0.1±0.2
10.	1001	1002	*α*-Phellandrene	0.0	1.8	0.1	0.0	tr	0.4±0.8
11.	1007	1008	*δ*-3-Carene	0.0	0.1	0.9	0.8	tr	0.4±0.5
12.	1016	1014	*α*-Terpinene	0.1	2.0	0.1	0.0	0.1	0.5±0.9
13.	1022	1020	*p*-Cymene	1.5	3.2	2.9	3.8	1.0	2.5±1.2
14.	1025	1024	Limonene	0.0	0.0	3.7	4.1	0.0	1.6±2.1
15.	1028	1026	1,8-Cineole	77.1	27.9	40.3	44.4	81.6	54.3±23.7
16.	1055	1054	*γ*-Terpinene	tr	0.6	0.0	0.0	0.0	0.1±0.3
17.	1095	1095	Linalool	0.4	0.3	2.2	1.9	0.4	1.0±0.9
18.	1100	1103[c]	Filifolone	0.0	0.1	0.9	0.8	0.0	0.4±0.5
19.	1122	1124	Chrysanthenone	0.0	0.1	0.4	0.3	0.0	0.2±0.2
20.	1143	1141	Camphor	8.9	9.7	10.4	11.4	7.8	9.6±1.4
21.	1147	1145	Camphene hydrate	0.0	tr	0.1	0.0	tr	0.0±0.0
22.	1160	1158	*trans*-Pinocamphone	0.1	0.1	0.6	1.0	0.0	0.4±0.4
23.	1162	1160	Pinocarvone	tr	tr	tr	0.0	0.0	0.0±0.0
24.	1167	1165	Borneol	2.4	0.8	3.5	4.6	1.7	2.6±1.5
25.	1172	1172	*cis*-Pinocamphone	0.0	tr	0.2	0.3	0.0	0.1±0.1
26.	1176	1174	Terpinen-4-ol	0.5	0.2	0.4	0.3	0.4	0.4±0.1
27.	1188	1186	*α*-Terpineol	2.3	0.2	0.7	0.6	1.0	1.0±0.8
28.	1207	1204	Verbenone	0.1	0.5	1.9	2.2	0.0	0.9±1.0
29.	1285	1283	Isobornyl acetate	0.2	0.4	0.2	0.1	tr	0.2±0.1
30.	1422	1417	(*E*)-Caryophyllene	0.3	0.1	tr	0.0	tr	0.1±0.1
			MH[d]	7.5	55.8	37.4	30.1	6.9	27.5±20.8
			MO	92.0	40.3	61.8	67.9	92.9	71.0±22.1
			SH	0.3	0.1	0.0	0.0	0.0	0.1±0.1
			SO	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			PP	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			O	0.0	3.0	0.4	0.3	0.1	0.8±1.3
			Total:	99.8	99.2	99.6	98.3	99.8	99.4±0.7

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] [c]Retention indices from NIST Chemistry WebBook relative to HP-5MS[2]; tr - trace (≤0.1 %). [d]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-XIII. Headspace volatiles of thyme, *Thymus vulgaris* samples

				Content, %			
No	RI[a]	AI[b]	Compound	s47	s48	s49	Mean±SD
1.	780	780[c]	Methyl 2-methylbutanoate	1.0	1.1	0.1	0.7±0.6
2.	925	924	*α*-Thujene	0.7	0.2	0.8	0.6±0.3
3.	932	932	*α*-Pinene	1.3	2.3	0.7	1.4±0.8
4.	947	946	Camphene	0.7	1.2	0.9	0.9±0.3
5.	970	969	Sabinene	tr	tr	0.2	0.1±0.1
6.	974	974	1-Octen-3-ol	1.1	1.2	0.4	0.9±0.4
7.	976	974	*β*-Pinene	0.3	0.2	0.2	0.2±0.1
8.	982	979	3-Octanone	0.1	0.1	0.4	0.2±0.2
9.	989	988	Myrcene	1.3	0.2	0.3	0.6±0.6
10.	991	988	3-Octanol	0.1	0.1	0.1	0.1±0.0
11.	1003	1002	*α*-Phellandrene	0.1	tr	tr	0.0±0.1
12.	1009	1008	*δ*-3-Carene	0.1	0.0	0.0	0.0±0.1
13.	1016	1014	*α*-Terpinene	1.3	0.1	0.9	0.8±0.6
14.	1024	1020	*p*-Cymene	69.6	83.3	45.8	66.2±19.0
15.	1026	1024	Limonene	0.8	0.7	2.7	1.4±1.1
16.	1028	1026	1,8-Cineole	1.5	1.6	3.3	2.1±1.0
17.	1056	1054	*γ*-Terpinene	8.2	tr	2.8	3.7±4.2
18.	1066	1065	*cis*-Sabinene hydrate	0.5	0.1	0.2	0.3±0.2
19.	1088	1086	Terpinolene	0.2	0.2	0.1	0.2±0.1
20.	1097	1095	Linalool	3.0	1.9	14.6	6.5±7.0
21.	1142	1141	Camphor	0.2	0.3	tr	0.2±0.2
22.	1151	1148	Menthone	tr	tr	0.2	0.1±0.1
23.	1166	1165	Borneol	0.4	0.5	0.8	0.6±0.2
24.	1176	1174	Terpinen-4-ol	0.3	0.5	0.3	0.4±0.1
25.	1188	1186	*α*-Terpineol	tr	0.1	6.2	2.1±3.6
26.	1197	1195	Estragole	0.2	0.0	0.0	0.1±0.1
27.	1234	1232	Thymol, methyl ether	1.1	0.6	2.9	1.5±1.2
28.	1243	1241	Carvacrol, methyl ether	0.8	0.4	1.1	0.8±0.4
29.	1250	1248	Thymoquinone	0.3	tr	3.2	1.2±1.8
30.	1286	1283	Isobornyl acetate	0.1	0.1	tr	0.1±0.1
31.	1291	1289	Thymol	3.8	2.2	2.7	2.9±0.8
32.	1300	1298	Carvacrol	0.2	0.2	0.0	0.1±0.1
33.	1346	1346	*α*-Terpinylacetate	0.0	0.0	7.2	2.4±4.2
34.	1421	1417	(*E*)-Caryophyllene	0.3	0.1	0.1	0.2±0.1
			MH[d]	84.6	88.4	55.4	76.1±18.1
			MO	6.0	5.1	32.8	14.6±15.7
			SH	0.3	0.1	0.1	0.2±0.1
			SO	0.0	0.0	0.0	0.0±0.0
			PP	6.4	3.4	9.9	6.6±3.3
			O	2.3	2.5	1.0	1.9±0.8
			Total:	99.6	99.5	99.2	99.4±0.2

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] [c]Retention indices from NIST Chemistry WebBook relative to HP-5MS[2]; tr - trace (≤0.1 %). [d]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-XIV. Headspace volatiles of cinnamon, *Cinnamomum verum* samples

				Content, %						
No	RI[a]	AI[b]	Compound	s50	s51	s52	s53	s54	s55	Mean±SD
1.	932	932	*α*-Pinene	3.0	3.1	2.7	1.8	0.8	3.3	2.5±1.0
2.	947	946	Camphene	1.1	1.8	2.0	1.4	0.6	1.7	1.4±0.5
3.	958	952	Benzaldehyde	0.1	1.1	0.5	0.5	0.6	1.0	0.6±0.4
4.	975	974	*β*-Pinene	0.8	0.6	1.5	0.6	0.3	0.2	0.7±0.5
5.	1023	1020	*p*-Cymene	0.5	0.6	0.2	0.2	0.1	1.0	0.4±0.3
6.	1028	1024	Limonene	1.0	1.2	0.6	0.6	0.3	1.2	0.8±0.4
7.	1030	1026	1,8-Cineole	18.3	21.6	15.7	16.5	10.5	13.1	16.0±3.9
8.	1098	1095	Linalool	0.9	0.4	0.8	0.2	0.4	0.2	0.5±0.3
9.	1166	1165	Borneol	0.2	0.5	1.3	1.8	1.6	1.7	1.2±0.7
10.	1177	1174	Terpinen-4-ol	1.6	1.7	1.7	2.2	1.5	1.4	1.7±0.3
11.	1190	1186	*α*-Terpineol	1.2	1.5	1.5	2.0	1.4	1.1	1.5±0.3
12.	1271	1267	(*E*)-Cinnamaldehyde	51.0	50.2	54.5	56.3	44.5	48.8	50.9±4.2
13.	1286	1283	Isobornyl acetate	6.3	7.6	8.1	8.9	12.1	4.5	7.9±2.6
14.	1378	1374	*α*-Copaene	7.6	3.8	2.4	2.0	11.9	10.2	6.3±4.2
15.	1416	1411	*α-cis*-Bergamotene	0.2	0.3	0.4	0.5	1.7	0.9	0.7±0.6
16.	1423	1417	(*E*)-Caryophyllene	4.1	1.7	1.5	1.0	3.3	3.4	2.5±1.3
17.	1502	1500	*α*-Muurolene	0.4	0.5	0.9	0.9	1.8	1.0	0.9±0.5
18.	1525	1522	*δ*-Cadinene	0.9	0.9	1.2	1.2	1.9	1.3	1.2±0.4
			MH[c]	6.4	7.3	7.0	4.6	2.1	7.4	5.8±2.1
			MO	28.5	33.3	29.1	31.6	27.5	22.0	28.7±3.9
			SH	13.2	7.2	6.4	5.6	20.6	16.8	11.6±6.2
			SO	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			PP	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			O	51.1	51.3	55.0	56.8	45.1	49.8	51.5±4.1
			Total:	99.2	99.1	97.5	98.6	95.3	96.0	97.6±1.7

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-XV. Headspace volatiles of bay laurel, *Laurus nobilis* samples

				Content, %)						
No	RI[a]	AI[b]	Compound	s56	s57	s58	s59	s60	s61	Mean±SD
1.	925	924	*α*-Thujene	0.1	0.1	0.2	0.2	0.1	0.1	0.1±0.1
2.	932	932	*α*-Pinene	1.3	0.8	1.7	1.2	0.4	1.5	1.2±0.5
3.	947	946	Camphene	0.3	0.1	0.2	tr	tr	0.2	0.2±0.1
4.	972	969	Sabinene	2.6	1.8	1.7	5.7	1.9	4.6	3.1±1.7
5.	975	974	*β*-Pinene	1.3	0.8	1.5	1.3	0.5	1.5	1.2±0.4
6.	989	988	Dehydro-1,8-cineol	0.0	0.1	0.1	0.2	0.2	0.1	0.1±0.1
7.	1016	1014	*α*-Terpinene	0.0	0.1	0.1	0.1	0.1	0.1	0.1±0.0
8.	1024	1020	*p*-Cymene	0.8	0.8	1.2	0.5	0.4	0.4	0.7±0.3
9.	1033	1026	1,8-Cineole	86.7	90.9	89.6	86.5	92.1	85.7	88.6±2.6
10.	1058	1054	*γ*-Terpinene	0.1	0.2	0.2	0.2	0.1	0.2	0.2±0.1
11.	1066	1065	*cis*-Sabinene hydrate	0.2	0.1	0.2	0.4	0.3	0.4	0.3±0.1
12.	1086	1086	Terpinolene	0.0	0.0	tr	tr	tr	tr	0.0±0.0
13.	1098	1095	Linalool	2.9	0.5	0.7	0.7	0.8	0.6	1.0±0.9
14.	1139	1135	*trans*-Pinocarveol	0.0	0.1	0.1	tr	tr	tr	0.1±0.1
15.	1163	1160	Pinocarvone	0.0	0.1	0.1	tr	tr	tr	0.1±0.1
16.	1165	1162	*δ*-Terpineol	0.0	0.1	0.1	0.1	0.1	0.2	0.1±0.1
17.	1178	1174	Terpinen-4-ol	1.4	1.5	0.8	0.4	1.1	1.1	1.1±0.4
18.	1190	1186	*α*-Terpineol	0.7	0.2	0.2	0.4	0.7	1.1	0.6±0.4
19.	1197	1195	Myrtenal	0.0	0.1	0.1	tr	tr	tr	0.1±0.1
20.	1286	1284	Isobornyl acetate	0.0	0.1	0.1	tr	tr	0.2	0.1±0.1
21.	1317	1316	*δ*-Terpinyl acetate	0.0	0.1	0.1	0.1	0.1	0.1	0.1±0.0
22.	1350	1346	*α*-Terpinyl acetate	1.0	1.3	0.7	1.8	0.9	1.8	1.3±0.5
			MH [c]	6.4	4.7	6.8	9.2	3.5	8.6	6.5±
			MO	93.0	95.2	92.9	90.6	96.3	91.3	93.2±
			SH	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			SO	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			PP	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			O	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			Total:	99.4	99.9	99.7	99.8	99.8	99.9	99.8±0.2

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] tr - trace (≤0.1 %). [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-XVI. Headspace volatiles of nutmeg, *Myristica fragrans* samples

				Content, %			
No	RI[a]	AI[b]	Compound	s62	s63	s64	Mean±SD
1.	925	924	*α*-Thujene	2.2	3.9	0.4	2.2±1.8
2.	932	932	*α*-Pinene	12.8	20.1	2.7	11.9±8.7
3.	947	946	Camphene	0.3	0.3	0.5	0.4±0.1
4.	972	969	Sabinene	7.6	10.3	0.3	6.1±5.2
5.	974	974	*β*-Pinene	6.7	11.8	1.0	6.5±5.4
6.	989	988	Myrcene	0.3	0.6	0.0	0.3±0.3
7.	1004	1002	*α*-Phellandrene	0.5	0.7	1.3	0.8±0.4
8.	1008	1008	*δ*-3-Carene	0.0	0.3	0.2	0.2±0.2
9.	1016	1014	*α*-Terpinene	4.4	5.8	6.7	5.6±1.2
10.	1024	1020	*p*-Cymene	6.9	7.1	5.9	6.6±0.6
11.	1026	1024	Limonene	2	3	1.1	2.0±1.0
12.	1028	1025	*β*-Phellandrene	2.1	3.2	2.3	2.5±0.6
13.	1029	1026	1,8-Cineole	0.2	0.0	0.8	0.3±0.4
14.	1056	1054	*γ*-Terpinene	6.3	7.4	6.0	6.6±0.7
15.	1066	1065	*cis*-Sabinene hydrate	0.8	0.8	0.0	0.5±0.5
16.	1088	1086	Terpinolene	0.8	0.6	0.9	0.8±0.2
17.	1096	1095	Linalool	2.2	1.7	0.6	1.5±0.8
18.	1176	1174	Terpinen-4-ol	21.1	9.2	59.1	29.8±26.1
19.	1191	1186	*α*-Terpineol	1.8	0.9	3.2	2.0±1.2
20.	1286	1283	Isobornyl acetate	0.3	0.0	0.0	0.1±0.2
21.	1289	1285	Safrole	5.3	0.6	2.6	2.8±2.4
22.	1358	1356	Eugenol	5.0	0.0	0.0	1.7±2.9
23.	1376	1374	*α*-Copaene	0.5	0.0	0.4	0.3±0.3
24.	1403	1403	Methyl eugenol	1.1	0.4	0.5	0.7±0.4
25.	1421	1417	(*E*)-Caryophyllene	0.0	0.0	0.3	0.1±0.2
26.	1521	1517	Myristicin	7.1	7.6	0.9	5.2±3.7
27.	1526	1521	Eugenol acetate	0.5	0.0	0.0	0.2±0.3
			MH[c]	52.9	75.1	39.3	55.8±18.1
			MO	26.4	12.6	53.7	30.9±20.9
			SH	0.5	0	0.7	0.4±0.4
			SO	0.0	0.0	0.0	0.0±0.0
			PP	19	8.6	4	10.5±7.7
			O	0	0	0	0.0±0.0
			Total:	98.8	96.3	97.4	97.5±1.3

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-XVII. Headspace volatiles of clove *Syzygium aromaticum* samples

				Content, %				
No	RI[a]	AI[b]	Compound	s65	s66	s67	s68	Mean±SD
1.	887	889	2-Heptanone	3.4	0.5	0.0	1.5	1.4±1.5
2.	898	894	2-Heptanol	0.2	0.0	0.0	0.1	0.1±0.1
3.	923	921	Methyl hexanoate	0.2	0.0	0.0	0.0	0.1±0.1
4.	931	932	*α*-Pinene	0.0	0.0	0.2	0.0	0.1±0.1
5.	974	974	*β*-Pinene	0.0	0.0	0.3	0.0	0.1±0.2
6.	998	997	Ethyl hexanoate	0.4	0.0	0.0	0.0	0.1±0.2
7.	1002	1002	*α*-Phellandrene	0.0	0.0	0.1	0.0	0.0±0.1
8.	1008	1008	*δ*-3-Carene	0.0	0.0	0.6	0.0	0.2±0.3
9.	1022	1020	*p*-Cymene	0.0	0.0	0.1	0.0	0.0±0.1
10.	1026	1024	Limonene	0.0	0.0	0.7	0.0	0.2±0.4
11.	1029	1026	1,8-Cineole	0.0	0.0	0.1	0.0	0.0±0.1
12.	1040	1038	2-Heptyl acetate	1.7	0.2	0.3	0.5	0.7±0.7
13.	1056	1054	*γ*-Terpinene	0.0	0.0	0.1	0.0	0.0±0.1
14.	1090	1087	2-Nonanone	0.8	0.0	0.0	0.0	0.2±0.4
15.	1094	1088	Methyl benzoate	0.1	0.0	0.0	0.0	0.0±0.1
16.	1096	1095	Linalool	0.0	0.0	0.0	1.0	0.3±0.5
17.	1170	1169	Ethyl benzoate	0.1	0.0	0.0	0.0	0.0±0.1
18.	1195	1190	Methyl salicylate	0.4	0.0	0.0	0.0	0.1±0.2
19.	1358	1356	Eugenol	73.0	82.6	39.7	78.9	68.6±19.6
20.	1376	1374	*α*-Copaene	0.7	0.0	1.2	0.0	0.5±0.6
21.	1422	1417	(*E*)-Caryophyllene	17.0	13.7	53.0	14.5	24.6±19.0
22.	1456	1452	*α*-Humulene	0.8	0.8	2.5	0.9	1.3±0.8
23.	1525	1521	Eugenol acetate	0.7	0.9	0.0	0.9	0.6±0.4
			MH[c]	0.0	0.0	2.1	0.0	0.5±1.1
			MO	0.0	0.0	0.1	1.0	0.3±0.5
			SH	18.5	14.5	56.7	15.4	26.3±20.4
			SO	0.0	0.0	0.0	0.0	0.0±0.0
			PP	73.7	83.5	39.7	79.8	69.2±20.1
			O	7.3	0.7	0.3	2.1	2.6±3.2
			Total:	99.5	98.7	98.9	98.3	98.9±0.5

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-XVIII. Headspace volatiles of turmeric, *Curcuma longa* samples

No	RI[a]	AI[b]	Compound	Content, %		
				s69	s70	Mean±SD
1.	923	924	*α*-Thujene	0.2	0.2	0.2±0.0
2.	931	932	*α*-Pinene	2.3	2.6	2.5±0.2
3.	969	969	Sabinene	0.1	0.1	0.1±0.0
4.	973	974	*β*-Pinene	0.1	0.1	0.1±0.0
5.	986	988	Myrcene	0.6	0.6	0.6±0.0
6.	1001	1002	*α*-Phellandrene	56.6	57.2	56.9±0.4
7.	1007	1008	*δ*-3-Carene	0.9	1.0	1.0±0.1
8.	1013	1014	*α*-Terpinene	0.5	0.4	0.5±0.1
9.	1021	1020	*p*-Cymene	7.1	9.5	8.3±1.7
10.	1025	1024	Limonene	1.6	1.8	1.7±0.1
11.	1028	1025	*β*-Phellandrene	1.7	1.9	1.8±0.1
12.	1027	1026	1,8-Cineole	10.5	9.4	10.0±0.8
13.	1055	1054	*γ*-Terpinene	0.9	0.7	0.8±0.1
14.	1085	1086	Terpinolene	1.2	0.8	1.0±0.3
15.	1419	1417	(*E*)-Caryophyllene	1.2	1.0	1.1±0.1
16.	1480	1479	ar-Curcumene	2.0	2.5	2.3±0.4
17.	1492	1493	*α*-Zingiberene	4.5	2.9	3.7±1.1
18.	1506	1505	*β*-Bisabolene	0.5	0.4	0.5±0.1
19.	1521	1521	*β*-Sesquiphellandrene	2.3	1.9	2.1±0.3
20.	1667	1668	ar-Turmerone	2.8	2.4	2.6±0.3
			MH[c]	73.8	76.9	75.4±2.2
			MO	10.5	9.4	10.0±0.8
			SH	10.5	8.7	9.6±1.3
			SO	2.8	2.4	2.6±0.3
			PP	0.0	0.0	0.0±0.0
			O	0.0	0.0	0.0±0.0
			Total:	97.6	97.4	97.5±0.1

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-XIX. Headspace volatiles of ginger, *Zingiber officinale* samples

				Content, %		
No	RI[a]	AI[b]	Compound	s71	s72	Mean±SD
1.	795	801	Hexanal	0.0	0.2	0.1±0.1
2.	895	894	2-Heptanol	0.0	0.2	0.1±0.1
3.	931	932	*α*-Pinene	0.0	1.9	1.0±1.3
4.	947	946	Camphene	1.5	8.2	4.9±4.7
5.	973	974	*β*-Pinene	0.0	0.5	0.3±0.4
6.	982	981	6-Methyl-5-hepten-2-one	0.0	1.7	0.9±1.2
7.	986	988	Myrcene	0.0	1.2	0.6±0.8
8.	1001	1002	*α*-Phellandrene	0.0	0.4	0.2±0.3
9.	1021	1020	*p*-Cymene	0.0	0.6	0.3±0.4
10.	1025	1024	Limonene	0.0	2.3	1.2±1.6
11.	1027	1025	*β*-Phellandrene	0.0	9.4	4.7±6.6
12.	1027	1026	1,8-Cineole	2.3	12.3	7.3±7.1
13.	1055	1054	*γ*-Terpinene	0.0	0.2	0.1±0.1
14.	1085	1086	Terpinolene	0.0	0.3	0.2±0.2
15.	1088	1087	2-Nonanone	0.0	0.2	0.1±0.1
16.	1093	1095*	Rose furan	0.0	1.0	0.5±0.7
17.	1095	1095	Linalool	0.0	1.7	0.9±1.2
18.	1142	1141	Camphor	0.0	0.2	0.1±0.1
19.	1146	1148	Camphene hydrate	0.0	0.1	0.1±0.1
20.	1165	1163	Borneol	0.0	3.7	1.9±2.6
21.	1171	1173	Rosefuran epoxide	0.0	0.4	0.2±0.3
22.	1174	1174	Terpinen-4-ol	0.0	0.3	0.2±0.2
23.	1188	1186	*α*-Terpineol	0.0	1.4	0.7±1.0
24.	1283	1284	Isobornyl acetate	0.0	0.2	0.1±0.1
25.	1366	1371	*α*-Ylangene	0.0	0.4	0.2±0.3
26.	1375	1374	*α*-Copaene	0.0	1.1	0.6±0.8
27.	1391	1389	*β*-Elemene	0.0	0.5	0.3±0.4
28.	1402	1405	Sesquithujene	0.0	0.2	0.1±0.1
29.	1462	1458	*allo*-Aromadendrene	0.0	0.4	0.2±0.3
30.	1476	1465	*cis*-Muurola-4(14),5-diene	0.0	0.5	0.3±0.4
31.	1480	1479	ar-Curcumene	16.5	9.2	12.9±5.2
32.	1492	1493	*α*-Zingiberene	46.1	21.9	34.0±17.1
33.	1498	1493	*trans*-Muurola-4(14),5-diene	3.2	2.9	3.1±0.2
34.	1505	1505	*β*-Bisabolene	11.4	6.7	9.1±3.3
35.	1507	1505	(*E*,*E*)-*α*-Farnesene	1.3	0.0	0.7±0.9
36.	1521	1521	*β*-Sesquiphellandrene	16.7	7.0	11.9±6.9
			MH[c]	1.5	15.5	8.5±9.9
			MO	2.3	19.9	11.1±12.4
			SH	95.2	50.8	73.0±31.4
			SO	0.0	0.0	0.0±0.0
			PP	0.0	0.0	0.0±0.0
			O	0.0	3.7	1.9±2.6
			Total:	99.0	99.4	99.2±0.3

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-XX. Headspace volatiles of black paper, *Piper nigrum* samples

				Content, %						
No	RI[a]	AI[b]	Compound	s73	s74	s75	s76	s77	s78	Mean±SD
1.	925	924	*α*-Thujene	0.1	1.3	1.8	1.4	0.8	2.7	1.4±0.9
2.	932	932	*α*-Pinene	2.7	4.7	4.4	12.9	3.5	7.4	5.9±3.8
3.	947	946	Camphene	tr	0.1	0.1	0.2	0.0	0.0	0.1±0.1
4.	972	969	Sabinene	0.3	7.3	19.1	5.3	2.1	13.1	7.9±7.1
5.	975	974	β-Pinene	4.5	8.6	6.3	14.9	5.9	11.3	8.6±3.9
6.	989	988	Myrcene	0.4	0.9	1.3	1.2	0.5	0.9	0.9±0.4
7.	1003	1002	*α*-Phellandrene	0.7	0.8	3.0	1.8	0.9	1.8	1.5±0.9
8.	1009	1008	*δ*-3-Carene	5.4	3.7	11.2	11.5	6.1	9.6	7.9±3.3
9.	1016	1014	*α*-Terpinene	0.0	0.2	0.1	0.3	0.2	0.3	0.2±0.1
10.	1024	1020	*p*-Cymene	0.5	0.3	0.9	0.7	0.4	0.8	0.6±0.2
11.	1028	1024	Limonene	8.0	14.4	13.3	21.8	11.0	19.0	14.6±5.1
12.	1056	1054	*γ*-Terpinene	0.0	0.6	0.3	0.5	0.3	0.5	0.4±0.2
13.	1086	1086	Terpinolene	0.1	0.2	0.3	0.0	0.0	0.0	0.1±0.1
14.	1097	1095	Linalool	0.6	0.4	1.2	0.4	0.3	0.5	0.6±0.3
15.	1178	1174	Terpinen-4-ol	0.0	0.3	0.1	0.0	0.0	0.0	0.1±0.1
16.	1243	1239	Carvone	0.1	0.0	0.0	5.3	0.0	0.0	0.9±2.2
17.	1339	1335	*δ*-Elemene	0.7	0.8	0.3	0.0	0.5	0.0	0.4±0.3
18.	1379	1374	*α*-Copaene	4.6	4.2	1.2	0.3	2.7	1.2	2.4±1.8
19.	1394	1389	*β*-Elemene	2.0	0.7	0.3	0.0	0.5	0.0	0.6±0.7
20.	1417	1411	*α-cis*-Bergamotene	0.0	0.1	0.0	0.0	0.1	0.0	0.0±0.1
21.	1420	1417	(*E*)-Caryophyllene	55.9	46.1	31.0	16.3	58.2	24.1	38.6±17.3
22.	1437	1432	*α-trans*-Bergamotene	0.0	0.1	0.0	0.0	0.2	0.0	0.1±0.1
23.	1458	1452	*α*-Humulene	3.3	1.5	1.4	0.8	2.3	1.2	1.8±0.9
24.	1486	1484	Germacrene D	0.0	0.1	0.0	0.7	0.0	0.0	0.1±0.3
25.	1491	1489	*β*-Selinene	4.0	0.4	0.8	0.0	1.1	0.3	1.1±1.5
26.	1499	1498	*α*-Selinene	3.0	0.4	0.7	0.0	0.8	0.3	0.9±1.1
27.	1507	1505	*β*-Bisabolene	0.6	0.7	0.0	0.0	0.4	1.7	0.6±0.6
28.	1526	1522	*δ*-Cadinene	1.4	0.4	0.2	0.0	0.5	0.2	0.5±0.5
29.	1559	1559	Germacrene B	0.0	0.0	0.0	0.0	0.0	1.3	0.2±0.5
			MH[c]	22.7	43.1	62.1	72.5	31.7	67.4	49.9±20.4
			MO	0.7	0.7	1.3	5.7	0.3	0.5	1.5±2.1
			SH	75.5	55.5	35.9	18.1	67.3	30.3	47.1±22.5
			SO	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			PP	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			O	0.0	0.0	0.0	0.0	0.0	0.0	0.0±0.0
			Total:	98.9	99.3	99.3	96.3	99.3	98.2	98.6±1.2

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]Adams' retention indices.[1] [c]Abbreviations: MH - monoterpene hydrocarbons, MO - oxygenated monoterepenes, SH - sesquiterpene hydrocarbons, SO - oxygenated sesquiterpenes, PP - phenylpropanoids. Others - aliphatic alcohols, aldehydes, ketones, esters.

TABLE S-XXI. Headspace volatiles of garlic, *Allium sativum* samples

				Content, %						
No	RI[a]	NI[b]	Compound	s79	s80	s81	s82	s83	s84	Mean±SD
1.	853	859	Diallyl sulfide	3.2	16.8	2.0	12.4	2.3	26.6	10.6±10.0
2.	913	919	Methyl allyl disulfide	4.6	5.8	3.8	7.6	3.9	9.0	5.8±2.1
3.	927	931	(*Z*)-Methyl 1-propenyl disulfide	tr	0.0	0.0	tr	0.0	0.0	0.0±0.0
4.	936	940	(*E*)-Methyl 1-propenyl disulfide	0.2	0.0	0	0.2	0.3	0.0	0.1±0.1
5.	967	972	Dimethyl trisulfide	0.8	3.2	0.6	6.5	0.5	2.7	2.4±2.3
6.	1077	1077	Diallyl disulfide	28.6	12.8	17.9	10.8	20.5	21.5	18.7±6.4
7.	1136	1144	Methyl allyl trisulfide	17.6	21.9	13.2	27	11.3	16.1	17.9±5.8
8.	1186	1191	3-Vinyl-1,2-dithia-cyclohex-4-ene	0.3	0.0	0.0	0.2	0.0	0.0	0.1±0.1
9.	1210	1202	3-Vinyl-1,2-dithia-cyclohex-5-ene	0.5	0.4	0.0	0.8	0.0	0.0	0.3±0.3
10.	1215	1215	1,4-Dimethyltetrasulfide	0.0	0.3	0.0	0.7	0.0	0.0	0.2±0.3
11.	1300	1304	Diallyl trisulfide	39.4	38.1	59.9	32.2	55.2	23.2	41.3±13.9
			Sulfides	3.2	16.8	2.0	12.4	2.3	26.6	10.6±10.0
			Disulfides	34.2	19	21.7	19.6	24.7	30.5	25.0±6.2
			Cyclic disulfides	0.8	0.4	0.0	1.0	0.0	0.0	0.4±0.4
			Trisulfides	57.8	63.2	73.7	65.7	67.0	42.0	61.6±10.9
			Tetrasulfides	0.0	0.3	0.0	0.7	0.0	0.0	0.2±0.3
			Total sulfides:	95.2	99.3	97.4	98.4	94.0	99.1	97.2±2.2

[a]Experimental linear retention indices relative to C8–C40 alkanes on the HP-5MS. [b]retention indices from NIST Chemistry WebBook relative to HP-5MS[2]; tr - trace (≤0.1 %).

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