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Characteristic Impact Odorants of *Changpo* (*Acorus calamus* var. *angustatus* Bess) Root Essential Oil

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Abstract This study was conducted to determine firstly the composition of the essential oil from fresh *changpo* (*Acorus calamus* var. *angustatus* Bess) roots quantitatively and qualitatively by use of two internal standards, and secondly volatile compounds which are primarily responsible for the aroma of *changpo* roots. Simultaneous steam distillation and extraction method was used for essential oil extraction, and aroma extract dilution analysis (AEDA) and sniffing test by gas chromatography/olfactometry (GC/O) were used to detect the characteristic impact odorants. According to the instrumental analysis of *changpo* root essential oil, *cis, trans*-farnesol (47.56 mg/kg of fresh wt), octanoic acid (23.73 mg/kg of fresh wt), *trans*-2-dodecenal (20.28 mg/kg of fresh wt) and *trans, trans*-farnesol (13.81 mg/kg of fresh wt) were the most abundant compounds. Geranyl acetate, *trans*-nerolidol and *trans, trans*-farnesyl acetate were evaluated as the characteristic impact odorants of *changpo* roots from results of AEDA and sniffing test. Especially, geranyl acetate was considered as the most similar odor component to *changpo* roots by organoleptic evaluation with GC/O.

Keywords: *changpo* root, aroma extract dilution analysis, gas chromatography/olfactometry, sniffing test, characteristic impact odorants

Introduction

Changpo (*Acorus calamus* var. *angustatus* Bess) is a perennial aquatic herb belonging to the Araceae family (1). *Changpo* flavor is widely accepted in Korea and China due to its attractive flavor. *Changpo* leaves have long been used as perfume, seasoning, and bathing products, especially for hair rinse and soap due to its refreshing aroma (2). The roots of *changpo* have been used as a domestic folk medicine for the remedy of diarrhea, indigestion, and bronchopneumonia in Korea and China. In Iran the roots of *changpo* were used as a tonic, insecticide, flavoring, and tea, as well as in the treatment of rheumatism (3). The importance of aromatic plants is considerable owing to their applications in folk medicine and their potential for commercial value in various fields as spices, beverages, perfumery, cosmetics, pharmaceutics, and aromatherapy. Essential oils from aromatic and medicinal plants have been known since antiquity to possess biological properties. There has been increasing world wide interest in the volatile flavors from natural aromatic medicinal plants (3-7).

There have been a few studies on the chemical composition (8), antimicrobial activity (9), narcotic effect (10), and nervous sedative effect (11) of *changpo*. Despite the pleasant flavor of this plant, no detailed report on the characteristic odor components of *changpo* roots evaluated by gas chromatography/olfactometry (GC/O) has been published to date. Therefore, this study was carried out to investigate the chemical composition of *changpo* root essential oil and to elucidate the characteristic impact odorants of the essential oil by GC/O and aroma extract dilution analysis (AEDA) technique.

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Materials and Methods

Materials Fresh *changpo* roots, harvested in May 2003, were collected from a farm located in Kyunggi Province, Korea. Authentic chemicals were obtained from the following reliable commercial sources: Aldrich Chemical Co. (Milwaukee, WI, USA), Fluka Fine Chemicals (Buchs, Switzerland), Funakoshi Co., Ltd. (Tokyo, Japan), Nacalai Tesque Inc. (Kyoto, Japan), PolyScience Co. (Nile, IL, USA), Sigma Chemical Co. (St. Louis, MO, USA), Theta Co. (Newtown Square, PA, USA), Tokyo Kasei Kogyo Co. (Tokyo, Japan), and Wako Pure Chemical Industries (Osaka, Japan). Some chemicals were provided by Bolak Co., Ltd (Osan, Korea) and French-Korean Aromatics (Youngin, Korea).

Preparation of essential oil Fresh *changpo* roots totaling 900 g were cut into small pieces of size (0.5 × 0.5 × 0.5 cm). Four hundred and fifty grams of cut roots was mixed with 1.4 L of water and then subjected to simultaneous steam distillation and solvent extraction with 125 mL of diethyl ether/pentane (1:1, v/v) as solvent for 1.5 hr using a modified Likens-Nickerson apparatus as described by Schultz *et al.* (12). The extraction was performed two times, and the total extract was dried by adding anhydrous sodium sulfate and then concentrated by evaporation. Finally, the essential oil sample was concentrated under reduced pressure at room temperature.

GC and GC/MS An Agilent 6890N gas chromatograph equipped with a DB-Wax (60 m × 0.25 mm i. d., film thickness 0.25 mm) fused-silica capillary column (J & W Scientific, Folsom, CA, USA) and a flame ionization detector (FID) was used. The column temperature was programmed to ramp from 70 (2 min) to 230°C (20 min) at 2°C/min. Injector and detector temperatures were set at 250°C. Nitrogen was the carrier gas at a flow rate of 1 mL/

min. The linear retention indices were calculated for all volatile components using a homologous series of *n*-alkanes (C_7-C_{29}) under the same GC conditions. 1-Heptanol and methyl myristate were used as internal standards for quantitative analysis of *changpo* root essential oil. The ratio of *changpo* oil for the two internal standards was 150 : 1 : 1. The weight percentage of each peak was calculated according to the FID correlation factor (13). One microliter of essential oil was injected and the split ratio was 50 : 1.

Gas chromatography combined with mass spectrometry was used for identifying the volatile components that had been detected. The analysis was carried out with Varian Saturn 2000R 3800 GC (Walnut Creek, CA) linked with a Varian Saturn 2000R MS. The oven condition, injector and detector temperatures, and column were the same as those described above for the Agilent 6890N GC. An essential oil sample of 0.2 μL was injected and the split ratio was 34 : 1. Helium was the carrier gas at a flow rate of 1.1 mL/min.

Identification of Components Individual components were identified by comparing their mass spectra with those of reference compounds in the data system of the Wiley library and NIST Mass Spectral Search Program (ChemSW Inc., NIST 98 version database) connected to a Varian Saturn 2000R MS. Other identifications were made by comparison of both mass spectrum and GC retention data with those of authentic compounds previously analyzed and stored in the data system. The volatile flavor components were also matched by co-injection with authentic compounds whenever available data was not obtained from retention indices and mass spectra.

GC/O An Agilent 6890N GC equipped with a DB-Wax fused-silica capillary column (60 m × 0.53 mm i.d., film thickness 1 μm, J&W Scientific, Folsom, CA, USA), FID, and olfactometer (Gerstel GmbH & Co., Mûlheim, Germany), including olfactory detector port, olfactory intensity device, and humidifier, were employed for GC/O. The oven condition, and injector and detector temperatures were the same as those given above for GC. The carrier gas was nitrogen (2 mL/min) and the split ratio was 10 : 1. The outlet of the column was split into two ways : one way leading to the detector and the other to the sniffing port. The panel was composed of previously trained individuals.

AEDA The essential oil of *changpo* roots was stepwise (3-fold) diluted with acetone until the sniffer could not detect any significant odor in a run (14-16), and aliquots of the dilutions were evaluated by three assessors. Odor potencies of each volatile in the *changpo* essential oil were evaluated by sniffers, together with the odor description. The sniffers also evaluated *changpo* root-like, and the most similar *changpo* root-like odor components perceived at the sniffing port. This evaluation was performed three times by three assessors. The highest dilution at which an individual component could be detected was defined as the flavor dilution (FD) factor for that odorant. Sweet, green, mild green, gaseous, woody, resinous, warm, fruity, dry, floral, oily, perfume-like, and pine-like were the terms used to describe the odorants. The lexicon was developed by sniffing the sample several times and selecting 13 of the most frequently used terms. On the basis of the AEDA results, relative flavor activity (RFA) was calculated using the following equation (16) : RFA = $\log 3^n/S^{0.5}$, where n is the FD-factor and S is the peak area percentage of a component.

Results and Discussion

Constituents of the essential oil of *changpo* roots The detected constituents from the essential oil of *changpo* roots are listed in Table 1, together with their concentrations. The data are mean values of triplicate measurements. The components are listed in order of their elution on the DB-Wax column. One hundred and twenty-seven components were identified in fresh *changpo* roots. The essential oil contained 29 hydrocarbons, 15 aldehydes, 37 alcohols, 7 ketones, 23 esters, 8 oxides and epoxides, 3 acids, 4 phthalides, and 1 miscellaneous component.

The essential oil obtained from the *changpo* roots was exclusively characterized by a high percentage of sesquiterpene alcohols, which alone accounted for 26.86% of the weight percent. Furthermore, the root oil was characterized by a large presence of aliphatic aldehydes, especially *trans*-2-dodecenal (no. 82), *cis, trans*-Farnesol (no. 118), octanoic acid (no. 99), and *trans, trans*-farnesol (no. 116) were the most abundant compounds of the essential oil from *changpo* roots.

Characteristic impact odorants of *changpo* roots The odor activity of each compound in a mixture was determined by sniffing the GC effluent through a series of dilutions by AEDA technique. Each volatile component was separated by GC and the odors were determined at a sniffing port of the GC/olfactometer. The aroma note of the eluting compounds from capillary gas chromatography was evaluated by AEDA and expressed as FD-factor. The highest dilution of individual components detected by the assessors was defined as its FD-factor. The FD-factor was expressed as a power of three. Odor descriptions for compounds detected with GC/O are given in Table 1.

The FD-factors of volatile constituents detected by AEDA ranged 1 and 11 (Table 1). The aroma-active volatiles (FD ≥5) in *changpo* root essential oil are given in Table 2. Geranyl acetate (no. 72) and *trans*-nerolidol (no. 95) showed the highest FD-factors of 11, followed by *trans, trans*-farnesyl acetate (no. 115) with a high FD-factor of 10. Geranyl propionate (no. 79) and isothymol (no. 113) showed a relatively high FD-factor of 7. The higher FD-factors were often related to the aroma-active compounds, and to the top note of the aroma. However, FD-factor does not always coincide with characteristic odor components (16, 17). High FD-factor of a compound may simply have been caused by its high content in the sample.

In this study, RFA, based on the results of quantitative analysis and AEDA, was calculated in addition to the FD-factor. RFA is also an important factor in the assessment of the characteristics of an aroma together with the FD-factor (16, 17). The following RFAs of major aroma-active compounds of *changpo* root essential oil were detected by GC/O: geranyl acetate, 37.1; *trans, trans*-farnesyl acetate,

Table 1. Volatile flavor components of *changpo* root essential oil

No.	Compound	Retention index	Concentration (mg/kg of fresh wt)	FD factor [a]	Odor description [b]	Identification
1	Methyl propyl acetate	990	0.02			RI [c], MS [d]
2	Decane	1004	0.22			RI, MS
3	α-Pinene	1048	0.54	6	Tree-like	RI, MS, Co-GC [e]
4	Camphene	1090	0.20	2	Green	RI, MS, Co-GC
5	Undecane	1101	0.59			RI, MS, Co-GC
6	Sabinene	1133	0.07	3	Gaseous	RI, MS, Co-GC
7	δ-3-Carene	1156	0.05			RI, MS, Co-GC
8	Myrcene	1165	tr [f]	3	Woody	RI, MS, Co-GC
9	α-Phellandrene	1177	1.10	4	Resinous, green	RI, MS, Co-GC
10	α-Terpinene	1194	0.02	4	Woody	RI, MS, Co-GC
11	3-Methyl butanol	1204	1.98	3	Green, warm	RI, MS
12	Limonene	1222	0.14	2	Green	RI, MS, Co-GC
13	β-Phellandrene	1234	tr	3	Woody	RI, MS
14	*cis*-β-Ocimene	1246	0.02	4	Green	RI, MS, Co-GC
15	γ-Terpinene	1257	0.02	2	Woody	RI, MS, Co-GC
16	*p*-Cymene	1275	tr	2	Green	RI, MS, Co-GC
17	2-Ethyl-2-hexenal	1316	tr	2	Fruity, resinous	RI, MS
18	6-Butyl-1,4-cycloheptadiene [g]	1331	tr	2	Sweet, green	MS
19	6-Methyl-5-hepten-2-one [g]	1342	0.07	3	Mild green	MS
20	Hexanol	1351	tr			RI, MS, Co-GC
21	2-Hexanol	1362	tr	2	Mild green	RI, MS
22	*trans*-3-Hexenol	1368	0.02	3	Dry, green	RI, MS
23	Tetradecane	1396	tr			RI, MS
24	Amylbenzene	1414	tr	4	Floral	RI, MS
25	*cis*-Linalool furan oxide	1423	0.02	2	Sweet	RI, MS, Co-GC
26	Butyl heptanoate	1428	tr	2	Sweet, green	RI, MS
27	Tetradecene	1433	tr			RI, MS
28	α-Thujone	1438	0.02	4	Green, woody	RI, MS
29	Hepten-1-yl acetate	1444	tr	3	Green	RI, MS
30	β-Thujone	1447	0.02	4	Green	RI, MS
31	*cis*-Limonene oxide	1451	0.20	4	Sweet	RI, MS, Co-GC
32	*trans*-Linalool oxide	1459	0.20	2	Fruity	RI, MS, Co-GC
33	*trans*-Limonene oxide	1472	0.02	3	Fruity	RI, MS, Co-GC
34	Octyl acetate	1479	0.02	2	Oily, green	RI, MS
35	Citronellal	1485	tr	3	Sweet	RI, MS, Co-GC
36	Pentadecane	1497	0.59			RI, MS
37	Decanal	1505	0.29	3	Sweet, green	RI, MS, Co-GC
38	Benzaldehyde	1519	0.83	3	Sweet, fruity	RI, MS, Co-GC
39	*d*-Camphor	1527	0.07			RI, MS, Co-GC
40	Borneol	1541	0.83	3	Floral	RI, MS
41	β-Cubebene	1545	0.02	3	Woody	RI, MS
42	Ethyl nonanoate	1550	0.05	3	Floral	RI, MS, Co-GC
43	Linalool	1558	3.36	3	Green, floral	RI, MS, Co-GC
44	Linalyl acetate	1565	0.93	3	Green, floral	RI, MS, Co-GC
45	α-Cedrene	1572	0.02	3	Dry, woody	RI, MS
46	Longifolene	1577	0.37	3	Dry, woody	RI, MS
47	Bornyl acetate	1593	0.05	4	Floral	RI, MS
48	β-Caryophyllene	1598	0.05	2	Woody	RI, MS
49	Terpinen-4-ol	1603	0.15	4	Warm, woody	RI, MS, Co-GC

Table 1. Continued

	No. Compound	Retention index	Concentration (mg/kg of fresh wt)	FD factor[a]	Odor description[b]	Identification
50	Undecanal	1611	0.51	2	Woody	RI, MS
51	*trans*-2-Decenal	1615	0.02	2	Warm, green	RI, MS
52	Citronelly formate	1625	0.44	2	Sweet	RI, MS
53	γ-Elemene	1636	0.05	4	Dry, woody	RI, MS, Co-GC
54	*trans*-2-Decenol	1648	0.15	4	Sweet	RI, MS
55	*l*-Menthol	1650	0.17			RI, MS, Co-GC
56	Ethyl decanoate	1654	0.44	6	Sweet	RI, MS, Co-GC
57	*cis*-β-Farnesene	1658	0.12	4	Mild green	RI, MS, Co-GC
58	Nonanol	1663	0.15	3	Mild green	RI, MS
59	Citrorelly acetate	1669	0.64	5	Floral	RI, MS, Co-GC
60	α-Humulene	1677	0.07	2	Floral	RI, MS
61	α-Murrolene	1680	0.27	4	Floral	RI, MS
62	*trans*-Piperitol	1889	0.05	4	Fruity	RI, MS
63	Decyl acetate	1692	0.24	5	Herbaceous	RI, MS, Co-GC
64	Neral	1696	0.37	5	Floral	RI, MS, Co-GC
65	α-Terpineol	1709	1.25	2	Floral, green	RI, MS, Co-GC
66	Dodecanal	1719	0.12	3	Floral	RI, MS, Co-GC
67	Valencene	1727	0.02	4	Floral, sweet	RI, MS
68	Neryl acetate	1733	1.03	3	Floral	RI, MS, Co-GC
69	*cis*-Carvone	1743	0.05	2	Fruity	RI, MS
70	*cis*-Linalool pyran oxide	1751	0.07	2	Fruity	RI, MS
71	*trans*-2-Undecenal	1761	0.02	2	Fruity	RI, MS
72	Geranyl acetate[h]	1768	0.05	11	Green, floral	RI, MS, Co-GC
73	Citronellol	1774	0.07	2	Green, floral	RI, MS, Co-GC
74	*n*-Decyl alcohol	1778	0.05	1	Green, floral	RI, MS
75	Cumin aldehyde	1784	0.15	4	Green, floral	RI, MS
76	Perilla aldehyde	1788	0.10	2	Green, oily	RI, MS
77	Methyl laurate	1814	0.42	5	Green, oily	RI, MS, Co-GC
78	Tridecanal	1824	4.75	6	Floral	RI, MS
79	Geranyl propionate	1830	0.24	7	Floral	RI, MS
80	Isopiperitone	1834	0.44	5	Green, floral	RI, MS
81	Geraniol	1852	1.05	2	Floral	RI, MS, Co-GC
82	*trans*-2-Dodecenal	1867	20.28	6	Green	RI, MS
83	Isopentyl caprate	1888	0.54	2	Green	RI, MS
84	Perilla alcohol	1896	0.49	2	Green, oily	RI, MS
85	2-Dodecen-4-one	1905	2.33	6	Green	RI, MS
86	Perilla alcetate	1916	0.49	4	Green, oily	RI, MS
87	2-Phentyl ethanol	1927	0.22	4	Green	RI, MS
88	Tetradecanal	1939	1.44	5	Dry, green	RI, MS
89	Dehydro carveol	1949	0.56	5	Green, oily	RI, MS
90	Heptanoic acid	1963	0.32	3	Sweet, green	RI, MS
91	2-Acetyl pyrrole	1974	0.54	5	Oily	RI, MS
92	*cis*- Caryophyllene epoxide	1987	6.73	3	Oily, green	RI, MS
93	*cis*-Nerolidol	1997	0.34	3	Oily, green	RI, MS
94	Caryophyllene oxide	2004	0.64	5	Oily	RI, MS
95	*trans*-Nerolidol[i]	2015	0.64	11	Sweet, floral	RI, MS
96	Ledol	2022	0.69	5	Fruity	RI, MS
97	Methyl tetradecanoate	2036	3.80	3	Sweet, green	RI, MS, Co-GC
98	*trans*-Dodec-2-enol	2044	0.29	2	Oily, green	RI, MS
99	Octanoic acid	2070	23.73	3	Fruity, sweet	RI, MS

Table 1. Continued

No.	Compound	Retention index	Concentration (mg/kg of fresh wt)	FD factor[a]	Odor description[b]	Identification
100	Elemol	2088	0.96	4	Floral	RI, MS
101	3-Methyl phenol	2107	0.44	2	Perfume-like	RI, MS
102	Cedrol	2119	0.22	2	Perfume-like	RI, MS
103	2-Pentadecanol	2128	11.1	3	Green, tree-like	RI, MS
104	Cedryl acetate	2143	1.52	3	Green, tree-like	RI, MS
105	Hexadecanol	2152	0.42	3	Green	RI, MS
106	Ethyl pentadecanoate	2161	0.78	3	Green	RI, MS, Co-GC
107	Eugenol	2174	0.93	3	Fruity, woody	RI, MS
108	Muurolol	2180	0.44	3	Woody	RI, MS
109	γ-Eudesmol	2188	2.45	3	Green, floral	RI, MS
110	Methyl pentadecanoate	2201	0.29	2	Oily, sweet	RI, MS, Co-GC
111	Isoeugenol	2213	0.42	2	Oily, green	RI, MS
112	α-Cadinol	2220	0.83	3	Green	RI, MS
113	Isothymol	2227	0.37	7	Tree-like, green	RI, MS
114	Heptadecanal	2249	2.35	2	Oily, floral	RI, MS
115	*trans, trans*-Farnesyl acetate[i]	2259	0.39	10	Fruity, green	RI, MS
116	*trans, trans*-Fanesol	2283	13.81	3	Green	RI, MS
117	*p*-Mentha-1,8-dien-10-ol[g]	2292	0.69	2	Oily, sweet	MS
118	*cis, trans*-Farnesol	2321	47.56	3	Green, floral	RI, MS
119	Octadecanol	2360	0.32	3	Oily, sweet	RI, MS
120	Ethyl heptadecanoate	2365	0.20	3	Oily	RI, MS, Co-GC
121	Nerol oxide	2383	1.47	3	Oily, sweet	RI, MS
122	Undecanoic acid	2419	1.67	3	Oily	RI, MS
123	14-Hydroxy-β-caryophyllene	2445	0.29	5	Green, oily	RI, MS
124	Isobutylidene phthalide	2563	1.52	5	Oily, green	RI, MS
125	Ligustilide	2629	1.20	4	Oily, green	RI, MS
126	3-Butyl dihydrophthalide	2643	0.54	3	Oily, green	RI, MS
127	*n*-Butylidene dihydrophthalide	2676	1.13	3	Oily, green	RI, MS

[a]Flavor dilution factor (3^n) of *changpo* root oil.
[b]Odor description of *changpo* root oil by GC/O.
[c]Identification based on retention index.
[d]Identification based on comparison of mass spectra.
[e]Identification based on co-injection with authentic compounds.
[f]Trace, less than 0.005%.
[g]Tentatively identified.
[h]Most similar *changpo* root-like odor compound perceived at the sniffing port.
[i]Changpo root-like odor compounds perceived at the sniffing port.

11.9; geranyl propionate, 10.6; and *trans*-nerolidol, 10.3. Although the FD-factors of *trans*-2-dodecenal, tridecanal, and 2-dodecen-4-one were relatively high at 6, their RFAs were very low at 1, 2.1 and 2.9, respectively. It could be assumed that the high FD-factors of these compounds might have been due to their concentrations (20.28, 4.75, and 2.33 mg/kg of fresh wt, respectively) in the sample. With regard to the RFA (>10), only geranyl acetate, *trans, trans*-farnesyl acetate, geranyl propionate and *trans*-nerolidol contributed essentially to the important aroma characteristics of *changpo* roots.

The FD-factor or RFA has proven to be a useful criterion to reconstruct the original aroma from odor-active compounds detected by AEDA (16, 17). However, the FD-factor and RFA often have no relation to the aroma characteristic of each compound (16, 17). The use of RFA is not involved in the decision on characteristic odor components, but rather in the consideration of relative contribution in odor activity. Therefore, the sniffing test of the original *changpo* root essential oil by on-line GC was adopted finally to determine the characteristic odorants of *changpo*. Organoleptic evaluation by GC-sniffing was particularly enforced for several compounds with high FD-factors (≥7) and/or high RFA (≥10). Among these compounds, geranyl acetate (FD-factor 11, RFA 37.1), *trans*-nerolidol (FD-factor 11, RFA 10.3) and *trans, trans*-farnesyl acetate (FD-factor 10, RFA 11.9) were regarded as the *changpo* root-like odors by GC-sniffing. The results of sniffing test were correlated with those of FD-factor and RFA by AEDA. Especially, geranyl acetate (no. 72) was evaluated as the odorant with the greatest similarity to *changpo* roots by GC-sniffing.

The results reported here suggest that geranyl acetate (no. 72), *trans*-nerolidol (no. 95) and *trans, trans*-farnesyl acetate (no. 115) were regarded as the characteristic impact odorants of *changpo* root essential oil, while the odorant characteristic of geranyl acetate was the most similar to that of *changpo* root aroma.

Table 2. Most odor-active volatiles (FD ≥ 5) in the essential oil of *changpo* roots as detected by GC/O

Peak No.[a]	Compound	Concentration (mg/kg of fresh wt)	FD-factor (3^n)	RFA
3	α-Pinene	0.54	6	6.1
56	Ethyl decanoate	0.44	6	6.7
59	Citronellyl acetate	0.64	5	4.7
63	Decyl acetate	0.24	5	7.5
64	Neral	0.37	5	6.2
72	Geranyl acetate	0.05	11	37.1
77	Methyl laurate	0.42	5	5.8
78	Tridecanal	4.75	6	2.1
79	Geranyl propionate	0.24	7	10.6
80	Isopiperitone	0.44	5	5.6
82	*trans*-2-Dodecenal	20.28	6	1
85	2-Dodecen-4-one	2.33	6	2.9
88	Tetradecanal	1.44	5	3.1
89	Dehydro carveol	0.56	5	5
91	2-Acetyl pyrrole	0.54	5	5.1
94	Caryophyllene oxide	0.64	5	4.7
95	*trans*-Nerolidol	0.64	11	10.3
96	Ledol	0.69	5	4.5
113	Isothymol	0.37	7	8.6
115	*trans, trans*-Farnesyl acetate	0.39	10	11.9
123	14-Hydroxy-β-caryophyllene	0.29	5	6.9
124	Isobutylidene phthalide	1.52	5	3

[a]Peak no. corresponding with the peak numbers in Table 1.

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