

## Chemical Constituents of the Essential Oil of *Stachys lavandulifolia* Vahl from Iran

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### Abstract

The essential oil of *Stachys lavandulifolia* Vahl (Lamiaceae) was isolated by hydrodistillation of the aerial parts of the plant, with a yield of 0.25%. The chemical composition of volatile oil was analyzed by capillary GC and GC/MS. The main components were germacrene-D (13.2%),  $\beta$ -phellandrene (12.7%),  $\beta$ -pinene (10.2%), myrcene (9.4%),  $\alpha$ -pinene (8.4%) and Z- $\beta$ -ocimene (5.8%).

**Keywords:** *Stachys lavandulifolia*; Lamiaceae; essential oil; GC-MS.

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### Introduction

In the flora of Iranica genus, *Stachys* is represented by thirty-one species. *Stachys lavandulifolia* is grown in many parts of Iran, Iraq and Anatolia (1). The plant is known as Chaye-kuhi in Iran and its' english name is Betony. It is used as the herbal tea in gastrointestinal disorders (2). Hydroalcoholic extract of the aerial parts of *S. inflata* shows potent anti-inflammatory activity in rat. The methanolic extract of the tuber of *S. sieboldii* has anti-anoxia action in mice (3, 4). Ramezani et al. reported spathulenol and caryophyllene oxide as the main constituents of *S. lavandulifolia* (5). In the present study a sample of *S. lavandulifolia* with different chemical composition has been reported.

### Experimental

#### Plant Material and Isolation Procedure

The plant material was collected in May

2002 from the Fasham area near Tehran. A voucher specimen has been deposited in the Herbarium of the Faculty of Pharmacy, Shaheed Beheshti University of Medical Sciences (herbarium no. 0783). The aerial parts of the plant were air-dried. The oil was obtained by hydrodistillation using a Clevenger-type apparatus for 4 hours. The yield of oil was 0.25%.

#### Identification of the oil components

The analytical Gas Chromatography (GC) method was carried out using a Varian GC 3600 chromatograph with DB-5 (methyl phenyl siloxane 25 m X 0.25 mm, 0.25  $\mu$ m film thickness), N<sub>2</sub> as the carrier gas with a split ratio of 1:20, and a flame ionization detector. Temperature programming was performed from 60°-240°C at 3°/min, with injector and detector temperatures, 240°C and 260°C respectively. GC/MS was performed on a cross-linked 5% phenyl methyl siloxane (HP-5, 30 m X 0.25 mm, 0.25  $\mu$ m film thickness) with He as the carrier gas at a split ratio of 1:20 and quadropole

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mass spectrometer (Helwett- Packard 6890) operating at 70 eV ionization energy. EIMS spectra were obtained in the scan mode at m/e range of 35-400 amu. The chromatographic conditions were as above. Retention indices were determined by using retention times of n-alkanes, which has been injected after the oil, under the same chromatographic conditions. The retention indices for all the components were determined according to the Van Den Dool method using n-alkanes as standard (6). The constituents were identified by comparison of retention indices (RRI, HP-5) with those reported in the literature and by comparison of their mass spectra with those held in Wiley library of mass spectra or with the published mass spectra (7,8).

### Results and Discussion

The yield of the oil obtained from *S. lavandulifoila* was 0.25%. The yield of the oils extracted from other species were, 0.18% from *S. setifera* ssp. *iranica* 0.18% from *S. chrysantha*, and 0.12% from *S.candida* (9, 10). The *S. lavandulifolia* oil was examined by GC and GC-MS. The list of compounds identified in the oil of *S. lavandulifolia* can be seen in Table 1. Seventy-nine compounds were identified, representing 98.2% of the essential oil, in which the major components were germacrene-D (13.2%),  $\beta$ -phellandrene (12.7%),  $\beta$ -pinene (10.2%) myrcene (9.4%),  $\alpha$ -pinene (8.4%) and Z- $\beta$ -ocimene (5.8%). In a previous study the main components of the oil were reported to be spathulenol (35.0%) and caryophyllene oxide (25.6%), this finding was completely different from our study, in which only 1.5% spathulenol was present in the oil. The major component of the *S. obliqua* oil was germacrene-D, which was also the main component of the *S. lavandulifolia* oil (11). The main components of the oils of *S. aegyptica* ( $\alpha$ -pinene) and *S. glutinosa* ( $\alpha$ -pinene and  $\beta$ -phellandrene) were presented as the major components of the *S. lavandulifolia* oil (12,13).  $\beta$ -Pinene, one of the main components of *S. recta* and *S. balansae* oils, was present at an amount of 8.4% in *S. lavandulifolia* oil (14).

**Table 1.** Composition of the essential oil of *Stachys lavandulifolia*.

Peak no.	Compound name	RI	% in oil
1	Hexanal	800	t
2	E-2-Hexenal	850	0.1
3	Heptanal	900	t
4	$\alpha$ -Thujene	928	0.5
5	<b><math>\alpha</math>-Pinene</b>	<b>937</b>	<b>8.4</b>
6	Camphene	949	0.3
7	Sabinene	974	0.3
8	<b><math>\beta</math>-Pinene</b>	<b>982</b>	<b>10.2</b>
9	<b>Myrcene</b>	<b>995</b>	<b>9.4</b>
10	$\alpha$ -Phellandrene	1006	t
11	$\delta$ -3-Carene	1011	0.2
12	$\alpha$ -Terpinene	1017	0.5
13	<b><math>\beta</math>-Phellandrene</b>	<b>1033</b>	<b>12.7</b>
14	Z- $\beta$ -Ocimene	1043	5.8
15	E- $\beta$ -Ocimene	1050	0.9
16	$\gamma$ -Terpinene	1061	1.4
17	Z-Sabinene-hydrate	1068	0.2
18	Terpinolene	1088	0.3
19	Linalool	1101	0.5
20	Nonanal	1104	0.1
21	<i>p</i> -menth-2-en-1-ol	1120	0.1
22	$\alpha$ -Campholene aldehyde	1125	0.1
23	allo-ocimene	1128	0.2
24	E-Pinocarveol	1137	0.2
25	E-verbenaol	1143	0.1
26	pinocarvone	1160	0.1
27	borneol	1165	t
28	terpinen-4-ol	1177	0.3
29	$\alpha$ -Terpineol	1190	0.3
30	methyl salicylate	1192	t
31	myrtenal	1195	0.2
32	+ myrtenol		
33	$\beta$ -cyclocitral	1218	t
34	nerol	1226	t
35	cuminal	1237	0.1
36	geraniol	1254	0.1
37	bornyl acetate	1283	t
38	E-anethole	1285	0.6
39	<i>p</i> -cymen-7-ol	1290	t
40	$\delta$ -elemene	1337	0.1
41	$\alpha$ -cubebene	1348	0.1
42	eugenol	1357	0.1
43	cyclosativene	1365	0.2
44	$\alpha$ -copaene	1378	4.4
45	$\beta$ -bourbonene	1382	0.5
46	$\beta$ -elemene	1391	1.3
47	Z-jasmone	1394	t
48	$\alpha$ -gurjunene	1406	0.2
49	$\beta$ -caryophyllene	1415	t
50	E- $\alpha$ -bergamotene	1433	0.7
51	Z- $\beta$ -Farnesene	1441	0.8
52	$\alpha$ -humulene	1450	0.2
53	E- $\beta$ -Farnesene	1458	3.4
54	<b>germacrene-D</b>	<b>1480</b>	<b>13.2</b>
55	bicyclogermacrene	1498	4.0
56	$\beta$ -bisabolene	1508	0.8
57	$\gamma$ -cadinene	1513	0.5
58	$\delta$ -cadinene	1526	3.1
59	cadina-1,4-diene	1531	0.1
60	$\alpha$ -cadinene	1536	0.1
61	$\beta$ -calacorene	1560	0.1
62	Spathulenol	1577	1.8
63	globulol	1583	0.2
64	<i>T</i> -cadinol	1642	1.0
65	$\alpha$ -muurolol	1647	0.3
66	valeranone	1672	0.5
67	$\alpha$ -bisabolol	1685	0.9
68	heptadecane	1697	0.1
69	benzyl benzoate	1763	0.2
70	methyl hexadecanoate	1924	t
71	palmitic acid	1975	0.3
72	trans-phytol	2116	3.1
73	octadecanoic acid	2178	0.1
74	docosane	2197	0.1
75	tricosane	2298	0.2
76	tetracosane	2399	t
77	hexacosane	2595	0.1
78	heptacosane	2696	t
79	octacosane	2795	0.8
<b>monoterpenes</b>			<b>54.0%</b>
<b>sesquiterpenes</b>			<b>38.6%</b>

t=trace (<0.05%)

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