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Chemical composition of *Scutellaria litwinowii* Bornm. & Sint. ex Bornm. essential oil from Iran

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Abstract

Background: The plants of the genus *Scutellaria*, belonging to family Lamiaceae, have been used for their antiviral, antithrombotic, sedative, anti-inflammatory and antioxidant properties. In this study, the chemical composition of the essential oil of *Scutellaria litwinowii*

Materials and Methods: In this study, the essential oil of *Scutellaria litwinowii* (Lamiaceae) was obtained (yield 0.2% (v/w)) by hydrodistillation using a clevenger-type apparatus.

The essential oil was analyzed by GC-FID and GC-MS.

Results: A total of 65 compounds, representing 99.9% of the oil, were identified and the major components of essential oil were β-farnesene (13.4%), germacrene-D (11.6%), bicyclogermacrene (6.6%), α-cis bergamotene (6%) and α-copaene (5.2%). Generally, the major groups were sesquiterpene hydrocarbons (74.3%) and oxygenated sesquiterpenes (18.6%).

Conclusion: In the essential oil obtained from the aerial parts of *S. litwinowii*, monoterpene hydrocarbons and oxygenated monoterpenes were present at low amounts.

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Introduction

The genus *Scutellaria*, belonging to family Lamiaceae, includes more than 300 species of erect or spreading annual or perennial herbs (Hassanzadeh and Emami et al, 2011). This genus (commonly known as skullcaps) is widely distributed in Europe, the United States and East Asia (Shang et al, 2010). From this genus, the Iranian flora comprises 20 species and 2 hybrids, of which 10 species and 2 hybrids are endemic (Hassanzadeh and Emami et al, 2011). The plants of this genus are used as traditional herbal medicines throughout the world. *Scutellaria* species are used for their antiviral, antithrombotic, sedative, anti-inflammatory and antioxidant properties. Modern pharmacology demonstrated anticancer, anti-HIV, antibacterial, antiviral, anti-inflammatory and anticonvulsant properties of some *Scutellaria* species (Shang, et al, 2010). For example, *S. litwinowii* has cytotoxic and apoptogenic properties on human cancer cell lines (Tayarani-Najaran et al, 2009).

Several studies have reported the volatile constituents of *Scutellaria* species (Yaghmai 1988; Skaltsa et al, 2000; Ghannadi and Mehregan 2003; Yu et al, 2004; Mirzmahdi and Dini 2005; Rosselli et al, 2007; Firouznia et al, 2009; Takeoka et al, 2009; Cicek et al, 2011; Formisano et al, 2011; Pant et al, 2012; Valarezo et al, 2012). The composition of the essential oils of *S. lateriflora* (Yaghmai 1988), *S. pinnatifida* and *S. litwinowii* has been reported from Iran. Germacrene-D and (E)-β-farnesene (20.3%) were the major components of the essential oil of *S. pinnatifida* and *S. litwinowii*, respectively (Firouznia and Rustaiyan , 2009). In this study, the essential oil of *S. litwinowii* was analyzed by GC-FID and GC-MS.

Materials and Methods

Plant materials and isolation procedure

Aerial parts of *S. litwinowii* were collected during the flowering stage from Pivehzhan village, Khorasan Razavi Province, the Northeast of Iran, in April 2011. A voucher specimen (No.14175) was deposited at the Herbarium of Faculty of Pharmacy, Mashhad University of Medical Sciences, Mashhad, Iran. The essential oil of air-dried aerial parts was obtained following 3- hrhydrodistillation using a Clevenger-type apparatus. The yield was 0.2% v/w.

GC and GC-MS analysis

Gas chromatography (GC) was carried out using a Shimadzu GC-17 equipped with a FID detector, fused-silica BP-5 column (25

m × 0.22 mm, film thickness 0.25 µm). The operating conditions were as follows: oven temperature 50 ºC for 5 min and increased to 280 °C at 5°C/min, injector temperature 280 °C, detector temperature 300 °C, carrier gas N_2 and split ratio 1:10. GC-MS analysis was carried out using an Agilent 6890 apparatus with a HP-5MS column (30 m × 0.25 mm, film thickness 0.25 µm). The column temperature was kept at 50 ºC for 5 min and increased to 280 ºC at a rate of 5 ºC/min. The flow rate of He as carrier gas was 0.8 ml/min. Mass spectra were taken at 70 eV.

Identification and quantification of compounds

The constituents of the oil were identified by calculation of their retention index under temperature-programmed conditions for *n*-alkanes (C_6-C_{24}) and the essential oil on a BP-5 column under the same chromatographic conditions. Each compound was identified by comparison of its mass spectra and retention indices (RI) with those of authenticated samples and those given in the literature (Adams 2004). Quantification of the relative amount of each component was performed according to the area percentage method without consideration of calibration factor.

Results

Hydrodistillation of dried aerial parts of *S. litwinowii* yielded 0.2% (v/w) of a yellowish essential oil. The essential oil constituents of *S. litwinowii* identified by GC and GC-MS are shown in Table 1.

Sixty-five components, representing 99.9 % of the oil, were characterized and the major components of essential oil were β-farnesene (13.4%), germacrene-D (11.6%), bicyclogermacrene (6.6%), α-cis-bergamotene (6%) and α-copaene (5.2%). The oil was rich in sesquiterpene hydrocarbons (74.3%) and oxygenated sesquiterpenes (18.6%). Notably, the monoterpene portion represented only 1.4% of the oil.

Table 1. Chemical composition of the essential oil of *S. litwinowi.*

No	compound	*RI	%
1	α-pinene	957	0.1
2	Sabinene	993	0.6
3	Decane	1020	t
4	Linalool	1119	0.3
5	Nonanol	1183	0.1

6	Terpinene-4-ol	1191	0.1
7	α-terpineol	1205	0.2
8	Unknown	1221	0.1
9	Unknown	1246	t
10	Geraniol	1269	t
11	Decanol-۵	1286	0.1
12	Tridecane	1304	0.1
13	p-vinyl-guaiacol	1326	0.1
14	δ-elemene	1344	0.1
15	α-cubebene	1356	0.7
16	Eugenol	1369	1.7
17	Cyclosativene	1372	0.6
18	α-copaene	1383	5.2
19	β-bourbonene	1390	2.3
20	β-cubebene	1394	2.0
21	Tetrad cane	1402	0.4
22	α-funebrene	1409	1.2
23	α-gurjunene	1414	1.5
24	α-cedrene	1416	0.2
25	α-*cis* bergamotene	1423	6.0
26	Caryophyllene	1426	3.5
27	β-copaene	1433	0.6
28	α-*trans*-bergamotene	1439	2.2
29	Aromadendrene	1443	0.1
30	β-farnesene	1447	3.2
31	*Cis*-muurola-3,5-diene	1454	0.3
32	β-farnesene	1464	13.4
33	*Trans* cadina-1(6),4-diene	1479	0.7
34	Germacrene D	1487	11.6
35	*Trans*-muurola-4(14),5-diene	1496	0.6
36	Bicyclogermacrene	1503	6.6
37	β-bisabolene	1508	1.0
38	α-cuprenene	1515	4.4
39	γ-bisabolene	1518	2.8
40	α-cedrene	1526	3.7
41	α-*cis* bergamotene	1531	0.5
42	Caryophyllene	1533	0.4
43	β-copaene	1537	0.4
44	α-*trans*-bergamotene	1553	1.5

45	Aromadendrene	1561	0.7
46	β-farnesene	1567	0.5
47	Caryophyllene oxide	1578	1.7
48	Viridiflorol	1582	0.8
49	Fokienol	1590	1.2
50	Rosifoliol	1593	1.0
51	Epi-cedrol	1599	0.3
52	Junenol	1611	0.3
53	α-acorenol	1613	0.2
54	β-acorenol	1626	2.1
55	Epi-α-muurolol	1629	0.3
56	β-eudesmol	1636	1.9
57	α-cadinol	1646	0.5
58	Epi-β-bisabolol	1650	1.6
59	Epi-α-bisabolol	1663	2.7
60	α-bisabolol	1674	0.6
61	Germacra-4(15),5,10(14)-trien-1-α-ol	1676	0.3
62	Heptadecane	1679	0.3
63	Octadecane	1683	0.9
64	Nonadecane	1776	0.5
65	Caryophyllene oxide	1870	0.6
39	Viridiflorol	957	0.1
40	Fokienol	993	0.6
41	Rosifoliol	1020	t
42	Epi-cedrol	1119	0.3
43	Junenol	1183	0.1
44	α-acorenol	1191	0.1
45	β-acorenol	1205	0.2
46	Epi-α-muurolol	1221	0.1
47	β-eudesmol	1246	t
48	α-cadinol	1269	t
49	Epi-β-bisabolol	1286	0.1
50	Epi-α-bisabolol	1304	0.1
51	α-bisabolol	1326	0.1
52	Germacra-4(15),5,10(14)-trien-1-α-ol	1344	0.1
53	Heptadecane	1356	0.7
54	Octadecane	1369	1.7

55	Nonadecane	1372	0.6
56	Caryophyllene oxide	1383	5.2
57	Viridiflorol	1390	2.3
58	Fokienol	1394	2.0
59	Rosifoliol	1402	0.4
60	Epi-cedrol	1409	1.2
61	Junenol	1414	1.5
62	α-acorenol	1416	0.2
63	β-acorenol	1423	6.0
64	Epi-α-muurolol	1426	3.5
65	β-eudesmol	1433	0.6

* RI: The Kovats retention indices relative to *n*-alkanes (C_6-C_{24}) was determined on BP-5 capillary column.
t: Trace, less than 0.05%.

Discussion

The composition of the essential oils of some species of *Scutellaria* has been previously reported (Yaghmai 1988; Skaltsa et al, 2000; Ghannadi and Mehregan 2003; Yu et al, 2004; Mirzamahdi and Dini 2005; Rosselli et al, 2007; Firouznia et al, 2009; Takeoka, et al, 2009; Cicek et al, 2011; Formisano, Rigano et al, 2011; Pant et al, 2012; Valarezo et al, 2012).

Germacrene-D (39.7%) and β-caryophyllene (15.0%) were the major components of the essential oil of *S. pinnatifida* ssp. *alpina* and hydrocarbon sesquiterpenes were the principal group of the oil (Ghannadi and Mehregan, 2003). Unlike *S. pinnatifida* ssp. *alpina*, *S. orientalis* ssp. *alpina* and *S. barbata* had hexahydrofarnesyl acetone, as the major component of the essential oil (Yu et al, 2004; Formisano et al, 2011). The major components of the oil of *S. albida* ssp. *albida* were linalool (52.6%) and *trans*-nerolidol (9.0%) (Skaltsa et al, 2000). The essential oil of *S. lateriflora* and *S. grossa* was characterized with higher amounts of δ-cadinene (27.0%) and linalool (37.0%), respectively (Yaghmai 1988; Pant et al, 2012).

To our knowledge, one study was conducted on the composition of the essential oil of *S. litwinowii.* Similar to our data, Tabatabaei-Anaraki and colleagues reported β-farnesene (20.3%) and germacrene-D (16.9%) as the major components of the oil obtained from the aerial parts of *S. litwinowii* (Firouznia et al, 2009). In this study, the essential oil of *S. litwinowii* was analyzed and β-farnesene and germacrene-D represented lesser amount (26%) as compared to a previous study (37.2%).

Conclusion

In the essential oil obtained from the aerial parts of *S. litwinowii*, monoterpene hydrocarbons and oxygenated monoterpenes were present at low amounts.

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Conflict of interest

The authors have no competing interests to declare.

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