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ESSENTIAL OIL COMPOSITION OF *DRACOCEPHALUM MOLDAVICA* L. FROM IRAN

Katayoun Morteza-Semnani[1*], Mohammad Akbarzadeh[2] and Kamran Moshiri[1]

[1]*Department of Medicinal Chemistry, Faculty of Pharmacy, Mazandaran University of Medical Sciences Sari, Iran*
[2]*Research Center of Natural Resources of Mazandaran, Sari, Iran*

ABSTRACT

The essential oil of *Dracocephalum moldavica* L. (Labiatae) collected from the suburb of Sari, North of Iran, was isolated by hydrodistillation and analyzed by means of GC and GC/MS. Ninety components were identified in the this oil. The major constituents of the essential oil were limonene (19.8%), α-pinene (14.4%), methyl geranate (8.5%), geranyl acetate (7.9%), carvacrol (7.8%) and geranial (5.4%). The essential oil of *D. moldavica* is rich in monoterpenoids.

Keywords: *Dracocephalum moldavica*, Labiatae, Essential oil composition, Limonene, α-Pinene, Geranyl acetate

INTRODUCTION

The genus *Dracocephalum* compromises about 50 species (Zargari, 1993); there are approximately 8 native *Dracocephalum* spp., which are found wild in many regions of Iran (Rechinger, 1982; Mozaffarian, 1996). *Dracocephalum moldavica* L. belonging to the family Labiatae, is an aromatic plant, which grows wild in Azerbaijan, Gilan, Mazandaran and Yazd provinces of Iran (Zargari, 1993; Rechinger, 1982). The seeds are bitter; astringent, tonic, carminative; good for disease of the brain. The seeds are used in fevers as a demulcent. In Europe, the plant is considered tonic, astringent and vulnerary (Kirtiakar and Basu, 2001). In 2000, antioxidant activity of *D. moldavica* extract in rapeseed oil was evaluated (Povilaityte and Venskutonis, 2000). In 2001, chemical constituents from the whole plant of *D. moldavica* were studied, the compounds were isolated using RA polystyrene resin and silica gel column chromatography and the structures were elucidated by means of spectral method, four compounds were identified as tilianin, agastachoside, acacetin and oleanolic acid (Li and Ding, 2001). In 2004, eight compounds were identified as apigenin, luteolin, kaempferol, isorhamnetin, tilianin, agastachoside, acacetin-7-*O*-(6-*O*-malonyl-β-D-glucopyranoside) and syringaresinol (Gu *et al*., 2004). In 2003, triacylglycerols and diacylglycerols in 16 plant oil samples including *D. moldavica* were analyzed by HPLC-MS with atmospheric pressure chemical ionization and UV detection at 205 nm on two Nova-Pak C18 chromatographic columns connected in series (Holcapek *et al*., 2003).

A literature survey has shown that there are few reports on the volatile constituents of *D. moldavica* (Hawthorne *et al*., 1993; Shatar and Altantsetseg, 2000). Thus we decided to investigate the chemical constituents of the essential oil of *D. moldavica* growing in Iran.

MATERIALS AND METHODS

Plant material

The aerial parts of *D. moldavica* were collected in June 2004 from the suburb of Sari, Mazandaran province, North of Iran and identified by Department of Botany, Research Center of Natural Resources of Mazandaran. A voucher specimen (herbarium No. 473) was deposited in the herbarium of Research Center of Natural Resources of Mazandaran.

Isolation of essential oil

The air-dried aerial parts of *D. moldavica* were subjected to hydrodistillation using a Clevenger-type apparatus for 4 h to yield 0.56% of yellowish oil. After preparation the oil was subjected to GC and GC-MS analysis.

Gas chromatography analysis (GC)

Gas chromatographic analysis was carried out on a Perkin-Elmer 8500 gas chromatograph with FID detector and a DB-5 capillary column (30 m $\times$ 0.25 mm; film thickness 0.25 μm). The operating conditions were as follows:

carrier gas helium with a flow rate of 2 mL/min, split ratio was 1:30, the oven temperature was programmed 4 min. Isothermal at 60°C and then 60-220 °C at 4 °C/min., injector and detector temperatures were set at 240 °C.

Gas chromatography-Mass spectrometry analysis (GC-MS)

GC-MS was carried out on Hewlett Packard 6890 series, using a DB-5 capillary column (30 m × 0.25 mm, film thickness 0.25 μm) which was programmed as follows: 60°C for 5min and then up to 220 °C at 4 °C/min. The carrier gas was helium at a flow rate of 2 mL/min. The carrier gas was helium at a flow rate of 2 ml/min; split ratio, 1: 40; ionization energy, 70 eV; scan time, 1 s; acquisition mass range, *m/z* 40-400.

Identification of components

The components of the oil were identified by their retention time, retention indices relative to C_9-C_{28} n-alkanes, computer matching with the WILEY275.L library and as well as by comparison of their mass spectra with those of authentic samples or with data already available in the literature (Adams, 2001; Davies, 1990; Engel *et al*., 1998).

The percentage of composition of the identified compounds was computed from the GC peak area without any correction factor and was calculated relatively.

RESULTS AND DISCUSSION

As shown in Table 1, 90 components were identified in the oil of *D. moldavica*, which presented about 92.3% of the total composition of the oil. The major constituents of the essential oil were limonene (19.8%), *α*-pinene (14.4%), methyl geranate (8.5%), geranyl acetate (7.9%), carvacrol (7.8%) and geranial (5.4%). The oil of *D. moldavica* comprised 1 hemiterpenoids (0.1%), 55 monoterpenoids (88.1%), 19 sesquiterpenoids (2.8%) and 15 non-terpenoids (1.3%). The essential oil of *D. moldavica* is rich in monoterpenoids.

In 2005, *δ*-3-carene (9.7%), limonene (9.2%), carvacrol (8.3%), 1,8-cineole (6.9%) and carvone (5.1%) were reported as the major constituents of the essential oil of *D. kotschyi* collected from the suburb of Sari, Mazandaran province, North of Iran (Morteza-Semnani and Saeedi, 2005).

In 1993, supercritical fluid extraction (SFE) and hydrodistillation were compared as methods to extract essential oil from *D. moldavica*. In SFE method, geranyl acetate (56.1%), carvacrol (13.7%), thymol (10.2%), geranial (7.1%) and neryl acetate (6.9%) and in hydrodistillation method, geranyl acetate (65.8%), carvacrol (14.9%) and thymol (7.0%) were identified as the major components (Hawthorne *et al*., 1993).

In 2000, Shatar and Altantsetseg reported linalool (67.0%) and carvone (5.9%) as the main compounds of *D. moldavica* cultivated in Mongolia (Shatar and Altantsetseg, 2000).

As mentioned previously, variations in the oil composition of different researches may be because of the collection time, chemotypes, drying conditions, mode of distillation, geographic and climatic factors.

Table 1. The chemical composition of the essential oil of *Dracocephalum moldavica*

No.	Component	KI[a]	GC area %
1	n-Hexane	600	trace[b]
2	3-Methylbutanal	649	0.1
3	*α*-Thujene	933	trace
4	*α*-Pinene	941	14.4
5	Camphene	955	0.1
6	Verbenene	969	0.2
7	*β*-Pinene	980	1.2
8	6-Methyl-5-hepten-2-one	988	0.3
9	3-*p*-Menthene	989	trace
10	Dehydro-1,8-cineole	995	0.1
11	Myrcene	996	0.4
12	1,4,8-*p*- Menthatriene	1012	0.1
13	*α*-Terpinene	1019	1.1
14	*p*-Cymene	1027	1.3
15	Limonene	1031	19.8
16	(E)-*β*-Ocimene	1052	0.3
17	Bergamal	1058	trace
18	*γ*-Terpinene	1062	1.1

19	*cis*-Sabinene hydrate	1072	trace
20	*trans*-Linalool oxide	1074	0.1
21	*cis*-Linalool oxide	1089	0.1
22	*p*-Mentha-2,4(8)-diene	1090	0.2
23	6,7-Epoxymyrcene	1095	0.1
24	Linalool	1099	0.8
25	*trans*-Vertocitral C	1109	trace
26	6-Camphenol	1117	0.2
27	*trans*-*p*-Mentha-2,8-dien-1-ol	1124	0.2
28	1,5,8-*p*-Menthatriene	1126	trace
29	α-Campholenal	1128	1.2
30	*trans*-Pinocarveol	1140	0.3
31	*cis*-Verbenol	1142	0.3
32	*trans*-Verbenol	1146	0.7
33	Nerol oxide	1160	trace
34	Sabina ketone	1161	0.1
35	cis-Chrysanthenol	1166	0.1
36	Pinocarvone	1167	0.1
37	*p*-Mentha-1,5-dien-8-ol	1172	0.7
38	*cis*-Pinocamphone	1176	0.2
39	Terpinen-4-ol	1178	0.7
40	Thuj-3-en-10-al	1185	0.2
41	*trans*-*p*-Mentha-1(7),8-dien-2-ol	1190	0.1
42	α-Terpineol	1191	0.5
43	Myrtenal	1198	0.2
44	*trans*-Dihydrocarvone	1203	0.1
45	*trans*-Carveol	1219	1.2
46	*cis*-Carveol	1230	0.1
47	*cis*-*p*-Mentha-1(7),8-dien-2-ol	1233	0.1
48	Neral	1240	4.8
49	*trans*-Chrysanthenyl acetate	1241	trace
50	Geraniol	1255	2.7
51	Geranial	1269	5.4
52	Perilla aldehyde	1274	0.1
53	Limonen-10-ol	1292	0.3
54	Thymol	1293	1.2
55	Carvacrol	1302	7.8
56	Methyl geranate	1326	8.5
57	Limonene aldehyde	1331	0.2
58	2-Phenylethylpropanoate	1356	0.1
59	(*Z*)-α-Damascone	1360	0.3
60	Eugenol	1361	0.2
61	Neryl acetone	1364	0.3
62	(*Z*)-β-Damascenone	1366	0.1
63	α-Copaene	1379	0.2
64	Geranyl acetate	1383	7.9
65	β-Bourbonene	1390	0.1
66	β-Cedrene	1423	0.1
67	β-Duprezianene	1425	trace
68	Alloaromadendrene	1462	0.1
69	Germacrene D	1488	0.2
70	Bicyclogermacrene	1502	0.2
71	δ-Cadinene	1525	0.1
72	*E*-Nerolidol	1565	0.1
73	3Z-Hexenyl benzoate	1569	trace
74	Spathulenol	1580	1.2
75	Caryophyllene oxide	1585	0.1
76	Geranyl isovalerate	1609	trace
77	Geranyl valerate	1659	trace
78	n-Heptadecane	1700	trace
79	Sesquicineol-2-one	1704	0.1

80	14-Hydroxy-α-muurolene	1783	trace
81	β-Eudesmol acetate	1794	0.1
82	n-Octadecane	1802	trace
83	(*Z*)-epi-β-Santalol acetate	1809	trace
84	(2*Z*,6*E*)-Farnesyl acetate	1824	0.1
85	(2*E*,6*E*)-Farnesyl acetate	1849	0.1
86	n-Nonadecane	1902	trace
87	2-Octadecanone	1996	trace
88	1-Octadecanol	2079	0.5
89	n-Heneicosane	2102	trace
90	n-Tricosane	2303	trace
Total			**92.3**

[a] KI = Kovats index on DB-5 column; [b] trace = less than 0.05%.

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