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Essential Oil Composition of the *Dracocephalum moldavica* L from Xinjiang in China

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ABSTRACT

The essential oil of Dracocephalum moldavica L from Xinjiang in China was isolated by hydrodistillation in yield of 0.15 %(w/w). The chemical composition of the essential oil was analyzed by GC and GCMS. Fifty-one compounds accounting for 99.45% of the total oil were identified. The major components wereα-Citral (32.55%),β-Citral (23.53%), Acetic acid, geranial ester(21.32%), Trans-Geraniol(3.38%), Nerolacetate(3.38%), Octane(2.14%), and 2,4,6-Trimethyl -3-cyclohexene-1-carboxaldehyde (1.3%). Monotenepers were the main group of compounds.

Keywords: Dracocephalum moldavica L, essential oil composition, GC-MS.

INTRODUCTION

Dracocephalum moldavica L. is a perennial herb belonging to the Lamiaceae (Labiatae) family. is an annual herbaceous aromatic plant belonging to the family Lamiaceae (Labiatae). It is native to central Asia and is naturalized in eastern and central Europe(1). In China, it is predominantly found in the north of the country, especially in XinJiang Province. This plant, with the common local name of Xiangqinglan or Uygur's name Badelajibuya, has been of interest to Uygur traditional medicine, especially in north XinJiang Province. It is used as a food ingredient, as a tea, as a herbal drug for its reputed medicinal properties, e.g. for the treatment of stomach and liver disorders, headaches and congestion (2–4).

MATERIALS AND METHODS

Plant material

The aerial parts of Dracocephalum moldavica L growing Liyu mountain of Urumqi in Xinjiang were collected during flowering. Voucher specimens were deposited in Traditional Chinese Medicine College Museum of Chinese herbal samples of Xinjiang Medical University.

Preparation of extract

The sample was weighed (100g, 3times), then steam distilled with a Clevenger-type apparatus for 6 h; the oil was collected and dried over anhydrous sodium sulfate, then stored at 4°C until analyzed.

Gas Chromatography

GC-MS analyses were carried out using a Shimadzu QP-2010 GC-MS system operating in the EI mode at 70 eV with scanning from 41 to 450 amu at 0.5 s, using a DB-5 (30 m, 0.25 mm, film thickness 0.25μm) capillary column. The temperature program was 40–250°C at a rate of 5°C/min. Injector and transfer line temperatures were 250°C, the ion source temperature was 200°C. Helium was used as the carrier gas, flow rate 1 mL/min. Split ratio, 1:100.

Table 1. Composition of the Dracocephalum moldavica L essential oil

Compound	RRI	Area (%)	Identification Method
α-Citral	1268	32.55	MS,RRI
β-Citral	1239	23.53	MS,RRI
Acetic acid, geranial ester	1377	21.32	MS,RRI
trans-Geraniol	1250	3.38	MS,RRI
Nerol acetate	1358	3.38	MS,RRI
Octane	800.2	2.14	MS,RRI
2,4,6-Trimethyl-3-cyclohexene-1-carboxaldehyde	1180	1.3	MS,RRI
p-Xylene	868	0.84	MS,RRI
Verbenol	1161	0.74	MS,RRI
Caryophyllene oxide	1590	0.72	MS,RRI
Cyclohexane, 1,2-dimethyl-, trans-	802.7	0.7	MS,RRI
cis-Geraniol	1224	0.69	MS,RRI
2-(2-Methyl-1-cyclohexen-1-yl)propanal	1207	0.57	MS,RRI
Methyl geranate	1321	0.5	MS,RRI
Ethylcyclohexane	831.6	0.47	MS,RRI
Linalool oxide trans	1071	0.44	MS,RRI
β-Linalool	1100	0.44	MS,RRI
(-)-cis-Myrtanol	1177	0.39	MS,RRI
6,8-Nonadien-2-one, 6-methyl-5-(1-methylethylidene)-	1393	0.34	MS,RRI
Cyclohexane, 1,3-dimethyl-, trans-	808.1	0.32	MS,RRI
Piperitone	1256	0.3	MS,RRI
α-Cyclocitral	1150	0.28	MS,RRI
Nonane	900.2	0.24	MS,RRI
3-Decyn-2-ol	1195	0.24	MS,RRI
6-Methyl-5-heptene-2-one	983.6	0.23	MS,RRI
Cyclogeraniolane	837.5	0.22	MS,RRI
Benzene, ethyl-	858.5	0.22	MS,RRI
No match			
0.22			
No match			
0.2			
β-bourbonene	1389	0.2	MS,RRI
Hexahydrofarnesyl acetone	1848	0.19	MS,RRI
Heptane, 2,3-dimethyl-	852.7	0.17	MS,RRI
3,6-Dihydro-4-methyl-2-(2-methyl-1-propenyl)-2H-pyran	1152	0.16	MS,RRI
2(10)-Pinen-3-one	1165	0.16	MS,RRI
Cyclopentane, 1-ethyl-3-methyl-, trans-	795	0.15	MS,RRI
α-Xylene	892	0.15	MS,RRI
Germacrene D	1486	0.15	MS,RRI
1,2,3-Trimethyl-cyclopent-2-enecarboxaldehyde	1102.5	0.14	MS,RRI
2H-1-Benzopyran, 3,4,4a,5,6,8a-hexahydro-2,5,5,8a-tetramethyl-(2a,4a,8a.)-	1292	0.14	MS,RRI
Spathulenol	1583	0.14	MS,RRI
No match			
0.13			
4,11,11-Trimethyl-8-methy lenebicyclo[7,2,0]undec-4-ene	1425	0.13	MS,RRI
Rhodinol	1170	0.12	MS,RRI
Heptane, 2,6-dimethyl-	825.8	0.11	MS,RRI
1-Octen-3-ol	979	0.11	MS,RRI
Cubenol	1621	0.11	MS,RRI
cis-Linalool Oxide	1087	0.1	MS,RRI
Ethy lidenecyclooctane	1140	0.1	MS,RRI
Methacrylic anhydride	1143	0.1	MS,RRI
Undecylenic alcohol	1383	0.09	MS,RRI
Octane, 2-methyl-	862	0.07	MS,RRI
Melonal	1083	0.07	MS,RRI
Hexane, 2,3,3-trimethyl-	818.8	0.05	MS,RRI
(2Z)-2-Dodecene	1236	0.05	MS,RRI

RRI: retention indices relative to C6-C22 n-alkanes on the DB-5 column

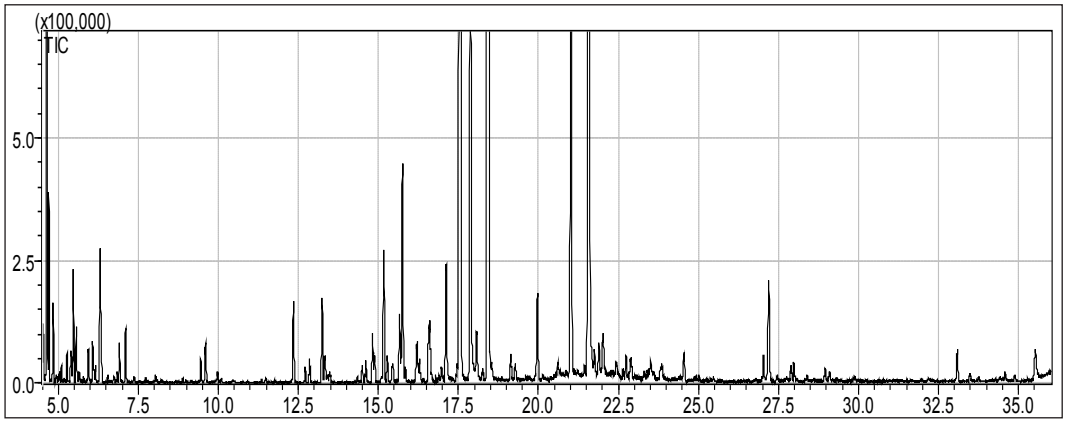

Fig 1. GC-MS chromatogram of Essential Oil Composition of the Dracocephalum moldavica L

Identification of the Components

The identification of the components was made by comparison of their retention time with respect to the n-alkane series (C6-C22) internal standards. The mass spectra and relative retention indices (RRI) were compared with those of commercial (NIST 05 and NIST 05 S). Area percentages were obtained from the TIC response without the use of an internal standard.

RESULTS AND DISCUSSION

The volatile light salmon pink oil (0.15% wt/wt) was obtained by hydrodistillation of whole grass and analyzed by GC-MS (Figures 1). A total of 51 out of 54 compounds representing 99.45% of the oil was identified (Table 1). The major components were α-Citral (32.55%), β-Citral (23.53%), Acetic acid, geranial ester (21.32%), Trans-Geraniol (3.38%), Nerol acetate (3.38%), Octane (2.14%), and 2,4,6-Trimethyl-3-cyclohexene-1-carboxaldehyde (1.3%). Monotenepers were the main group of compounds. Citral are known to be antibiotics (6). The antifungal and bactericidal properties of Citral have been reported (7-8). Citral also is a new inducer of caspase-3 in tumor cell lines (9). The high proportion of Citral in this plant could contribute to its medicinal properties.When the results of studies on literature values were compared with those of Table 1, the oils showed differences and similarities. The reason for this variability can be understood if we take into account all the factors influencing the chemical composition of the oils, namely, climatic, seasonal, and geographic condition, harvest period, and distillation technique,among others.

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