Chemistry of Natural Compounds, Vol. 41, No. 6, 2005

ESSENTIAL OIL COMPOSITION OF *Nepeta involucrata* FROM IRAN

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UDC 547.913

The essential oil of Nepeta involucrata *(Bunge) Bornm. (Lamiaceae) obtained by hydrodistillation from the aerial parts during the flowering stage was analyzed by GC and GC-MS. Forty-eight compounds representing 97.2% of total oil were identified. The main compounds of the oil were 1,8-cineol (23.1%), germacrene-D (15.1%), and* β*-pinene (12.2%). No traces of nepetalactone isomers were found as oil constituents.*

Key words: *Nepeta involucrata*, Lamiaceae, essential oil.

The genus *Nepeta* L. belongs to the family Lamiaceae, subfamily Nepetoideae and tribe Mentheae [1]. It is one of the largest genera of *Nepetoideae* and consists of about 300 species distributed in southwest Asia and Europe. In flora of Iran 63 species included in 12 sections have already been recognized [2], but on the basis of recently introduced new species and records, the number of species has now increased to 75 [3–9].

The literature review on the essential oil composition of Iranian *Nepeta* species revealed that the oil of some species is characterized by nepetalactone isomers as the first main compound, e.g., *N. racemosa* (74%) [10], (83.6%) [11], *N. cephalotes* (35.1%) [12], *N. persica* (30.5%) [13], *N. crassifolia* (93.2%) [14], *N. pogonosperma* (57.6%) [15], and *N. meyeri* (56.6%) [16], while in some other species such as *N. asterorticha* (17.5%) [17] and *N. binaludensis* (25.9%) [18] nepetalactones constitute the second major component of the oil. No traces of nepetalactone isomers were found as the oil constituent in *N. glomerulosa* subsp. *carmanica* [19], *N. ispahanica* [18], *N. denudate* [12], *N. heliotropifolia* [20], *N. glomerulosa* [21], *N. fissa* [22], and *N. macrosiphon* [23]. 1,8-Cineol was found to be the principal component of some other *Nepeta* species such as *N. ispahanica* (65.2%), *N. binaludensis* (42.3%) [18], *N. denudate* (48%) [12], *N. heliotropifolia* (19%) [20], and *N. crispa* (47.9%) [24]. In continuation of our studies on characterization of the essential oil composition of Iranian *Nepeta* species [24], we now report on the chemical composition of the essential oil of *N. involucrata*, which has not been investigated previously.

Hydrodistillation of the aerial parts of *N. involucrata* gave a yellow oil in a yield of 0.2% (w/w) based on the dry weight of the plant. Forty-eight components were identified in the oil, accounting for 97.2% of the total oil. The qualitative and quantitative essential oil composition can be seen in Table 1, where compounds are listed in order of their elution on a DB-1 column. The oil was characterized by a high percentage of oxygenated monoterpenes (38.3%), in which 1,8-cineol (23.1%) was the major compound similar to those of *N. ispahanica* (65.2%), *N. binaludensis* (42.3%), *N. denudate* (48%), *N. heliotropifolia* (19%), and *N. crispa* (47.9%). The monoterpene hydrocarbons constituted 27.8% of the oil, with β-pinene (12.2%) as the main component followed by sabinene (6.7%) and α-pinene (4.9%). Comparison of the oil composition of *N. involucrata* with those of other *Nepeta* species reported from Iran showed that no traces of nepetalactone isomers were found, similar to *N. glomerulosa* subsp. *carmanica*, *N. ispahanica*, *N. denudate*, *N. heliotropifolia*, *N. glomerulosa*, *N. fissa*, and *N. macrosiphon*. Sesquiterpene hydrocarbons comprised 23.2% of the oil, with germacrene-D (15.1%) as the principal constituent. Oxygenated sesquiterpenes constituted 7.9% of the oil, with spathulenol (2.3%) as the main component.

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0009-3130/05/4106-0683

TABLE 1. Chemical Composition of the Essential Oil of *Nepeta involucrata*

Compound	RI	%	Ident. method	Compound	RI	%	Ident. method
α-Thujene	922	0.1	RI, MS	Carvone	1219	1.4	RI, MS, CoI
α-Pinene	934	4.9	RI, MS, CoI	Perilla aldehyde	1250	0.3	RI, MS
Sabinene	968	6.7	RI, MS	α-Copaene	1380	0.6	RI, MS
β-Pinene	975	12.2	RI, MS, CoI	β-Bourbonene	1389	1.7	RI, MS
Myrcene	982	1.4	RI, MS	β-Cedrene	1421	1.1	RI, MS
α-Terpinene	1011	0.6	RI, MS	β-Caryophyllene	1424	0.1	RI, MS
1,8-Cineol	1026	23.1	RI, MS, CoI	β-Cubebene	1432	0.4	RI, MS
(Z)-Ocimene	1035	0.2	RI, MS	β-Gurjunene	1434	0.4	RI, MS
γ-Terpinene	1050	1.1	RI, MS, CoI	γ-Gurjunene	1446	0.1	RI, MS
trans-Sabinene hydrate	1056	0.2	RI, MS	β-Ionone	1466	0.1	RI, MS
Terpinolene	1081	0.6	RI, MS	γ-Muurulene	1475	0.1	RI, MS
Linalool	1083	0.1	RI, MS, CoI	Germacrene-D	1484	15.1	RI, MS
cis-Verbenol	1106	0.1	RI, MS	Bicyclogermacrene	1496	1.4	RI, MS
α-Campholenal	1109	0.6	RI, MS	δ-Cadinene	1517	2.1	RI, MS
trans-*p*-Menth-2-en-1-ol	1111	0.1	RI, MS	2,3,3-Trimethyl-2-(3-methyl-1,3-	1542	1.5	MS
trans-Pinane	1115	0.2	RI, MS	butadienyl)-cyclohexanone			
cis-Limonene oxide	1119	0.1	RI, MS	Spathulenol	1571	2.3	RI, MS
trans-Limonene oxide	1124	0.1	RI, MS	Caryophyllene oxide	1579	2.2	RI, MS
trans-Pinocarveol	1129	1.8	RI, MS	δ-Cadinol	1630	0.1	RI, MS
trans-Verbenone	1132	0.8	RI, MS	α-Cadinol	1632	0.2	RI, MS
Pinocarvone	1144	1.2	RI, MS	α-Cedrol	1638	0.3	RI, MS
p-Menth-1-en-8-ol	1151	1.3	MS	τ-Muurolol	1643	1.3	RI, MS
4-Terpineol	1165	1.9	RI, MS	Monoterpene hydrocarbons	27.8		
α-Terpineol	1176	3.3	RI, MS	Oxygenated monoterpenes	38.3		
Myrtenol	1182	0.6	RI, MS	Sesquiterpene hydrocarbons	23.2		
trans-Piperitol	1192	0.1	RI, MS	Oxygenated sesquiterpenes	7.9		
trans-Carveol	1199	0.9	RI, MS	Total	97.2		

RI: retention indices relative to C_6-C_{24} *n*-alkanes on the DB-1 column.
MS: mass spectrum.
CoI: coinjection with an authentic sample.

EXPERIMENTAL

Plant Material and Isolation Procedure. The aerial parts of *N. involucrata* were collected from Takab (West Azerbaijan province) in June 2003 at the full flowering stage. A voucher specimen (MP-324) has been deposited in the Medicinal Plants and Drugs Research Institute Herbarium, Shahid Beheshti University, Tehran, Iran. Air-dried aerial parts (100 g) were subjected to hydrodistillation for 3 h using a Clevenger-type apparatus. The distillate was dried over anhydrous sodium sulfate and was stored at 4°C until analysis.

Oil Analysis Procedure. GC analysis of the oil was conducted using a Varian CP-3800 instrument equipped with a fused silica DB-1 column (25 m × 0.25 mm i.d., film thickness 0.25 μm). Nitrogen was used as the carrier gas at a constant flow of 1.1 mL/min. The oven temperature was held at 60°C for 1 min, then programmed to 250°C at a rate of 4°C /min, and then held for 10 min. The injector and detector (FID) temperatures were kept at 250°C and 280°C, respectively. GC-MS analysis was carried out on a Thermoquest-Finnigan Trace GC-MS equipped with a fused silica DB-1 column (60 m × 0.25 mm i.d., film thickness 0.25 μm). The oven temperature was raised from 60°C to 250°C at a rate of 5°C/min, then held at 250°C for 10 min; the transfer line temperature was 250°C. Helium was used as the carrier gas at a flow rate of 1.1 mL/min; the split ratio

was 1/50. The quadrupole mass spectrometer was scanned over the 45–465 amu range with an ionizing voltage of 70 eV and an ionization current of 150 μA. The constituents of the volatile oil were identified by calculation of their retention indices under temperature-programmed conditions for *n*-alkanes (C_6–C_{24}) and the oil on a DB-1 column under the same chromatographic conditions. Identification of individual compounds was made by comparison of their mass spectra with those of the internal reference mass spectra library or with authentic compounds and confirmed by comparison of their retention indices with authentic compounds or with those reported in the literature [25–27]. Quantitative data were obtained from FID area percentages without the use of correction factors.

ACKNOWLEDGMENT

We are grateful to Shahid Beheshti University Research Council for financial support of this work.

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