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THE ESSENTIAL OIL COMPOSITION OF *Ballota nigra*

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The genus *Ballota* (Labiatae) comprises 3 species, which are distributed in Iran [1]. *Ballota nigra* L. has been found in Azerbaijan, Golestan, Kurdestan, and Mazandaran provinces of Iran [2, 3]. *B. nigra* has antiaging, antiemetic, antitussive, antioxidant, and antispasmodic activity [4]. In Iranian herbal medicine, it has already been used as tonic and anticonvulsant, diuretic, anthelminthic, and for treatment of nervous disorders [3]. A literature survey has shown that there is one report on the volatile constituents of *B. nigra* ssp. *foetida* [5]. Diterpenes and tannins have been found in *B. nigra* [6]. The medicinal properties attributed to the essential oil of the genus *Ballota*, prompted us to investigate the chemical constituents of the oil of *B. nigra*.

The hydrodistillation of the dried flowering aerial parts of *B. nigra* gave a light yellowish oil with a yield of 0.5% (v/w). As shown in Table 1, 42 components were identified in this oil, which presented about 95.4% of the total composition of the oil. The major constituents of the essential oil were caryophyllene oxide (7.9%), *epi*-α-muurolol (6.6%), δ-cadinene (6.5%), and α-cadinol (6.3%). The oil of *B. nigra* comprised 35 sesquiterpenoids (89.9%), one diterpenoid (0.1%), and 6 nonterpenoids (5.4%). The essential oil of the flowering aerial parts of *B. nigra* is rich in sesquiterpenoids.

In 2003, Bader *et al*. reported germacrene D as the main compound of *B. nigra* ssp. *foetida* collected from Amman Jordan; monoterpenes were little represented, while sesquiterpenes were present in large amounts [5]. In 2002, Couladis *et al*. reported caryophyllene oxide, phytol, and γ-muurolene as the major componenets of *B. pseudodictamnus* [7]. The difference in the oil composition of the present study and previous research may be due to the collection time, chemotypes, drying conditions, mode of distillation, and geographic and climatic factors.

Plant Material. The flowering aerial parts of *B. nigra* were collected in June 2005 from the suburb of Nour, Mazandaran province, North of Iran and identified by the Department of Botany, Research Center of Natural Resources of Mazandaran. A voucher specimen (herbarium No. 108) was deposited at the Herbarium of the Department of Botany, Research Center of Natural Resources of Mazandaran.

Identification of Components. The dried flowering aerial parts were subjected to hydrodistillation using a Clevenger-type apparatus for 4 h. The oil after preparation was submitted to GC and GC-MS analysis. 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, oven temperature programmed 4 min, isothermal at 60°C and then 60–220°C at 4°C/min., injector and detector temperatures set at 240°C.

Gas Chromatography-mass spectrometry was carried out on Hewlett Packard 6890 series, using a DB-5 capillary column (30 m $\times$ 0.25 mm, film thickness 0.25 μm) programmed as follows: 60°C for 5 min and then up to 220°C at 4°C/min. The carrier gas was helium at a flow rate of 2 mL/min. 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. Library, as well as by comparison of their mass spectra with those of authentic samples or with data already available in the literature [8, 9]. The percentage composition of the identified compounds was computed from the GC peak area without any correction factor and was calculated relative to it.

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TABLE 1. The Chemical Constituents of the Essential Oil of *Ballota nigra*

Components	KI[a]	GC area, %	Components	KI[a]	GC area, %
n-Hexane	602	0.3	δ-Cadinene	1524	6.5
2-Methylhexane	662	0.2	*trans*-Calamenene	1531	2.6
3-Methylhexane	670	0.1	Germacrene D-4-ol	1577	3.2
n-Heptane	702	0.1	Caryophyllene oxide	1585	7.9
α-Cubebene	1353	2.2	Humulene epoxide II	1609	1.2
α-Ylangene	1377	2.4	1,10-di-*epi*-Cubenol	1620	1.3
β-Bourbonene	1390	4.1	1-*epi*-Cubenol	1630	1.1
β-Elemene	1393	2.8	Alloaromadendrene epoxide	1643	1.6
(*E*)-Caryophyllene	1419	4.0	*epi*-α-Muurolol	1644	6.6
β-Cedrene	1423	2.2	α-Cadinol	1656	6.3
α-*trans*-Bergamotene	1436	2.2	7-*epi*-α-Eudesmol	1666	1.1
γ-Elemene	1439	2.7	α-Bisabolol	1688	3.2
α-Guaiene	1441	1.1	Eudesma-4(15),7-dien-1-β-ol	1689	0.1
Aromadendrene	1443	3.4	*cis*-14-nor-Muurol-5-en-4-one	1690	0.6
trans-Muurola-3,5-diene	1455	0.1	(2*Z*,6*E*)-Farnesyl acetate	1824	0.5
Alloaromadendrene	1461	1.2	6,10,14-Trimethyl-2-pentadecanone	1845	4.0
9-*epi*-(*E*)-Caryophyllene	1467	1.4	(2*E*,6*E*)-Farnesyl acetate	1849	0.8
γ-Gurjunene	1478	1.1	Carissone	1930	0.1
γ-Muurolene	1482	3.2	Sclarene	1977	0.1
Germacrene D	1486	3.8	*n*-Octadecanol	2079	0.7
α-Amorphene	1487	3.0	Total		95.4
γ-Amorphene	1498	4.3			

[a]KI = Kovat's index on DB.

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