CHEMICAL CONSTITUENTS OF THE ESSENTIAL OIL OF *Nepeta oxyodonta*

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Water-distilled essential oil from the aerial parts of Nepeta oxyodonta *Boiss. was analyzed by GC/MS for the first time. Fifty-eight components were identified. The major components were (E)-caryophyllene (12.6%), spathulenol (8.5%),* β*-bourbonene (8.1%), germacrene-D (7.4%),* α*-cadinol (7.3%), germacrene-D-4-ol (6.8%), T-cadinol (5.6%), and caryophyllene oxide (5.3%).*

Key words: *Nepeta oxyodonta*, essential oil, GC/MS analysis, (E)-caryophyllene.

The genus *Nepeta*, which belongs to the Lamiaceae family, consists of about 250 species [1]. The genus is represented in the flora of Iran by 67 species, including 39 endemics [2, 3]. In Iran, members of this genus are called "Punesa" and some of them have been traditionally used in folk medicine as herbal drugs [4].

In the genus *Nepeta* attention has been mainly directed towards the composition of oils of the Iranian and Turkish species. The essential oils of some *Nepeta* spp. are characterized by the presence of high concentrations of stereoisomers of nepetalactones [5–12]. However, there are *Nepeta* spp. poor in nepetalactones [13, 14], and some may even contain no nepetalactones [15–24].

Nepeta oxyodonta Boiss. is a herbaceous wild plant endemic to Iran [2], and no phytochemical studies on this plant have yet been carried out. In continuation of our investigations on the chemical composition of the essential oils of various *Nepeta* species growing in Iran [15, 16], the chemical composition of the essential oil from *N. oxyodonta* is reported for the first time.

The aerial parts of *N. oxyodonta* yielded 0.1% (v/w) of a clear yellowish oil with an aromatic odor. The identified components and their percentages are given in Table 1, where the components are listed in order of their elution on the HP-5 column. Fifty-eight components were identified. (E)-Caryophyllene (12.6%), spathulenol (8.5%), β-bourbonene (8.1%), germacrene-D (7.4%), α-cadinol (7.3%), germacrene-D-4-ol (6.8%), T-cadinol (5.6%), and caryophyllene oxide (5.3%) were found to be the major constituents of the oil.

Many of the identified components in the *N. oxyodonta* oil are common in the oils of other *Nepeta* species that have been studied previously. Generally, the genus *Nepeta*, according to the presence or absence of nepetalactones in their oils, could be classified into two groups. Nepetalactones are absent in the oils of some *Nepeta* species [15–24]. As can be seen in Table 1, nepetalactones were not also detected in the oil of *N. oxyodonta*.

EXPERIMENTAL

The aerial parts of *N. oxyodonta* were collected from Charmahal and Bakhtiari Province (southwest of Iran) in June at an altitude of 2700 m. The plant was identified at the Botany Department of the Faculty of Sciences, Isfahan University, Isfahan, Iran and a voucher specimen has been deposited in the Herbarium of the Faculty of Pharmacy and Pharmaceutical Sciences, Isfahan University of Medical Sciences, Isfahan, Iran.

The air-dried aerial parts of *N. oxyodonta* were reduced to a coarse powder and the oil was isolated by hydrodistillation using a Clevenger-type apparatus for 3 h. The oil was subsequently dried over anhydrous sodium sulfate.

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TABLE 1. Composition of the Essential Oil of *Nepeta oxyodonta*

RI	Compound	%	RI	Compound	%
852	*trans*-2-Hexenal	0.4	1403	(Z)-Caryophyllene	0.1
928	α-Thujene	0.2	1406	α-Gurjunene	0.2
937	α-Pinene	3.2	1416	(E)-Caryophyllene	12.6
975	Sabinene	1.6	1428	β-Gurjunene	1.1
979	β-Pinene	1.4	1433	*cis*-α-Bergamotene	0.2
991	Myrcene	0.2	1442	*cis*-β-Farnesene	0.6
995	2-Octanol	0.1	1451	α-Humulene	0.9
1017	α-Terpinene	0.1	1459	*allo*-Aromadendrene	1.9
1025	*p*-Cymene	0.1	1479	Germacrene-D	7.4
1030	Limonene	0.1	1485	β-Ionone	0.3
1032	1,8-Cineole	3.3	1488	*cis*-β-Guaiene	0.2
1049	*trans*-β-Ocimene	0.1	1493	Bicyclogermacrene	1.7
1060	γ-Terpinene	0.2	1496	α-Muurolene	0.5
1068	*cis*-Sabinene hydrate	0.1	1506	(E,E)-α-Farnesene	0.1
1087	Terpinolene	0.1	1510	γ-Cadinene	0.4
1099	Linalool	0.3	1522	δ-Cadinene	2.8
1103	Nonanal	0.2	1523	β-Sesquiphellandrene	0.6
1122	*p*-Menth-2-en-1-ol	0.1	1529	Cadina-1,4-diene	0.1
1126	α-Campholene aldehyde	0.1	1535	α-Cadinene	0.2
1140	*cis*-Verbenol	0.2	1565	Ledol	0.4
1146	*trans*-Verbenol	0.2	1576	Germacrene D-4-ol	6.8
1178	Terpinen-4-ol	0.5	1578	Spathulenol	8.5
1191	α-Terpineol	0.3	1582	Caryophyllene oxide	5.3
1195	Myrtenol	0.3	1591	Viridiflorol	1.6
1204	Decanal	0.1	1598	Cedrol	0.9
1335	Bicycloelemene	0.2	1606	Humulene epoxide II	1.3
1374	α-Copaene	1.6	1641	T-Cadinol	5.6
1382	β-Bourbonene	8.1	1648	β-Eudesmol	1.8
1390	β-Elemene	1.3	1654	α-Cadinol	7.3

RI: Retention indices on HP-5 capillary column.
%: Calculated from TIC data.

GC/MS analysis was carried out on a Hewlett-Packard 6890 gas chromatograph fitted with a fused silica HP-5MS capillary column (30 m × 0.25 mm; coating thickness 0.25 mm). The oven temperature was programmed from 60–280°C at 4°C/min. Helium was used as a carrier gas at a flow rate of 2 mL/min. The gas chromatograph was coupled to a Hewlett-Packard 6890 mass selective detector. The MS operating parameters were: ionization voltage, 70 eV; ion source temperature, 200°C. Identification of components of the volatile oil was based on retention indices relative to *n*-alkanes and computer matching with the WILEY275.L library, as well as by comparison of the fragmentation patterns of the mass spectra with those reported in the literature [25, 26].

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