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CONSTITUENTS OF THE ESSENTIAL OIL OF *Berula angustifolia* FROM IRAN

K. Javidnia,[1,2*] R. Miri,[1,2] and M. Assadollahi[1]

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Berula angustifolia (L.) Mertens & W. D. Koch (Apiaceae, Subfamily Apioideae, Tribe Apieae) is a perennial, probably a monotypic species distributed in damp places in Europe, Asia, East and South Africa, North America, and many parts of Iran. The synonyms of this plant are *Berula erecta*, *Sium erectum*, and *Sium angustifolium* [1, 2]. Here we report on the composition of the essential oil of *Berula angustifolia* which, to the best of our knowledge, has not been reported previously.

In Table 1, data on the constituents of this species are given. Analysis of the essential oil of *Berula angustifolia* led to identification of 44 compounds, which represent 94.0% of the total oil. The main components of the oil were piperitenone oxide (14.6%), limonene (13.9%), α-zingiberene (12.8%), and (*E*)-β-farnesene (9.6%). It has been shown in different studies that piperitenone oxide is a relaxant of intestinal smooth muscle, and it is also found to be highly toxic and repellent against malarial vector [3, 4].

TABLE 1. The Chemical Composition of the Essential Oil of *Berula angustifolia*

Compound	RI	%	Compound	RI	%
α-Pinene	934	0.1	(*E*)-β-Farnesene	1458	9.6
β-Pinene	976	0.8	Germacrene-D	1483	3.1
Myrcene	991	0.2	*ar*-Curcumene	1485	1.4
Octanal	1000	1.1	(*E*)-β-Ionone	1489	0.5
Limonene	1029	13.9	α-Zingiberene	1495	12.8
(*Z*)-β-Ocimene	1040	1.2	(*E,E*)-α-Farnesene	1595	3.0
(*E*)-β-Ocimene	1050	0.3	β-Sesquiphellandrene	1521	2.7
γ-Terpinene	1059	0.2	Germacrene B	1557	2.8
Nonanal	1100	0.3	Spathulenol	1579	1.2
trans-p-Mentha-2,8-dien-1-ol	1124	0.7	*epi*-α-Cadinol	1642	0.9
cis-p-Mentha-2,8-dien-1-ol	1139	0.8	Selina-3,11-dien-6-α-ol	1645	1.4
Camphor	1147	0.3	α-Bisabolol	1690	3.0
Pinocarvone	1164	Tr.	Mint sulfide	1735	0.4
Decanal	1267	0.7	Neophytadiene*	1838	2.0
Isopiperitenone	1276	0.3	6,10,14-Trimethyl-2-pentadecanone	1844	0.2
Isobornyl acetate	1286	0.2	Neophytadiene*	1875	Tr.
Carvacrol	1303	0.3	Methyl hexadecanoate	1924	Tr.
trans-Carvyl acetate	1341	Tr.	Hexadecanoic acid	1976	0.7
Piperitenone oxide	1367	14.6	(*Z*)-Falcarinol	2034	3.1
β-Elemene	1393	1.6	Methyl linolenate	2090	0.3
β-Caryophyllene	1418	1.7	Phytol	2114	3.1
γ-Elemene	1434	2.2	Total		94.0
α-Humulene	1452	0.3			

*Correct isomer not identified. Tr.: trace (< 0.05%). RI: retention indices elative to C_8–C_{28} *n*-alkanes on HP5. The components are listed in order of elution from the HP-5 column.

1) Medicinal & Natural Product Chemistry Research Centre, Shiraz University of Medical Sciences, Shiraz, Iran, fax: +98 711 2332225, e-mail: javidniak@sums.ac.ir; 2) Department of Medicinal Chemistry, Faculty of Pharmacy, Shiraz University of Medical Sciences, Shiraz, Iran. Published in Khimiya Prirodnykh Soedinenii, No. 6, pp. 840–841, November–December, 2010. Original article submitted July 13, 2009.

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Plant Material and Isolation Procedure. The plant material was collected in June 2008 from Margon waterfalls in Fars province. The plant was identified by the Department of Biology, University of Shiraz (Iran). A specimen (Herbarium No. PC 87-1) has been deposited in the Herbarium of the Faculty of Sciences, Shiraz University. The aerial parts were air-dried at ambient temperature in the shade and hydrodistilled using a Clevenger-type apparatus for 4 h. The yield of oil was 0.04% (w/w) and the color of the oil was yellow. It was dissolved in *n*-hexane (Merck), dried over anhydrous sodium sulfate, and stored at 4–6°C.

Identification of the Oil Components. GC analysis was carried out using a Varian GC 3600 chromatograph with a DB-5 column (30 m × 0.25 mm; 0.25 μm film thickness). The oven temperature was increased from 60–240°C at 3°C/min, and the injector and detector temperatures were 240°C and 250°C, respectively. Quantitative data were obtained from electronic integration of peak areas without the use of correction factors.

GC/MS analysis was carried out using a Hewlett-Packard 6890 machine operating at 70 eV ionization energy, equipped with an HP-5 capillary column (phenyl methyl siloxane, 30 m × 0.25 mm; 0.25 μm film thickness) with He as the carrier gas and with a split ratio of 1:20. Retention indices were determined by using the retention times of *n*-alkanes injected after the oil under the same chromatographic conditions. The retention indices for all the components were determined according to the Van Den Dool method using *n*-alkanes as standard [5]. The compounds were identified by comparison of their retention indices (RRI, HP-5) with those reported in the literature and by comparison of their mass spectra with the Wiley and Mass finder 3 libraries or with the published mass spectra [6, 7].

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