ORIGINAL ARTICLE

A C G publications

Rec. Nat. Prod. 12:5 (2018) 426-431

records of natural products

Composition of the Essential Oil of *Salvia montbretii* Benth. from Turkey

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(Received December 27, 2017; Revised January 28, 2018; Accepted January 30, 2018)

Abstract: The composition of the essential oil produced from aerial parts of *Salvia montbretii* Benth.(Lamiaceae), was analyzed by GC and GC-MS. Forty-six compounds constituting about 97.7% of the essential oil were characterized.The main compounds were characterized as β-caryophyllene (32.8%), *β*-pinene (9.8%), α-humulene (8.2%), 12-hydroxy-β-caryophyllene acetate (6.6%), germacrene D (4.9%) and α-pinene (4.5%).

Keywords: *Salvia montbretii* Benth; oil composition; β-caryophyllene; α-humulene; *β*-pinene.

1. Introduction

Salvia L. is one of the largest genera in the family Lamiaceae with 900 species in the World. *Salvia* genus is represented by 100 species, 53% of whic are endemic in Turkey [1-3]. *Salvia montbretii* is named " kara salba" in South-East Anatolia, Turkey.

Numerous *Salvia* species are used both internally and externally as folk medicines all around the World. There are several reports on the medicinal uses of some species of the genus, mainly against cold, skin infections, wounds, pharyngitis, stomatitis, stomachache, headache, memory enhancement and galactorrhoea [4].

The chemical compositions of several *Salvia* species have been extensively investigated revealing the presence of terpenes, triterpenoids, diterpenoids, tannins, phenolics and essential oil [3- 18].

Previous phytochemical studies on *Salvia montbretii* Benth. have reported the presence of abiatane diterpenes and triterpenoids. Salvibretol, 1-oxosalvibretol, 6-hydroxysalvinolone, 7-hydroxytaxodione, 7,7´-bistaxodione, and 11,´-didehydroxy-7,7´-dihydroxytaxodione, montbretol, montbretyl 12-methyl ester, 14-hydroxy ferruginol, 3-β-O-cis-p-coumaroylmonogynol and 3-β-O-trans-p-coumaroylmonogynol were isolated from root of *S. montbretii* [15-17].

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The article was published by ACG Publications
www.acgpubs.org/RNP © September-October/ 2018EISSN:1307-6167
DOI: http://doi.org/10.25135/rnp.51.17.12.080

In previous study, water-distilled essential oil of *S. montbretii* was analyzed using GC and GC–MS and thymol (24.0%) and caryophyllene oxide (26.9%) were found to be the main components in the oil [19].

2. Materials and Methods

2.1. The Plant Material

Salvia montbretii was collected from Şanlıurfa: between Çatak –Bozova in Turkey on 20 May 2017. The voucher specimenhas been deposited at the Herbarium in the Recep Tayyip Erdoğan Unıversity (RTEUB 6079), Rize, Turkey (Voucher specimen no: FABAK 1478). The plant material was identified by Prof. Dr. Vagif ATAMOV (Recep Tayyip Erdoğan University, Faculty of Science and Literature, Department of Biology , Rize , Turkey).

2.2. Isolation of the Essential Oil

Aerial parts of the plant were water distilled for 3 h using a Clevenger-type apparatus.The essential oil was stored at 4°C in the dark until analyzed. Oil yield in the sample was less than 0.1%.

2.3. Gas Chromatography (GC) and Gas Chromatography -Mass Spectrometry (GC-MS) Analysis

The oil was analyzed by Gas Chromatography (GC) and Gas Chromatography-Mass Spectrometry (GC-MS) using a Agilent GC-MSD system (Mass Selective Dedector-MSD).

2.3.1. GC-MS Analysis

The GC-MS analysis was carried out with an Agilent 5975 GC-MSD system (Agilent, USA; SEM Ltd., Istanbul, Turkey). Innowax FSC column (60m × 0.25mm, 0.25μm film thickness) was used with helium as carrier gas (0.8 mL/min). GC oven temperature was kept at 60°C for 10 min and programmed to 220°C at a rate of 4°C/min, and kept constant at 220°C for 10 min and then programmed to 240°C at a rate of 1°C/min. Split ratio was adjusted 40:1. The injector temperature was at 250°C. The interphase temperature was at 280°C. MS were taken at 70 eV. Mass range was from m/z 35 to 450.

2.3.2. GC Analysis

GC analyses were performed using an Agilent 6890N GC system. FID temperature was set to 300°C and the same operational conditions were applied to a triplicate of the same column used in GC–MS analyses. Simultaneous auto injection was done to obtain equivalent retention times. Relative percentages of the separated compounds were calculated from integration of the peak areas in the GC-FID chromatograms.

2.4. Identification of Compounds

The components of essential oils were identified by comparison of their mass spectra with those in the Baser Library of Essential Oil Constituents, Adams Library, MassFinder Library, Wiley GC/MS Library [20-22] and confirmed by comparison of their retention indices. These identifications were accomplished by comparison of retention times with authentic samples or by comparison of their relative retention index (RRI) to a series of n-alkanes. Alkanes were used as reference points in the calculation of relative retention indices (RRI) [23]. Relative percentage amounts of the separated compounds were calculated from FID chromatograms. The analysis results are expressed as mean percentage ± standard deviation (SD) (n = 3) as listed in Table 1.

3. Results and Discussion

Essential oil of of *Salvia montbretii* was hydrodistilled from aerial parts for 3 h using a Clevenger apparatus and analysed by gas chromatography (GC), and gas chromatography-mass spectrometry (GC-MS).

Table 1. Composition of the essential oil of *Salvia montbretii* Benth.

RRI[a]	RRI[b]	Compounds	%	ID
1025[c]	1032	α-Pinene	4.5± 0.1	t_R, Ms
1117[c]	1118	β-Pinene	9.8± 0.3	t_R, Ms
1122[c]	1132	Sabinene	1.6± 0.2	t_R, Ms
1160[c]	1174	Myrcene	1.4± 0.0	t_R, Ms
1212[c]	1203	Limonene	2.7± 0.1	t_R, Ms
1213[c]	1213	1,8-Cineole	1.4± 0.1	t_R, Ms
1232[c]	1246	(Z)-β-Ocimene	0.2± 0.0	t_R, Ms
1245[c]	1255	γ-Terpinene	2.9± 0.1	t_R, Ms
1249[d]	1266	(E)-β-Ocimene	0.5± 0.1	t_R, Ms
1282[c]	1280	*p*-Cymene	0.5± 0.1	t_R, Ms
1282[c]	1290	Terpinolene	0.2± 0.0	t_R, Ms
1391[d]	1400	Nonanal	0.2± 0.0	Ms
1399[d]	1406	α-Fenchone	0.2± 0.0	Ms
1414[d]	1424	Hexyl butyrate	0.1± 0.0	Ms
1443[f]	1444	Dimethyl tetradecane	0.3± 0.0	Ms
1468[d]	1479	δ-Elemene	0.3± 0.0	Ms
1487[d]	1484	Bicycloelemene	0.4± 0.1	Ms
1488[c]	1497	α-Copaene	0.7± 0.1	Ms
1496[d]	1506	Decanal	0.3± 0.1	Ms
1523[c]	1535	β-Bourbonene	0.8± 0.0	t_R, Ms
1543[c]	1553	Linalool	0.3± 0.0	t_R, Ms
1554[d]	1565	Linalyl acetate	1.2± 0.1	t_R, Ms
1576[c]	1577	β-Ylangene	0.5± 0.0	Ms
1591[d]	1600	β-Elemene	0.5± 0.0	Ms
1600[g]	1600	Hexadecane		t_R, Ms
1598[d]	1612	β-Caryophyllene	32.8± 0.1	t_R, Ms
1602[d]	1617	Lavandulyl acetate	0.2± 0.1	Ms
1639[d]	1651	γ-Elemene	1.9± 0.1	Ms
1651[d]	1668	(Z)-β-Farnesene	2.4± 0.0	Ms
1663[c]	1687	α-Humulene	8.2± 0.0	t_R, Ms

Table 1 Continued…

1700[f]	1700	Heptadecane	0.8± 0.0	t_R, Ms
1708[c]	1726	Germacrene D	4.9± 0.0	Ms
1718[d]	1733	Neryl acetate	0.2± 0.0	Ms
1800[g]	1800	Octadecane	0.6± 0.1	t_R, Ms
1935[d]	1957	(E)-β-Ionone	t	Ms
1986[d]	2008	Caryophyllene oxide	2.3± 0.1	t_R, Ms
2124[c]	2131	Hexahydrofarnesyl acetone	1.3± 0.1	t_R, Ms
2126[c]	2144	Spathulenol	t	t_R, Ms
2164[d]	2205	Thymol	1.1± 0.1	t_R, Ms
2211[d]	2246	Carvacrol	t	t_R, Ms
2331[e]	2316	12-Hydroxy-β-caryophyllene acetate	6.6± 0.0	Ms
2392[d]	2392	Caryophyllenol II	0.5± 0.1	Ms
2571[c]	2622	Phytol	0.7± 0.0	Ms
2628[d]	2676	Manool	0.3± 0.0	Ms
2687[d]	2696	Tetradecanoic acid	0.6± 0.1	t_R, Ms
2913[d]	2931	Hexadecanoic acid	0.8± 0.3	Ms
		Grouped compounds (%)		
		Monoterpene hydrocarbones	24.1	
		Oxygenated monoterpenes	3.5	
		Sesquiterpenes hydrocarbones	53.4	
		Oxygenated sesquiterpenes	2.8	
		Others	13.9	
		Total %	97.7	

RRI[a]: RRI data from literature (c [18]; d [25] ; e [26] ; f [27] ; g [28]) for polar column values; RRI[b]: RRI Relative retention indices experimentally calculated against *n*-alkanes; *: correct isomer not identified %: calculated from the FID chromatograms and expressed as mean ± SD (n = 3); t: Trace (<0.1 %); ID: Identification Method; Identification method based on the relative retention indices (t_R) of authentic compounds on a HP Innowax column; Ms, identified on the basis of computer matching of the mass spectra with those of the in-house Baser Library of Essential Oil Constituents, Adams, MassFinder and Wiley libraries.

Forty-six compounds constituting about 97.7% of the essential oil were characterized. The main compounds were characterized as β-caryophyllene (32.8%), β-pinene (9.8%), α-humulene (8.2%), 12-hydroxy-β-caryophyllene acetate (6.6%), germacrene D (4.9%) and α-pinene (4.5%). The analysis results are given in Table 1.

However, according to Ozen et al., the main compounds of *S. montbretii* collected from South-eastern Turkey in June 2002 (DUF 9473; Diyarbakır: between Silvan – Batman), were reported thymol (24.0%) and caryophyllene oxide (26.9%) [19].

The sesquiterpene hydrocarbon *β*-caryophyllene is present in almost all of the *Salvia* species. *β*-caryophyllene; *S. aramiensis* Rech. f. (7.55%), *S. atropatana* Bunge (1.39%), *S.aucheri* Bentham var. *aucheri* (3.02%), *S. bracteata* Banks & Sol. (1.36%), *S. caespitosa* Montbret& Aucher ex Benth. (1.44%), *S. kronenburgii* Rech. f. (10.27%), *S. modesta* Boiss. (3.78%), *S. multicaulis* Vahl (2.09%), *S. pachystachys* Trautv (4.83%), *S. pisidica* Boiss. & Heldr. (1.53%), *S. potentillifolia* Boiss. Heldr. ex Benth. (1.09%) *S. rosifolia Sm.* (1.45%) and *S. sclarea L.* (1.05%) [3].

Salvia montbretii essential oil has high sesquiterpenes hydrocarbones content (53.4%). To the best of our knowledge, this is the first report on the GC and GC-MS determination of the essential oil composition of *S. montbretii* in this locality. These results provide further support to earlier observations on the existence of distinct chemotypes [3, 24] of the same species of *Salvia* naturally growing the same area.

Disclosure Statement

No potential conflict of interest was reported by the authors

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