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COMPOSITION OF ESSENTIAL OILS FROM *Salvia anatolica*, A NEW SPECIES ENDEMIC FROM TURKEY

G. Ozek,[1] T. Ozek,[1] K. H. C. Baser,[1] E. Hamzaoglu,[2] and A. Duran[3]

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The component composition of essential oils produced by steam distillation from flower heads, leaves, and stems of Salvia anatolica *(Lamiaceae), a recently described new species endemic from Turkey, was studied by GC/FID and GC/MS. A total of 127 volatile components representing 96% of the oil was identified in essential oil from flower heads and leaves. It was found that the principal oil components of flower heads and leaves were α-pinene (10.9%), β-pinene (6.7%), α-copaene (6.3%), heptacosane (6.2%), and hexadecanoic acid (5.0%). A total of 109 volatile compounds representing 87.9% of the oil was characterized in essential oil isolated from stems. The principal oil components of stems were identified as hexadecanoic acid (27.2%), tetradecanoic acid (15.2%), dodecanoic acid (5.5%), and α-copaene (5.0%).*

Key words: *Salvia anatolica*, Labiatae, essential oil, α-pinene, β-pinene, α-copaene, hexadecanoic acid.

Certain species of *Salvia* (Lamiaceae) growing in Turkey are reported to have spasmolytic, antiseptic, and antioxidant properties [1, 2]. The component compositions of essential oils from certain *Salvia* species growing in Turkey have been previously published [3-17].

S. anatolica Hamzaoglu et A. Duran was recently described as a new endemic species from the Eastern Anatolia region of Turkey [18]. It is a perennial with a woody rhizome and belongs to the Iran—Turan species.

Herein we present data on the component composition of essential oils from *S. anatolica*. Steam distillation of flower heads with leaves and stems of *S. anatolica* produced two samples of green oils in yields of 0.03 and 0.01%, respectively. The resulting oils were analyzed using GC/FID and GC/MS methods. Table 1 gives a list of compounds observed in essential oils of *S. anatolica*, their relative percent content, and relative retention indices (RRI) in the order of their elution from a column of HP-Innowax FSC. The essential oil constituents were classified into monoterpenes (hydrocarbon and oxidized forms), sesquiterpenes (hydrocarbons and oxidized forms), fatty acids and their esters, and hydrocarbons and esters. Table 1 also gives the percent content of the main classes of compounds.

A total of 127 constituents making up 96% of the oil was observed in essential oil from flower heads and leaves. Sesquiterpenes (38.4%) were the major group of compounds in the oil. Hydrocarbbon sesquiterpenes (23.3%) dominated over oxidized forms of sesquiterpenes (15.1%). The main component in this group was α-copaene (6.3%). Among *Salvia* taxons, α-copaene (15.5%) was previously noted as the main compound in oil from *S. aethiopis* L. [19]. The important sesquiterpenes in oil from *S. anatolica* were germacrene D (3.0%), δ-cadinene (2.7%), β-caryophyllene (2.3%), and (*Z*)-β-farnesene (2.3%). The most important of the oxidized sesequiterpenes were caryophyllene oxide (2.9%), spatulenol (2.4%), and β-eudesmol (2.0%).

Monoterpenes (28.7%) in oil from flower heads and leaves of *S. anatolica* consisted primarily of unoxidized forms (25.1%). Of these, α-pinene (10.9%), β-pinene (6.7%), and limonene (3.2%) were identified as the main representatives of this group. Oxidized monoterpenes (3.6%) were found in much lower quantities than the hydrocarbon forms. These included the hydrocarbons (19.6%) heptacosane (6.2%), nonacosane (3.9%), and pentacosane (3.1%) as the main representatives. Fatty acids and their esters (6.5%) included mainly hexadecanoic acid (5.0%).

1) Department of Pharmacognosy, Faculty of Pharmacy, Anadolu University, 26470, Eskisehir, Turkey, fax: +90-222-330-6809, e-mail: gozek@anadolu.edu.tr; 2) Department of Biology, Faculty of Science and Letters, Bozok University, Yozgat, Turkey; 3) Department of Biology, Faculty of Education, Selcuk University, 42090, Konya, Turkey. Translated from Khimiya Prirodnykh Soedinenii, No. 6, pp. 552-555, November-December, 2007. Original article submitted February 9, 2007.

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TABLE 1. Chemical Composition of Essential Oils from *Salvia anatolica* (Flower Heads, Leaves, Stems)

Component	RI	Content, %		Component	RI	Content, %	
		A	B			A	B
α-Pinene	1032	**10.9**	0.3	β-Copaene	1603	Tr.	0.1
α-Thujene	1035	0.1	-	2-Undecanone	1604	0.6	-
Camphene	1076	0.1	-	β-Caryophyllene	1612	2.3	0.4
β-Pinene	1118	6.7	0.2	Octylbutyrate	1623	-	0.2
Sabinene	1132	0.5	Tr.	Octyl-2-methylbutyrate	1634	-	0.2
Myrcene	1174	0.9	Tr.	β-Cyclocitral	1638	0.1	-
α-Terpinene	1188	0.1	Tr.	Myrtenal	1648	Tr.	-
Limonene	1203	3.2	Tr.	γ-Elemene	1650	-	0.2
1,8-Cineol	1213	1.9	-	Octyl-3-methylbutyrate(=Octylisovalerate)	1654	-	Tr.
β-Phellandrene	1218	0.4	Tr.	(*E*)-2-Decenal	1655	Tr.	-
(*Z*)-3-Hexenal	1225	0.1	-	γ-Gurjunene	1659	0.1	-
2-Pentylfuran	1244	0.1	Tr.	Phenylacetaldehyde	1663	0.1	-
(*Z*)-β-Ocimene	1246	1.1	Tr.	(*Z*)-β-Farnesene	1668	2.3	2.1
γ-Terpinene	1255	0.4	Tr.	α-Humulene	1687	1.0	0.2
(*E*)-β-Ocimene	1266	0.2	Tr.	Selina-4,11-diene(=4,11-Eudesmadiene)	1688	Tr.	Tr.
p-Cymene	1280	0.4	Tr.	γ-Muurolene	1704	0.3	0.1
Terpinolene	1290	0.1	-	α-Terpineol	1706	0.1	-
1-Tridecene	1350	-	Tr.	Borneol	1719	0.1	-
cis-Alloocimene	1382	-	Tr.	2-Undecanol	1720	0.1	-
(*Z*)-3-Hexenol	1391	0.1	-	Dodecanal	1722	-	0.1
3-Octanol	1393	Tr.	-	α-Zingiberene	1725	0.3	-
Nonanal	1400	0.2	-	Germacrene D	1726	3.0	0.6
Tetradecane	1404	-	Tr.	β-Selinene	1742	1.2	1.0
Hexylbutyrate	1424	-	Tr.	α-Selinene	1744	0.4	0.2
Hexyl-2-methylbutyrate	1438	Tr.	Tr.	Bicyclogermacrene	1755	0.2	0.2
Dimethyltetradecane	1445	-	Tr.	Naphthalene	1763	0.1	-
2,6-Dimethyl-1,3(*E*),5(*Z*),7-octatetraene	1446	Tr.	-	δ-Cadinene	1773	2.7	2.2
1-Octen-3-ol	1452	0.1	-	γ-Cadinene	1776	0.2	Tr.
2,6-Dimethyl-1,3(*E*),5(*E*),7-octatetraene	1460	Tr.	-	β-Sesquiphellandrene	1783	0.1	0.1
α-Cubebene	1466	Tr.	-	Kessane	1784	Tr.	-
Octylacetate	1483	0.1	0.1	*ar*-Curcumene	1788	1.0	0.7
Bicycloelemene	1495	-	0.1	Selina-3,7(11)-diene	1796	-	Tr.
α-Copaene	1497	**6.3**	**5.0**	Octadecane	1800	-	0.1
Dihydroedulan II	1505	Tr.	-	Myrtenol	1804	0.2	-
Decanal	1506	0.1	-	2-Tridecanone	1815	0.5	0.8
(*E*,*E*)-2,4-Heptadienal	1507	Tr.	-	(*E*,*E*)-2,4-Decadienal	1827	0.1	-
α-Burbonene	1521	Tr.	-	Tridecanal	1830	-	Tr.
Camphor	1526	0.1	-	(*E*)-β-Damascenone	1838	0.1	-
β-Burbonene	1528	0.8	0.1	(*E*)-Anethole	1845	0.2	-
Dihydroedulan I	1529	0.1	-	Calamenene	1853	0.3	0.5
Octylisobutyrate	1547	-	0.2	(*E*)-Geranylacetone	1868	0.5	0.1
(*E*)-2-Nonenal	1548	0.1	-	*epi*-Cubebol	1900	0.1	Tr.
β-Cubebene	1549	0.1	Tr.	Nonadecane	1904	0.1	0.1
Linalool	1553	0.3	-	2-Dodecanol	1925	0.1	-
Octanol	1562	0.2	-	Tetradecanal	1933	-	0.2
cis-Chrysanthenylacetate	1582	Tr.	-	α-Calacorene	1941	0.2	0.2
Pinocarvone	1586	0.1	0.1	Cubebol	1957	0.3	-
β-Ylangene	1589	0.1	0.1	(*E*)-β-Ionone	1958	0.5	-
Bornylacetate	1590	0.1	-	1-Dodecanol	1973	0.2	0.2
trans-β-Bergamoten	1594	-	0.1	Unident.	1979	-	1.0
β-Elemene	1600	0.1	0.2	γ-Calacorene	1984	0.1	0.1
Hexadecanone	1601	0.1	0.1	Isocaryophyllene oxide	2001	0.1	-

TABLE 1. (continued)

Component	RI	Content, %		Component	RI	Content, %	
		A	B			A	B
Caryophyllene oxide	2008	2.9	0.5	Ethyl-3-hydroxydodecanoate	2328	0.2	0.2
Methyltetradecanoate	2021	-	Tr.	Galaxolide (I)[a]	2343	-	0.1
2-Pentadecanone	2033	-	0.1	Galaxolide (II)[a]	2351	-	0.1
Salvial-4(14)-en-1-one	2037	0.3	0.2	Eudesma-4(15),7-dien-1β-ol	2376	0.8	0.3
Pentadecanal	2041	-	0.1	Hexylcinnamaldehyde	2377	-	0.1
Humulene epoxide-I	2045	0.2	-	Farnesylacetone	2378	0.1	1.0
(*E*)-Nerolidol	2050	0.1	0.2	Caryophylla-2(12),6-dien-5β-ol	2392	0.4	0.2
Ethyltetradecanoate	2059	-	0.1	(=Caryophyllenol II)			
Humulene epoixde-II	2071	**0.8**	-	Tetracosane	2400	0.5	0.1
Tridecanol	2077	0.1	0.1	Dihydroambrettolide	2402	-	Tr.
Cubenol	2080	0.2	-	Pentacosane	2500	3.1	2.5
1-*epi*-Cubenol	2088	0.2	-	Dodecanoic acid	2503	-	5.5
Heneicosane	2100	0.2	0.1	Ethyl-3-hydroxytridecanoate	2537	0.5	-
Guaiol	2103	-	Tr.	Geranyllinalol	2551	-	0.1
Hexahydrofarnesylacetone	2131	1.7	1.7	Methyllinolenate	2583	-	0.4
Spatulenol	2144	2.4	0.4	Hexacosane	2600	-	0.5
(*Z*)-3-Hexen-1-ylbenzoate	2148	0.2	-	Octadecanol	2607	-	0.9
Tetradecanol	2179	2.2	0.4	Ethyllinolenate	2615	-	0.5
Isothymol(=2-Isopropyl-4-methylphenol)	2181	1.7	-	Phytol	2627	0.9	0.8
T-Cadinol	2187	0.4	-	Tridecanoic acid	2629	-	0.2
Docosane	2200	-	Tr.	Manool	2680	-	Tr.
T-Muurolol	2209	0.2	0.1	Tetradecanoic acid(=Myristicinic acid)	2719	0.6	**15.2**
ar-Turmerol	2214	Tr.	-	Heptacosane	2722	**6.2**	**4.8**
Isocarvacrol(=4-Isopropyl-2-methylphenol)	2221	0.1	-	Octacosane	2800	-	0.6
Methylhexadecanoate(=methylpalmitate)	2226	0.2	0.1	Pentadecanoic acid	2822	-	1.6
Carvacrol	2239	0.1	-	Nonacosane	2900	3.9	0.1
α-Eudesmol	2250	0.4	-	Hexadecanoic acid(=Palmitinic acid)	2931	**5.0**	**27.2**
α-Cadinol	2255	Tr.	-	Total		96.0	87.9
β-Eudesmol	2257	2.0	0.7	Monoterpene hydrocarbons		25.1	0.6
Ethylhexadecanoate	2270	-	0.2	Oxidized monoterpenes		3.6	0.2
Alismol(=Guaia-6,10(14)-dien-4β-ol)	2274	0.2	0.1	Sesquiterpene hydrocarbons		23.1	14.5
Oxo-α-ylangene	2289	Tr.	-	Oxidized sesquiterpenes		15.0	5.6
Myristicin	2296	0.3	0.3	Fatty acids and fatty acid esters		6.5	51.2
Tricosane	2300	0.7	0.5	Hydrocarbons		19.6	12.4
Eudesma-4(15),7-dienol isomer[*a]	2315	1.0	-	Esters		0.3	0.7
Caryophylla-2(12),6(13)-dien-5α-ol (=Caryophylladienol II)	2324	0.2	-	Others		2.8	2.4

RRI are relative retention indices calculated relative to *n*-alkanes; %, calculated from FID data;

Tr, trace (<0.1%); A, oil of flower heads and leaves; B, oil of stems; *exact isomer not identified.

* Identification method, identification based on retention index of compounds on HP-Innowax column and agreement with mass spectra from catalogs of Baser, Adams, MassFinder, Wiley, and NIST.

[a] Identification method based on approximate similarity of mass spectra.

† Mass spectrum of unknown compound (EIMS, 70 eV, *m*/*z*, rel. int.): 292 (0.01), 266 (0.01), 253 (0.1), 206 (0.5), 191 (1), 176 (0.1), 151 (1), 134 (14), 119 (1), 91 (3), 83 (100), 79 (3), 77 (3), 55 (37), 41 (4), 39 (3).

A total of 109 constituents making up 87.9% of the oil was characterized in oil from stems of *S. anatolica*. Fatty acids and their esters were found in large quantities (51.2%) in oil from stems. The main representatives of this group were hexadecanoic (27.2%), tetradecanoic (15.2%), and dodecanoic (5.5%) acids. The next most important group in oil from stems was sesquiterpenes (20.1%). Sesquiterpene hydrocarbons (14.5%) prevailed compared with oxidized sesquiterpenes (5.6%).

α-Copaene (5.0%), δ-cadinene (2.2%), (*Z*)-β-farnesene (2.1%), and β-selinene (1.0%) were the main sesquiterpene hydrocarbons. The oxidized forms included hexahydrofarnesyl acetone (1.7%), farnesyl acetone (1.0%), and β-eudesmol (0.7%) as the most important representatives. A very small quantity (0.8%) of monoterpenes was observed in essential oil from stems.

Thus, the chemical composition of essential oils from *S. anatolica*, a new endemic species from the Eastern Anatolia region of Turkey, was studied for the first time using GC and GC/MS. Analysis of essential oils from *S. anatolica* using GC/FID and GC/MS methods showed that flower heads and leaves are rich in monoterpenes (28.7%) compared with oil from stems (0.8%). A literature search revealed that α-pinene and β-pinene were already proposed as the main constituents of essential oils from certain other *Salvia* species such as *S. tomentosa* Miller (6-29 and 5-33%, respectively), *S. wiedemanii* Boiss. (23-33 and 14-30%, respectively), *S. potentillifolia* Boiss. et Heldr. ex Benth. (10 and 8%, respectively), *S. limbata* C. A. Meyer (11-24 and 10-21%, respectively) [12, 16]. A high percentage of sesquiterpenes was found in both studied oils (38.1 and 20.1%, respectively). However, small differences were found in the content of certain main components. Oil from stems had a high content of fatty acids and their esters (51.2%).

According to the classification of the main chemical groups in essential oils from the genus *Salvia* [9], the new endemic species studied by us belongs to the α/β-pinenes group. Plants of the genus *Salvia* are of great scientific and commercial interest. However, certain wild species have not yet been studied. The results of our work provide useful data for the chemotaxonomy of *Salvia* species.

EXPERIMENTAL

Plant Material. Aerial parts of *S. anatolica* were collected at an elevation of 1695 m in Sivas province (Turkey) in June 2004. A voucher specimen is kept at the Herbarium of the Education Faculty of the Biology Department in Selcuk University in Konya, Turkey (A. Duran 6595).

Essential Oil Preparation. Flower heads with leaves and stems (air-dried raw material) of *S. anatolica* were steam distilled separately in a Clevenger apparatus for 3 h. The yields of essential oils were 0.03 and 0.01% for flower heads with leaves and stems, respectively. The oil yield was calculated per dry raw material. The resulting oils were dried over anhydrous Na_2SO_4. Oils were preserved in flasks of dark glass at 4°C and were prepared for GC/FID and GC/MS analysis.

GC/MS Analysis. The chemical composition of essential oils was studied using capillary GC/FID and GC/MS on Agilent GC—MSD systems. GC/MS analysis was performed on an Agilent 5975 GC—MSD system using an HP-Innowax FSC column (60 m × 0.25 mm dia., 0.25 μm thickness) and helium as carrier gas (0.8 mL/min). The GC/FID thermostat was kept at 60°C for 10 min and programmed to 220°C at a rate of 4°C/min, then kept constant at 220°C for 10 min and then programmed to 240°C at a rate of 1°C/min. The split ratio was adjusted at 40:1. The injector temperature was at 250°C. Mass spectra (EI, 70 eV) were recorded in the range 35-450 *m*/*z*. Alkanes (C_9-C_{20}) were used as reference points in the calculation of RRI.

GC Analysis. An identical column and conditions were used for GC/FID and GC/MS analyses. GC/FID analysis was carried out on an Agilent 6890N GC using an Innowax FSC column (60 m × 0.25 mm dia., 0.25 μm thickness) and nitrogen as carrier gas (flow rate from 1.2 to 0.9 mL/min). The GC thermostat was kept at 60°C for 10 min and programmed to 220°C at a rate of 4°C/min, then kept constant at 220°C for 10 min and then again programmed to 240°C at a rate of 1°C/min. The flow was set at 12 mL/min with a split ratio adjusted to 10:1. The FID temperature was 300°C. An elution order identical to that for GC/MS was achieved by simultaneous injection using the same column and operating conditions. The relative percent content of the separated constituents of the essential oils was calculated using the FID chromatograms.

Identification of Compounds. Volatile compounds were identified based on the agreement of retention indices and mass spectra of the studied components with the corresponding characteristics in the Baser Library of Essential Oil Constituents, which includes mass spectra and retention data for more than 3500 compounds. Wiley GC/MS Library, MassFinder, Adams Library, and NIST02 were also used.

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