

CHEMICAL COMPOSITION OF THE ESSENTIAL OILS OF *Stachys atherocalyx* AND *S. sylvatica* FROM IRAN

Shamsali Rezazadeh,^{1*} Morteza Pirali-Hamedani,²
Abbas Hadjiakhondi,³ Yousef Ajani,¹
Marzyeh Yarigar-Ravesh,² and Abbas Shafiee²

UDC 547.913

The genus *Stachys* (Lamiaceae) is distributed in the mediterranean regions and southwest Asia. About three hundred *Stachys* species are reported [1]; 34 of them are found in Iran, of which 13 are endemic [2, 3]. Several *Stachys* species are used in Iranian folk medicine as medicinal plants [4]. In addition, pharmacological studies confirmed that extracts or components of plants belonging to the genus *Stachys* exert significant antibacterial [5], anti-inflammatory [6], antitoxic [7, 8] and anti-anoxia [9] effects.

Biosystematic and chemotaxonomic studies have been carried out on *Stachys* species in which flavonoids and flavonoid glycosides, quinones, iridoids, phenolic acids, diterpenoids, and essential oils were reported [5–14]. As *Stachys atherocalyx* and *Stachys sylvatica* are used in Iranian folk medicine and potentially have medical importance, we decided to make an analysis of their essential oil composition.

The compounds identified by GC and GC-MS analyses from the essential oils of *Stachys atherocalyx* C. Koch. and *Stachys sylvatica* L. are presented in Table 1. Both essential oils were light yellow with a distinct sharp odor, and the total yield of both plants was 0.20% v/w. The yield from other species were: *S. chrysantha*, 0.18%; *S. candida*, 0.12%; *S. setifera*, 0.18%, *S. obliqua*, 0.075%; *Stachys schtschegleevii*, 0.2%; and *Stachys balansae*, 0.3% [5, 13, 14, 17].

In *Stachys atherocalyx* thirty six components were identified representing 98.1% of the total oil; spathulenol (22.1%) was the major component. Eighteen monoterpenes, representing 47.9%, thirteen sesquiterpenes, representing 42.9%, and two aromatic hydrocarbons, representing 1.6% of the total oil, were detected, in which 71.2% of them were oxygenated compounds. The more abundant sesquiterpene was β -bourbonene (5.7%), and the major monoterpenes that were found were β -pinene (9.6%), linalool (9.1%), linalyl acetate (8.9%), α -pinene (4.8%), and α -terpineol (4.3%). Also β -ionone (3.8%) was found with good abundance.

In *Stachys sylvatica* L. twenty-five components representing 93.9% of the total oil were identified. β -Caryophyllene (19.6%) was the major component, and nine sesquiterpenes and thirteen monoterpenes comprising 75.9% and 19.6% of the total oil were detected, respectively. Other major components were δ -cadinene (13.4%), spathulenol (12.5%), α -humulene (11.2%), δ -3-carene (7.4%), α -copaene (6.4%), and bicyclogermacrene (6.2%).

In spite of the large size of the genus *Stachys*, the composition of the essential oil in only a small number of species has been reported. Previous works on the oil of members of the *Stachys* genus showed varying compositions [5, 11–19]. For example, the principal constituents of the oil of *Stachys officinalis* from Yugoslavia were a mixture of β - and isocaryophyllene (22.9%) [12]; the oil of *Stachys candida* consisted of manoyl oxide (12.07%), caryophyllene oxide (11.5%), and β -caryophyllene (9.58%) [5]; in the oil of *Stachys balansae* from Turkey [15], β -caryophyllene (24.3%), β -pinene (24.1%), and α -pinene (16.0%) were the major components; also, in our previously reported study, we have found in *Stachys schtschegleevii* germacrene-D (25.8%), limonene (8.8%), valencene (6.1%), α -pinene (5.6%), bicyclogermacrene (4.5%), δ -cadinene (3.3%); and in *Stachys balansae* we have found germacrene-D (16.4%), α -pinene (12.1%), β -pinene (11.9%), and valeranone (10.4%) as the major components [17].

1) Department of Pharmacognosy, Institute of Medicinal Plants (ACECR), Karaj, Iran, P.O.Box: 13145-1446, fax: +98 21 6697 1191, e-mail: shrezazadeh@imp.ac.ir; 2) Department of Chemistry, Faculty of Pharmacy and Pharmaceutical Sciences Research Center, Tehran, Iran; 3) Department of Pharmacognosy and Medicinal Plants Research Center, Faculty of Pharmacy, Tehran University of Medical Sciences, Tehran, Iran. Published in *Khimiya Prirodnikh Soedinenii*, No. 5, pp. 621–622, September–October, 2009. Original article submitted March 5, 2008.

TABLE 1. The Chemical Compounds of the Essential Oils of *Stachys atherocalyx* C. Koch. and *Stachys sylvatica* L.

Compound	RRI*	<i>S. atherocalyx</i>	<i>S. sylvatica</i>	Compound	RRI*	<i>S. atherocalyx</i>	<i>S. sylvatica</i>
		%				%	
α -Pinene	936	4.82	2.93	Nerol	1228	0.42	–
Camphene	953	–	0.13	Pulegone	1237	–	0.37
Benzaldehyde	954	0.82	0.16	Carvone	1242	0.74	–
β -Pinene	978	9.6	–	α -Cubebene	1351	–	2.10
3-Octanol	993	0.32	–	Linalyl acetate	1258	8.86	–
δ -3-Carene	1011	0.42	7.38	<i>p</i> -Methoxyacetophenone	1348	0.74	–
Limonene	1027	1.10	–	Neryl acetate	1365	0.66	–
<i>cis</i> - β -Ocimene	1040	0.58	2.13	α -Copaene	1376	–	6.38
<i>trans</i> - β -Ocimene	1050	–	1.52	Geranyl acetate	1383	2.12	–
γ -Terpinene	1062	–	0.24	β -Bourbonene	1385	5.65	–
1-Octanol	1070	–	0.10	β -Cubebene	1393	0.76	–
<i>cis</i> -Linalool oxide	1074	0.74	–	α -Gurjunene	1409	–	0.74
<i>trans</i> -Linalool oxide	1088	1.0	–	β -Caryophyllene	1418	–	19.64
α -Terpinolene	1088	–	0.21	Neryl acetone	1433	0.58	–
Linalool	1098	9.14	–	α -Humulene	1458	–	11.17
Nonanal	1102	–	0.62	Germacrene D	1480	0.6	–
1-Octen-3-yl acetate	1110	3.38	–	β -Ionone	1485	3.78	–
<i>trans</i> -Thujone	1114	–	0.13	Valencene	1491	2.18	–
1-Terpineol	1134	–	0.13	α -Muurolene	1497	0.64	–
<i>trans</i> -Pinocarveol	1139	2.37	–	δ -Cadinene	1528	0.58	13.41
Camphor	1143	–	0.14	Bicyclogermacrene	1506	–	6.15
Pinocarvone	1162	0.52	0.15	Spathulenol	1584	22.08	12.51
Borneol	1165	0.66	–	Viridiflorol	1597	1.24	–
4-Terpineol	1177	–	0.61	α -Cadinol	1660	2.02	3.81
α -Terpinol	1189	4.3	–	Phytol	1949	2.02	–
Myrtenol	1194	1.62	–	Sum		98.09	93.9
<i>trans</i> -Carveol	1217	1.02	–				

*Relative retention index.

The main constituents of the essential oil of *Stachys iberica* subsp. *stenostachya* growing in Turkey were reported as linalyl acetate (42.2%), linalool (18.9%), geranyl acetate (8.2%), and α -terpineol (5.3%) [18]. Also the main constituents of the essential oil of *Stachys laetivirens* Kotschy & Boiss. ex Rech. fil., endemic in Turkey, were found to be nonacosane (23.1%) and phytol (17.9%) [19]. Pulegone (20.5%), piperitone oxide (17.4%), and α -terpinyl acetate (11.2%) were the major components of *Stachys setifera* [14], and myrtenyl acetate (48.7%), globulol (13.1%), caryophyllene oxide (8.4%), and spathulenol (5.6%) were the major components in the essential oil of *Stachys ixodes* [20]. *Stachys glutinosa* was rich in germacrene-D (19%), terpinen-4-ol (13.1%), α -pinene (13.1%), α -terpineol (10.1%), β -phellandrene (6.8%), and δ -terpinene (6.1) [21]. Spathulenol, β -pinene, and linalool, which are the three major components of the oil of *Stachys atherocalyx*, were at least one of the predominant components of the oil of *Stachys ixodes* [20], *Stachys laxa* [16], *Stachys schtschegleevii*, and *Stachys balansae* [17]. Also, the major components of the oil of *Stachys sylvatica* (β -caryophyllene, δ -cadinene, and spathulenol) were one of the main compounds in the oil of *Stachys* subsect swainsoniaeae [22] and *Stachys ixodes* [20]. This study showed the good similarity in composition of the oils of our studied species and some of those previously reported.

ACKNOWLEDGMENT

This work was supported by a grant from the Institute of Medicinal Plants (ACECR). The authors are grateful for their collaboration.

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