COMPOSITION OF THE ESSENTIAL OIL OF *Stachys acerosa* GROWING IN CENTRAL IRAN

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The essential oil of aerial parts of Stachys acerosa, *which belongs to the Lamiaceae family and grows in central Iran, was obtained by a hydrodistileation method and analyzed by GC and GC-MS apparatus. Fourteen compounds representing 98.8% of the oil were identified. Among them N-methylisatin (30%), α-pinene (25%), sabinene (12.3%), and 2-hydroxyacetophenone (11.2%) were the major constituents of the oil, which was obtained in 0.1% yield.*

Key words: *Stachys acerosa*, Lamiaceae, essential oil, *N*-methylisatin, α-pinene.

The genus *Stachys acerosa* Boiss., which belongs to the Lamiaceae family, is found in mild regions of the Mediteranean and in southwest Asia. This genus consists of 250 species widespread throughout the word. Among the 39 species present in Iran, 13 species are endemic and *Stachys acerosa* Boiss. which is named "sonbolei-kouhsary" or "sonbolei-kharalood", is one of them. The compositions of the oils of some *Stachys* species from Iran, such as *S. setifera* [1], *S. ixodes* [2], *S. persica* [3], *S. byzanthin* [4], *S. lanata* [5], *S. schtscheglee* [6], *S. pilifera* [7], *S. lavandolifolia* [8, 9], and *S. laxa* [10], have been reported. *Stachys* species have also been studied in biosystematic and chemotaxonomic studies [11, 12]. Because of the various uses of *Stachys acerosa* and their essential oils, we decided to study the constituents of the essential oil from *Stachys acerosa* of the Kashan area [13], central Iran. Masoudi et al [7] considered the oil of this species from Lalezar Mountain, province of Kerman, south of Iran. A literature survey revealed that the essential oil of the aerial part of this plant in central Iran has not been chemically studied to date. The present paper deals with the detailed analysis of the oil by capillary GC and GC-MS with the determination of the percentage composition.

The aerial parts of *Stachys acerosa* yielded 0.1% v/w of a yellowish oil which was determined by the gravimetric method and calculated as a percentage with respect to the mass of starting dry plant material. In this oil 14 components, which represented about 98.8% of the total composition, were identified and listed in Table 1 with their percentage compositions. The constituents are listed in order of their elution from HP-5MS column. This oil consisted mainly of six monoterpenes (49.3%) and one alkaloid (30%) and four sesquiterpenes (4.7%). The major components are *N*-methylisatin (30%), α-pinene (25%), sabinene (12.3%), and 2-hydroxyacetophenone (11.2%). According to a similar experiment [7] on the essential oil of *Stachys acerosa* in the province of Kerman, south of Iran, in June 1999, the monoterpenes are the main components (79.3%) relative to sesquiterpenes (11.2%). The major components in their results are *cis*-chrysantenyl acetate (41%) and linalool (23.5%), which are different from our results. As can be seen, the chemical composition of *S. acerosa* that we identified in central Iran is different from that from south of Iran. There was no *cis*-chrysantenyl acetate and linalool in our oil. Only three compounds, eugenol (1.6%), neryl acetate (0.4%), and δ-cadinene (0.8%), which exist in their oil, were identified in our oil at 1.9%, 0.3% and 2.9%, respectively. On the other hand, *N*-methylisatin, which is the major component in our oil, was not found in their oil. This difference between the oil compositions of one species of *Stachys* from two different areas can be related to climatological factors (from south to central Iran) and is discussed in phytological studies.

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TABLE 1. Composition of the Essential Oil of *Stachys acerosa* Boiss. from Central Iran

Compound[a]	Percentage	RI[b]	Compound[a]	Percentage	RI[b]
α-Pinene	25.0	930	α-Humulene	1.0	1450
Sabinene	12.3	970	*N*-Methylisatin[c]	30.0	1477
δ-3-Carene	3.8	1009	γ-Cadinne	0.2	1505
Limonene	5.3	1027	δ-Cadinene	2.9	1510
Isobornyl acetate	2.6	1275	Ethyl laurate	1.7	1515
2-Hydroxyacetophenone	11.2	1287	α-Bisabolol	0.6	1675
Eugenol	1.9	1330	Total	98.8	
Neryl acetate	0.3	1341			

[a]Compounds listed in order of their RI.
[b]RI (retention index) measured relative to n-alkanes (C9-C18) on a nonpolar HP-5 column.
[c]Tentatively identified according to mass spectra data; RI = 1477, MS data 70 eV, m/z (rel. int): 161 (100), 119 (20), 105 (48), 104 (76), MW (161).
%, Relative percentage obtained from peak area.

TABLE 2. Diversity and Percentage of Chemical Compositions of Some *Stachys* Species Essential Oils

Plant Name	Oil Yield (v/w), %	Monoterpenes, %	Sesquiterpenes, %	Major Component, %
*S. acerosa** [7]	0.2	79.3	11.2	*cis*-Chrysantenyl acetate (41)
S. glutinosa [14]	0.3	70.6	19.7	Terpinen-4-ol (13.1)
S. balansae [15]	0.1	64.1	29.2	β-Caryophyllene (24.3)
S. oblique [16]	0.1	63.5	33.4	Germacrene-D (25.4)
S. lavandolifolia [17]	0.4	60.1	14.9	β-Caryophyllene (11.3)
*S. acerosa***	0.1	49.3	4.7	*N*-Methylisatin (30)
S. athorekalyx [18]	0.1	47.8	29.6	Oct-1-en-3-ol (18.7)
S. recta [19]	0.1	47.4	13.9	Oct-1-en-3-ol (33.8)
S. laxa [10]	0.1	11.7	78.6	Germacrene-D (40.8)
S. officinalis [9]	0.5	6.3	72.0	β-Caryophyllene (22.9)

**S. acerosa* from south of Iran.
***S. acerosa* from central Iran.

Previous studies on essential oils of members of *Stachys* genus showed various compositions. Table 2 shows the diversity of major components among oils of some *Stachys* species which have been analyzed by some investigators [9, 10, 14–19]. Monoterpenes were the predominat fraction in the oils of most *Stachys* species; however, *S. officinalis* [9] and *S. laxa* [10] oils are reported as sesquiterpene-rich essential oils (78.6% and 72.0% respectively). As shown in table 2, an alkaloid, *N*-methylisatin, is the major component of *S. acerosa* (which growes in central Iran). Germacrene-D in both *S. laxa* [10] and *S. obliqua* [16] oils is the major compound. β-Caryophyllene in *S. officinalis* [9], *S. lavandolifolia* [17], and *S. balansae* [15] oils and oct-1-en-3-ol in *S. recta* [19] and *S. athorekalyx* [18] oils are major constituents. Comparison of the results with the literature showed significant differences for the oils, which can be attributed to either climatological factors or genetic differences of the plants.

EXPERIMENTAL

The aerial parts of *Stachys acerosa* were collected from the Kashan area (Isfahan Province, central area of Iran) at an altitude of ca. 1500 m in July 2004. The aerial parts (leaves and flowers/inflorescences) were dried in the shade (at room

temperature). The voucher specimens of the plant were deposited in the herbarium of the Research Institute of Forests and Rangelands, Kashan, Iran.

The air-dried aerial parts of the plant (100 g) were powdered and the volatile fraction was isolated by hydrodistillation in an all-glass Clevenger-type apparatus for 3 h according to the method recommended in the European Pharmacopoeia [20]. After decanting, the yellow oil (0.1 mL) was dried over anhydrous sodium sulfate and stored in a vial at low temperature (4°C) before analysis.

The oil was analyzed by GC and GC-MS. GC analysis was carried out on a Hewlett-Packard-6890 gas chromatograph equipped with an FID detector and an HP-5MS fused silica column (30 m × 0.25 mm i.d., film thickness, 0.25 μm). The column temperature was kept at 60°C for 3 min and then programmed to 220°C at a rate of 5°C /min and then kept constant at 220°C for 3 min. Injector and detector (FID) temperatures were 290°C. The flow rate of helium (carrier gas) was 1 mL/min. Volume injected, 0.1 μL of the oil; split ratio, 1:20. GC/MS analysis was performed on an HP-5973 mass selective detector coupled with an HP-6890 gas chromatograph, equipped with a cross-linked 5% PH ME siloxane HP-5MS capillary column (30 m × 0.25 mm i.d., film thickness, 0.25 μm) and operating under the same condition as described above. The MS operating parameters were as follows: ionization potential, 70 eV; ionization current, 2A; ion source temperature, 200°C; resolution, 1000.

Identification of components in the oil was based on retention indices (RI) relative to *n*-alkanes and computer matching with the WILEY 275.L library, as well as by comparison of the fragmentation pattern of the mass spectra with data published in the literature [21]. The percentage composition of the samples was computed from the GC peak areas.

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