

The Essential Oil of *Salvia sclarea* L. from Tajikistan

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Abstract: The essential oil from the aerial parts of *Salvia sclarea* L., growing wild in Tajikistan, were obtained by hydrodistillation and analyzed by gas chromatography – mass spectrometry. A total of 59 compounds were identified representing 94.2% of total oil composition. Major components of the essential oil were linalyl acetate (39.2%), linalool (12.5%), germacrene D (11.4%), α -terpineol (5.5%), geranyl acetate (3.5%), and (*E*)-caryophyllene (2.4%). The chemical composition, the large concentrations of linalool and linalyl acetate, and a cluster analysis based on principal components; of Tajik *S. sclarea* oil reveal it to be comparable to commercial *S. sclarea* oils.

Keywords: *Salvia sclarea* L.; essential oil composition; linalyl acetate; linalool; germacrene D.

1. Plant Source

Aerial parts of *S. sclarea* were collected from the Chormaghzak village, Yovon region of Tajikistan, (38.417502 N, 69.172175 E, 1300 m above sea level), on 25 July 2010. The plant was identified by F. S. Sharopov, and a voucher specimen (TJ2010-033) has been deposited in the herbarium of the Chemistry Institute of the Tajikistan Academy of Sciences.

2. Previous Studies

The genus *Salvia* is the largest in the Lamiaceae with over 700 species [1] and possibly as many as 900 species [2]. Some of its representatives, e.g., *S. sclarea* L. and *S. officinalis* L., are commercially important sources of essential oils. The essential oil of *S. sclarea* (clary sage) is used in the perfumery industry, soft drink and liquor production [3,4]. The oil has shown medicinal utility in aromatherapy for its anxiolytic effects [5] as well as digestive activities [6]. Sages are used for wound treatment, bathing, washing, skin and hair care [7]. *S. sclarea* oil has been evaluated for antioxidant [8], antibacterial [9,10], antifungal [6,11-13], antiinflammatory [14], antimalarial [15], anticholinesterase [16] and antiviral [17] and opioid receptor activities [18]. In this work we report the chemical composition of *S. sclarea* growing wild in Tajikistan. To our knowledge this is the first examination of the volatile components of Tajik *S. sclarea*.

3. Present Study

The air-dried samples of *S. sclarea* were crushed and hydrodistilled for 2 h using a Clevenger apparatus to give the essential oil in 0.3% yield.

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Table 1. Chemical composition of *Salvia sclarea* L. essential oil from Tajikistan.

RI	Compound	%	RI	Compound	%
941	α -Pinene	0.1	1419	(<i>E</i>)-Caryophyllene	2.4
978	β -Pinene	0.1	1428	β -Copaene	0.1
992	Myrcene	0.7	1453	α -Humulene	0.1
1004	α -Phellandrene	0.1	1467	(<i>2E</i>)-Dodecenal	0.1
1016	α -Terpinene	0.1	1484	Germacrene D	11.4
1024	<i>p</i> -Cymene	0.5	1487	β -Selinene	0.2
1028	Limonene	0.2	1497	Bicyclogermacrene	1.2
1030	1,8-Cineole	0.1	1501	α -Cuprenene	0.1
1036	Santolina alcohol	0.1	1505	Germacrene A	0.1
1038	(<i>Z</i>)- β -Ocimene	0.1	1510	(<i>E,E</i>)- α -Farnesene	0.3
1048	(<i>E</i>)- β -Ocimene	0.2	1517	<i>cis</i> -Dihydroagarofuran	0.1
1058	γ -Terpinene	0.3	1524	δ -Cadinene	0.4
1100	Linalool	12.5	1578	Spathulenol	0.2
1107	α -Thujone	0.4	1583	Caryophyllene oxide	0.2
1116	β -Thujone	0.5	1604	(<i>2R,5E</i>)-Caryophyll-5-en-12-al	0.3
1153	Menthone	0.1	1626	(<i>2S,5E</i>)-Caryophyll-5-en-12-al	0.2
1164	Borneol	0.1	1642	Unidentified sesquiterpenoid	0.6
1176	Terpinen-4-ol	0.1	1650	β -Eudesmol	0.5
1190	α -Terpineol	5.5	1653	α -Eudesmol	0.3
1215	Linalyl formate	0.1	1707	δ -Dodecalactone	0.1
1228	Nerol	1.1	1881	(<i>5E,9Z</i>)-Farnesyl acetone	0.3
1236	Pulegone	0.4	1914	(<i>5E,9E</i>)-Farnesyl acetone	0.1
1243	Carvone	0.1	1920	Unidentified sesquiterpenoid	1.3
1256	Linalyl acetate	39.2	1940	Unidentified diterpene	0.8
1284	1-Phenyl-2,4-pentadiyne	1.2	1955	Unidentified diterpene	0.8
1292	Thymol	1.5	1957	Unidentified diterpene	0.8
1301	Carvacrol	1.3	1970	Unidentified diterpene	1.5
1349	δ -Elemene	0.2	1987	(<i>E,Z</i>)-Geranyl linalool	0.2
1366	Neryl acetate	1.9	2002	(<i>Z,E</i>)-Geranyl linalool	0.1
1375	α -Copaene	1.0	2031	(<i>E,E</i>)-Geranyl linalool	0.1
1386	Geranyl acetate	3.5	2057	Manool	0.2
1390	β -Cubebene	0.6	2222	Sclareol	1.2
1405	Methyl eugenol	t	Total Identified		94.2

The essential oil of *S. sclarea* was analyzed by GC-MS using an Agilent 6890 GC with Agilent 5973 mass selective detector [MSD, operated in the EI mode (electron energy = 70 eV), scan range = 45-400 amu, and scan rate = 3.99 scans/sec], and an Agilent ChemStation data system. The GC column was an HP-5ms fused silica capillary with a (5% phenyl)-polymethylsiloxane stationary phase, film thickness of 0.25 μ m, a length of 30 m, and an internal diameter of 0.25 mm. The carrier gas was helium with a column head pressure of 48.7 kPa and a flow rate of 1.0 mL/min. Inlet temperature was 200°C and interface temperature was 280°C. The GC oven temperature program was used as follows: 40°C initial temperature, hold for 10 min; increased at 3°C/min to 200°C; increased 2°/min to 220°C. A 1% w/v solution of the sample in CH₂Cl₂ was prepared and 1 μ L was injected using a splitless injection technique. Identification of oil components was achieved based on their retention indices (RI, determined with reference to a homologous series of normal alkanes), and by comparison of their mass spectral fragmentation patterns with those reported in the literature [19] and stored on the MS library

[NIST database (G1036A, revision D.01.00)/ChemStation data system (G1701CA, version C.00.01.08)].

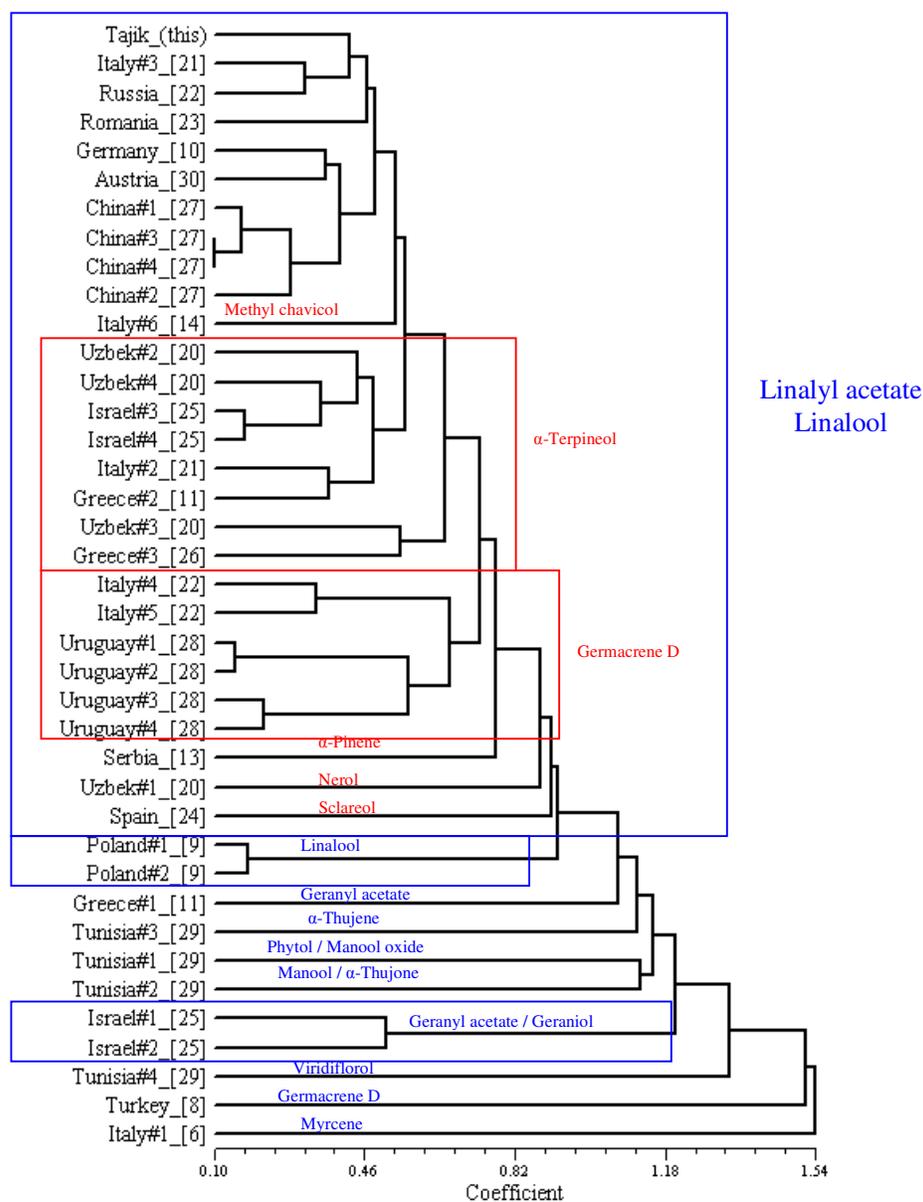


Figure 1. Dendrogram obtained by cluster analysis of the percentage composition of essential oils from *S. sclarea* samples, based on correlation and using the unweighted pair-group method with arithmetic average (UPGMA).

A total of 39 *Salvia sclarea* essential oil compositions from the published literature [6,8-11,13,14,20-30] were treated as operational taxonomic units (OTUs). The percentage composition of 35 principal essential oil components (linalyl acetate, linalool, α -terpineol, germacrene D, geranyl acetate, geraniol, (*E*)-caryophyllene, neryl acetate, α -thujene, sclareol, nerol, methyl chavicol, myrcene, caryophyllene oxide, geranial, phytol, (*E*)- β -ocimene, manool, α -copaene, manool oxide, limonene, bicyclogermacrene, viridiflorol, neral, α -thujone, (*Z*)- β -ocimene, camphor, spathulenol, δ -cadinene, α -

pinene, β -eudesmol, thymol, β -bourbonene, carvacrol, and linalyl formate) was used to determine the chemical relationship between the different *S. sclarea* essential oil samples by cluster analysis using the NTSYSpc software, version 2.2 [31]. Correlation was selected as a measure of similarity, and the unweighted pair-group method with arithmetic average (UPGMA) was used for cluster definition. The *S. sclarea* dendrogram is shown in Figure 1.

The chemical composition of Tajik *S. sclarea* essential oil is summarized in Table 1. A total of 59 compounds were identified representing 94.2% of the total composition. The oil was dominated by the monoterpenic ester linalyl acetate and the corresponding alcohol linalool. Other major components were α -terpineol and germacrene D. Commercial clary sage oil comes mainly from Russia, other former Soviet republics, the United States, China, France, and Bulgaria, and is composed largely of (–)-linalool (10-20%) and (–)-linalyl acetate (45-75%) [32]. Thus, for example, commercial Russian clary sage oil has been reported to contain 60% linalyl acetate and 21% linalool [10] while commercial Serbian clary sage oil had 53% linalyl acetate and 18% linalool [13].

In addition to the commercial grade clary sage oil, other chemotypes have been identified, including a geraniol/geranyl acetate-rich chemotype from Israel [25], a methyl chavicol-rich chemotype from Sardinia [14], a germacrene-D-rich chemotype from Sicily [33], and very recently, α -thujone, thujene, and manool oxide/phytol chemotypes from Tunisia [29]. The cluster analysis based on the principal clary sage essential oil components (Figure 1) reveals a large cluster with linalyl acetate and linalool predominating, with several subclusters based on concentrations of methyl chavicol, α -terpineol, germacrene D, α -pinene, nerol, and sclareol. In addition, there are chemotypes defined by high linalool, high geranyl acetate, high α -thujene, high phytol/manool oxide, high manool/ α -thujone, high geranyl acetate/geraniol, high viridiflorol, high germacrene D, and high myrcene concentrations (see Figure 1). Based on this current study, the clary sage oil from Tajikistan is rich in linalyl acetate and linalool, and compares favorably with commercial grade clary sage oil.

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