

GC and GC/MS Analysis of the Essential Oil of *Salvia hierosolymitana* Boiss. Growing Wild in Lebanon

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The essential oil of the aerial parts of *Salvia hierosolymitana* Boiss. (Lamiaceae), growing wild in Lebanon, was obtained by hydrodistillation and analysed by GC and GC-MS. Ninety-two compounds, representing 92.7% of the oil, were identified. The major components were hexadecanoic acid (15.5%), phytol (5.4%), hexahydrofarnesyl acetone (4.6%), (Z,Z)-9,12-octadecadienoic acid (4.5%) and 4-vinylguaiaicol (4.4%).

Keywords: *Salvia hierosolymitana*, essential oil, GC-MS, hexadecanoic acid, phytol, hexahydrofarnesyl acetone, (Z,Z)-9,12-octadecadienoic acid, 4-vinylguaiaicol.

Salvia hierosolymitana Boiss. is known as Jerusalem sage, with the Hebrew name *moriah* and with the Arabic name *Quwaysah al quds*, *Lisân al'ijlah* [1]; its leaves are eaten cooked and stuffed with rice. The plant blooms from April to June. Previously [2], we identified in this plant two new dammarane triterpenes, salvilymitone and salvilymitol, together with four known triterpenoids, ursolic, oleanolic, crataegolic, and 2- α -hydroxyursolic acids. Recently [3] *S. hierosolymitana* leaves were investigated for their topical anti-inflammatory properties and it was demonstrated that the chloroform extract shows a strong inhibition of the croton oil-induced ear oedema in mice, comparable to indomethacin. In this paper, as a continuation of our studies on the essential oils composition of *Salvia* spp. [4-8], we report for the first time the chemical composition of the essential oil of the aerial parts of *S. hierosolymitana*.

Ninety-two constituents, representing 92.7 % of the total oil, have been identified; their retention indices, percentage composition and identification methods

are given in Table 1, where the components are listed in order of elution from a HP 5MS column. The monoterpene fraction amounts to 17.0% of the oil and is characterized only by oxygen containing monoterpenes, amongst which the most abundant were α -thujone (2.9%), linalool (2.0%) and α -terpineol (1.5%). The sesquiterpene fraction (13.9%) was mainly composed of sesquiterpene hydrocarbons (9.5%) and among the nineteen compounds of this fraction only α -copaene (1.5%) and (*E*)- β -farnesene (1.2%) showed values higher than 1.0%. Spathulenol (1.4%) was the most abundant of the six oxygen containing sesquiterpene compounds. Noteworthy is the content of C-13 and C-18 terpenic ketones that amounted, respectively, to 7.6% and 5.3% of the oil. Among the C-13 ketones (*E*)- β -damascenone and β -ionone were present in nearly equal amounts (2.7% and 2.9%, respectively) while (*E*)-geranyl acetone was present in lower amount (1.2%). Hexahydrofarnesyl acetone (4.6%) was the main C-18 ketone. Noticeable also is the phytol content (5.4%). Other components of the oil were fatty acids (24.5%) and hydrocarbons (7.2%), which were the

most represented compounds, the former mostly represented by hexadecanoic acid (15.5%) and (Z,Z)-9,12-octadecadienoic acid (4.5%); 4-vinylguaiaicol was the unique phenolic compound determined.

Table 1: Essential oil composition of *Salvia hierosolymitana* Boiss. growing wild in Lebanon.

I ^a	I ^b	Component	Method ^c	% ^d
854	1231	2-Hexenal	I,MS	t
901	1238	(Z)-4-Heptenal	I,MS	0.2
963	1543	Benzaldehyde	I,Co-GC,MS	0.5
975	1312	1-Octen-3-one	I,MS	0.2
1002	1243	2-Pentylfuran	I,MS	0.2
1015	1507	(E,E)-2,4-Heptadienal	I,MS	0.1
1034	1213	1,8-Cineole	I,Co-GC,MS	0.6
1047	1482	cis-Linalool oxide (furanoid)	I,MS	0.9
1048	1663	Phenylacetaldehyde	I,Co-GC,MS	1.4
1055	1466	(E)-2-Octenal	I,MS	0.3
1058	1657	Acetophenone	I,Co-GC,MS	t
1065	1455	trans-Linalool oxide (furanoid)	I,MS	0.4
1092		1-Undecene	I,MS	0.1
1098	1553	Linalool	I,Co-GC,MS	2.0
1105	1430	α -Thujone	I,MS	2.9
1115	1451	β -Thujone	I,MS	0.8
1145	1532	Camphor	I,Co-GC,MS	0.7
1154	1572	(E,Z)-2,6-Nonadienal	I,MS	0.3
1176	1611	Terpinen-4-ol	I,Co-GC,MS	0.6
1179	1763	Naphthalene	I,Co-GC,MS	0.9
1184	1797	p-Methylacetophenone	I,MS	0.1
1189	1706	α -Terpineol	I,Co-GC,MS	1.5
1193	1648	Myrtenal	I,MS	0.9
1196	1804	Myrtenol	I,MS	0.3
1197		Safranal	I,MS	0.6
1206	1510	Decanal	I,MS	0.2
1208		α -Ionone	I,MS	0.5
1235	1857	Geraniol	I,MS	0.1
1237	1665	Pulegone	I,MS	1.7
1240	1656	Neral	I,MS	0.8
1259	1665	Linalyl acetate	I,Co-GC,MS	1.3
1278	2190	Nonanoic acid	I,Co-GC,MS	0.2
1290	2471	Indole	I,Co-GC,MS	1.0
1295	1658	Sabinyl acetate	I,MS	0.5
1312	2180	4-Vinylguaiaicol	I,MS	4.4
1343	1748	Piperitenone	I,MS	0.4
1363	1492	Cyclosativene	I,MS	0.3
1377	1497	α -Copaene	I,MS	1.5
1382	1838	(E)- β -Damascenone	I,MS	2.7
1385	1535	β -Bourbonene	I,MS	0.3
1411	1568	α -Cedrene	I,MS	0.5
1415	1612	β -Caryophyllene	I,MS	0.9
1426		Thujopsene	I,MS	t
1452	1673	(E)- β -Farnesene	I,MS	1.2
1454	1854	(E)-Geranyl acetone	I,MS	1.2
1455	1689	α -Humulene	I,MS	0.8
1463	1661	allo-Aromadendrene	I,MS	0.4
1478	1704	γ -Muuroleone	I,MS	0.6
1481	1743	β -Selinene	I,MS	0.5
1482	1957	β -Ionone	I,Co-GC,MS	2.9

Table 1 (Continued)

1485		Dihydroactinidiolide	I,MS	2.0
1495	1740	Valencene	I,MS	0.2
1498	1744	α -Selinene	I,MS	0.3
1515	1776	γ -Cadinene	I,MS	0.9
1520	1839	cis-Calamenene	I,MS	0.3
1526	1773	δ -Cadinene	I,MS	0.1
1541	1941	α -Calacorene	I,MS	t
1565	2057	Ledol	I,MS	0.5
1568	2467	Dodecanoic acid	I,Co-GC,MS	0.3
1578	2150	Spathulenol	I,MS	1.4
1580	1815	Tridecan-2-one	I,MS	t
1583		a Megastigmatrienone	MS	1.2
1588	2098	Globulol	I,MS	0.3
1592		1-Hexadecene	I,MS	0.3
1600	1600	Hexadecane	I,Co-GC,MS	0.1
1640	2187	T-Cadinol	I,MS	0.9
1642	2209	T-Muurolol	I,MS	0.8
1649	2255	α -Cadinol	I,MS	0.5
1672	2175	Tetradecanol	I,Co-GC,MS	0.2
1677	2256	Cadalene	I,MS	0.2
1694		Pentadecan-2-one	I,MS	0.5
1700	1700	Heptadecane	I,Co-GC,MS	0.4
1768	2672	Tetradecanoic acid	I,Co-GC,MS	1.8
1800	1800	Octadecane	I,Co-GC,MS	0.2
1835	2131	Hexahydrofarnesylacetone	I,MS	4.6
1873	2740	Pentadecanoic acid	I,MS	0.3
1900	1900	Nonadecane	I,Co-GC,MS	0.2
1918		(E,E)-Farnesyl acetone	I,MS	0.7
1950	2622	Phytol	I,MS	5.4
1957	2931	Hexadecanoic acid	I,Co-GC,MS	15.5
2099	3195	(Z,Z,Z)-9,12,15-Octadecatrienoic acid	I,Co-GC,MS	1.4
2100	2100	Heneicosane	I,Co-GC,MS	0.2
2104	3160	(Z,Z)-9,12-Octadecadienoic acid	I,Co-GC,MS	4.5
2120		(Z)-9-Octadecenoic acid	I,Co-GC,MS	0.5
2300	2300	Tricosane	I,Co-GC,MS	0.4
2400	2400	Tetracosane	I,Co-GC,MS	0.1
2500	2500	Pentacosane	I,MS	0.7
2600	2600	Hexacosane	I,MS	0.2
2700	2700	Heptacosane	I,MS	1.3
2800	2800	Octacosane	I,MS	0.2
2900	2900	Nonacosane	I,MS	1.1
3000		Triacotane	I,MS	0.2
3100		Entriacotane	I,MS	0.4
3200		Dotriacotane	I,MS	t
Total identified				92.7

^aHP-5 MS column; ^bHP Innowax; ^cI is the retention index, MS = mass spectrum, Co-GC = coinjection with authentic compound; ^d: t = trace, less than 0.05%.

The composition of the present oil differs from those of *S. multicaulis* Vahl. var. *simpliciflora* Boiss. [6] and *S. microstegia* Boiss. et Balansa [8], both collected in Lebanon. The former was characterized by a high content of sesquiterpene hydrocarbons (42.4%) and 10.1% of monoterpene hydrocarbons, while the latter showed a high content of oxygen

containing monoterpenes (30.6%) and a sesquiterpene fraction that is about twice that of the value of the present oil. Furthermore, both oils showed low contents of fatty acids (0.2% and 5.1%, respectively). This finding might be attributed to either environmental factors, such as light, nutrients and season [13,14] or to genetic differences [15,16].

Experimental

Plant material: Aerial parts of *S. hierosolymitana* Boiss were collected at the full flowering stage from plants growing wild on rocky soil in the Kadiska valley (North Lebanon) in June 2005. A voucher specimen (leg. & det. N. Arnold s. n., confirm. Th. Raus) was deposited in the Herbarium of the Botanischer Garten, Berlin Universität.

Essential oil isolation: The oil from air-dried and ground aerial parts of plants was isolated by hydrodistillation for 3 h, using a Clevenger-type apparatus according to the method recommended in the *European Pharmacopoeia* [9]. The oil was dried over anhydrous sodium sulphate and stored under N₂ at +4°C in the dark until tested and analysed. The sample yielded 0.12% of yellow oil (w/w), with a pleasant smell.

GC analysis: Analytical gas chromatography was carried out on a Perkin-Elmer Sigma 115 gas chromatograph fitted with a HP-5 MS capillary column (30 m x 0.25 mm i.d.; 0.25 µm film thickness). Helium was the carrier gas (1 mL min⁻¹). Column temperature was initially kept at 40°C for 5 min, then gradually increased to 250°C at 2°C min⁻¹, held for 15 min and finally raised to 270°C at 10°C min⁻¹. Diluted samples (1/100 v/v, in *n*-hexane) of

1 µL were injected manually at 250°C, and in the splitless mode. Flame ionization detection (FID) was performed at 280°C. Analysis was also run by using a fused silica HP Innowax polyethyleneglycol capillary column (50 m x 0.20 mm i.d.; 0.20 µm film thickness).

GC-MS analysis: GC-MS analysis was performed on an Agilent 6850 Ser. II apparatus, fitted with a fused silica HP-1 capillary column (30 m x 0.25 mm i.d.; 0.33 µm film thickness), coupled to an Agilent Mass Selective Detector MSD 5973; ionization voltage 70 eV; electron multiplier energy 2000 V. Gas chromatographic conditions were as reported above; transfer line temperature, 295°C.

Qualitative and quantitative analyses: Most constituents were identified by gas chromatography by comparison of their retention indices (*I*) with either those of the literature [10,11] or with those of authentic compounds available in our laboratories. The retention indices were determined in relation to a homologous series of *n*-alkanes (C₈-C₂₄) under the same operating conditions. Further identification was made by comparison of their mass spectra on both columns with either those stored in NIST 02 and Wiley 275 libraries or with mass spectra from the literature [10,12] and our home made library. Component relative concentrations were calculated based on GC peak areas without using correction factors.

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