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Chemical compositions of the essential oils of three *Salvia* species cultivated in Germany

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Abstract

The essential oils from three *Salvia* species from Heidelberg, Germany were analyzed by gas-liquid chromatography – mass spectrometry (GLC-MS). Intermedeol (57.4%), 1,8-cineole (15.5%), and linalyl acetate (36.3%) were found as the major components in the essential oils of *Salvia discolor*, *Salvia officinalis*, and *Salvia sclarea*, respectively. To our best knowledge, no previous works on the chemical composition of the essential oil of *S. discolor* have been reported.

Keywords: *Salvia discolor*, *Salvia officinalis*, *Salvia sclarea*, essential oil, chemotype.

1. Introduction

The genus *Salvia* is the largest genus in the Lamiaceae with over 900 species^[1, 2] and is widely distributed in the temperate, subtropical, and tropical regions all over the world^[3]. Around 400 *Salvia* species are used in traditional and modern medicine^[3]. Some of its representatives, e.g., *S. sclarea* L. and *S. officinalis* L., are commercially important sources of essential oils. The essential oils of *S. sclarea* and *S. officinalis* have been extensively investigated. However, no previous work on the chemical composition of the essential oil of *S. discolor* has been reported.

A previous study has revealed α -thujone, β -thujone, 1,8-cineole, camphor, α -humulene, linalool, germacrene D, viridiflorol, α -pinene, limonene, and borneol to be the major constituents of the essential oil of *S. officinalis*^[4]. Three chemotypes have been described for European *S. officinalis*^[3]: 1. α -pinene, camphor, β -thujone; 2. α -thujone, camphor, 1,8-cineole; and 3. β -thujone, camphor. Furthermore, three additional chemotypes have been described: A thujones-rich chemotype; a chemotype with intermediate concentrations of thujones, α -pinene, camphene, camphor and high borneol concentration; and a camphor, camphene, α -pinene-rich chemotype were grouped from populations growing in Montenegro^[5]. A cluster analysis of the compositions of 39 essential oils of *S. sclarea* from the published literature has shown that most of the essential oils belong to the chemotype rich in linalyl acetate and linalool^[6]. In addition, other chemotypes of *S. sclarea* such as geraniol/geranyl acetate-rich chemotype^[7], a methyl chavicol-rich chemotype^[8], a germacrene-D-rich chemotype^[9], and α -thujone, thujene, and manool oxide/phytol chemotypes^[10] have been identified.

In the present work, the essential oils from three *Salvia* species: *S. discolor* (Andean sage), *S. officinalis* (common sage) and *S. sclarea* (clary sage) which were cultivated in Heidelberg, Germany were analyzed by gas-liquid chromatography – mass spectrometry (GLC-MS).

2. Materials and Methods**2.1 Plant Material**

S. officinalis and *S. sclarea* were collected in July 2013, and *S. discolor* in October 2013, from an ornamental garden near Heidelberg, Germany. Fresh plant material was used for the investigation. The essential oils were obtained by hydrodistillation using a Clevenger-type apparatus.

2.2 Gas-liquid Chromatography – Mass Spectrometry (GLC-MS)

The essential oils of *Salvia* species were analyzed by GLC-MS using a Shimadzu GCMS-QP2010 Ultra operated in the EI mode [(electron energy = 70eV), scan range = 3.0 scans/sec], and GCMS solution software. The GC column was ZB-5 fused silica capillary column with a (5% phenyl)-polymethyl siloxane stationary phase a film thickness of 0.25 mm. The carrier

gas was helium with a column head pressure 80 psi and flow rate of 1.37 mL/min. Injector temperature was 250 °C and the ion source temperature was 200 °C. The GC oven temperature program was programmed for 50 °C initial temperature, increase in temperature rate 2 °C/min to 260 °C. A 5% w/v solution of the sample in CH₂Cl₂ was prepared and 0.1 µL was injected in splitting mode (30:1).

Identification of the oil components was based on their retention indices determined by reference to a homologous series of *n*-alkanes (Kovats RI), and by comparison of their mass spectral fragmentation patterns with those reported in the literature [11] and stored on the MS library (NIST 11, WILEY 10, FFNSC version 1.2). The percentages of each component are reported as raw percentages based on total ion current without standardization (set 100%).

3. Results and Discussion

Twenty-one components were identified representing 99.28% of the total *S. discolor* essential oil composition (Table 1, Fig. 1). The major components were intermedeol (57.37%), (*E*)-caryophyllene (17.81%), germacrene D (3.98%), α -humulene (3.11%) and linalool (3%). The eudesmenol sesquiterpenoid intermedeol has been found in small concentrations in the floral essential oil of *S. viridis* from Turkey [12]. To our knowledge, there have been no previous works on chemical compositions of the essential oil of *S. discolor*.

The chemical composition of the essential oil of *S. officinalis* from Germany was mainly dominated by oxygen-containing monoterpenoids (Table 1, Fig 2). 1,8-Cineole (15.52%),

camphor (13.49%), borneol (8.47%), α -humulene (8.21%), and α -thujone (8.05%), were found to be the major oil components. The *S. officinalis* oil composition from Germany is comparable to previous analyses from Iran [13] and Lithuania [14].

The results of the analysis of *S. sclarea* essential oil are presented in Table 1 and Figure 3. Thirty-six compounds were identified representing 99.72% of total *S. sclarea* essential oil composition. The oil was dominated by linalyl acetate (36.33%), linalool (23.47%), α -terpineol (8.12%) and sclareol (14.62%). It is very clear that the essential oil of *S. sclarea* growing in Germany belongs to the chemotype rich in linalyl acetate and linalool [6]. Sabinene, β -pinene, *p*-cymene, limonene, 1,8-cineole, linalool, and (*E*)-caryophyllene were found in all three *Salvia* species. In addition, γ -terpinene and α -humulene were found in both *S. discolor* and *S. officinalis* essential oils, and germacrene D, caryophyllene oxide were in both *S. discolor* and *S. sclarea* essential oils. The essential oils of *S. officinalis* and *S. sclarea* had 15 common components.

4. Conclusions

In conclusion, essential oils of *S. officinalis* and *S. sclarea* have more similarity to each other than *S. discolor* oil which is not surprising as *S. discolor* is a New World species whereas the former two are Old World species. *S. officinalis* cultivated in Germany is a α -thujone/camphor/1,8-cineole chemotype, cultivated *S. sclarea* is the linalyl acetate/linalool chemotype, and *S. discolor*, analyzed for the first time, is rich in intermedeol.

Table 1: Chemical compositions of the essential oils of three *Salvia* species

RI	Compound	Composition, %*		
		<i>S. discolor</i>	<i>S. officinalis</i>	<i>S. sclarea</i>
861	2-Methyloctane		0.07	
923	Tricyclene		0.20	
925	α -Thujene		0.18	
932	α -Pinene		4.27	0.21
933	Cyclofenchene	0.34		
949	Camphene		5.26	
972	Sabinene	0.24	0.82	0.17
978	β -Pinene	1.94	6.54	0.97
989	Myrcene		1.38	0.2
1017	α -Terpinene		0.15	
1024	<i>p</i> -Cymene	0.32	0.21	0.36
1029	Limonene	0.89	1.32	0.66
1032	1,8-Cineole	0.40	15.52	0.36
1035	(<i>Z</i>)- β -Ocimene		0.66	
1046	(<i>E</i>)- β -Ocimene		0.22	
1058	γ -Terpinene	0.26	0.41	
1070	<i>cis</i> -Linalool oxide (furanoid)			0.21
1070	<i>cis</i> -Sabinene hydrate		0.12	
1085	α -Terpinolene		0.23	
1086	<i>trans</i> -Linalool oxide (furanoid)			0.17
1099	Linalool	3.00	0.36	23.47
1101	<i>trans</i> -Sabinene hydrate		0.11	
1107	1-Octen-3-yl acetate	0.54		
1107	α -Thujone		8.05	
1118	β -Thujone		1.08	
1119	3-Octyl acetate	1.68		
1148	Camphor		13.49	0.19
1161	<i>trans</i> -Pinocamphone		0.37	
1169	3-Thujanol		0.14	
1171	δ -Terpineol		0.20	
1173	Borneol		8.47	
1176	<i>iso</i> -Pinocamphone		0.11	
1181	Terpinen-4-ol		0.23	

1187	(3Z)-Hexenyl butyrate			0.19
1195	α -Terpineol		0.47	8.12
1223	Nerol			0.76
1249	Linalyl acetate		0.17	36.33
1267	Geranial			0.31
1284	Bornyl acetate		2.31	
1331	Terpendiol			0.11
1346	α -Terpinyl acetate		0.48	
1358	Neryl acetate			1.05
1369	α -Ylangene		0.24	
1370	<i>iso</i> -Ledene		0.12	
1375	α -Copaene		0.36	0.28
1377	Geranyl acetate			2.30
1389	β -Elemene	0.36		
1400	α ,4-Dimethyl- γ -benzenebutanal			0.40
1407	α -Gurjunene		0.10	
1419	(<i>E</i>)-Caryophyllene	17.81	3.40	0.62
1426	Carvone hydrate			0.11
1427	β -Copaene		0.21	
1430	β -Gurjunene		0.34	
1438	Aromadendrene		2.86	
1446	Myrtayl-4(12)-ene		0.27	
1455	α -Humulene	3.11	8.21	
1460	<i>allo</i> -Aromadendrene		0.16	
1474	<i>trans</i> -Cadin-1(6),4-diene		0.81	
1479	α -Amorphene		0.07	
1480	Germacrene D	3.98		0.52
1487	Hydroxylinalool			0.17
1488	β -Selinene		0.21	
1490	Viridiflorene		1.23	
1494	α -Zingiberene	1.21		
1495	α -Selinene		0.13	
1498	α -Muurolene		0.16	
1507	β -Bisabolene	2.54		
1512	γ -Cadinene		0.31	
1518	δ -Cadinene		1.05	
1523	β -Sesquiphellandrene	0.55		
1541	α -Calacorene		0.10	
1547	α -Elemol	2.07		
1576	Spathulenol		0.25	0.18
1581	Caryophyllene oxide	0.30		1.11
1585	Globulol		0.14	
1594	Viridiflorol		4.15	0.78
1609	Humulene epoxide II		0.23	
1654	α -Eudesmol			1.22
1667	Intermedeol	57.37		
1702	δ -Dodecalactone			0.16
1782	Agarspirol acetate	0.37		
1884	Sclareol oxide			0.51
1949	Geranyl α -terpinene			0.17
1991	Manoyl oxide			0.12
2051	Manool		0.71	1.01
2057	<i>epi</i> -7-Manool			0.13
2214	Sclareol			14.62
Total identified		99.28	99.42	98.25

*total peak area = 100%

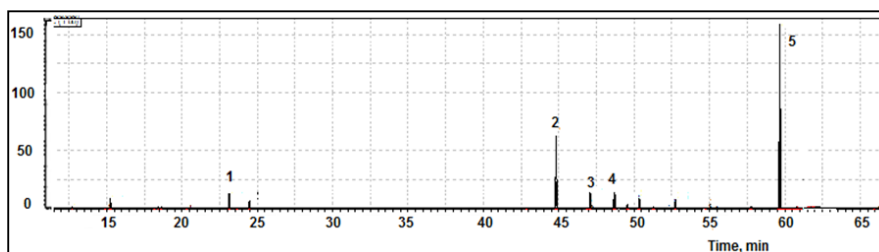


Fig 1: GLC-MS profile of the essential oil from *Salvia discolor*. 1 - linalool, 2 - *trans*-caryophyllene, 3 - α -humulene, 4 - germacrene D, 5 - intermedeol

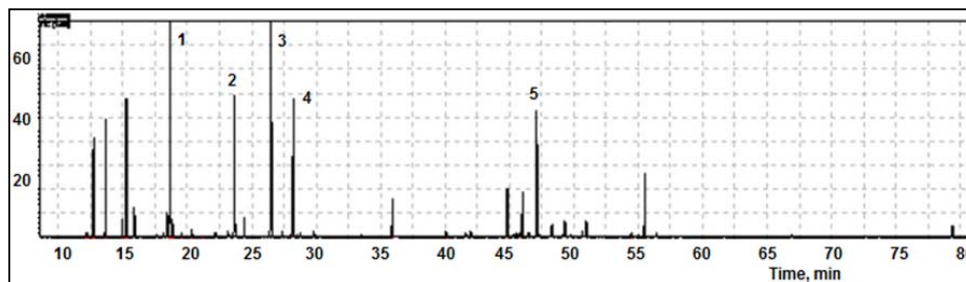


Fig 2: GLC-MS profile of the essential oil from *Salvia officinalis*. 1 - 1,8-cineol, 2 - α -thujone, 3 - camphor, 4 - borneol, 5 - α -humulene

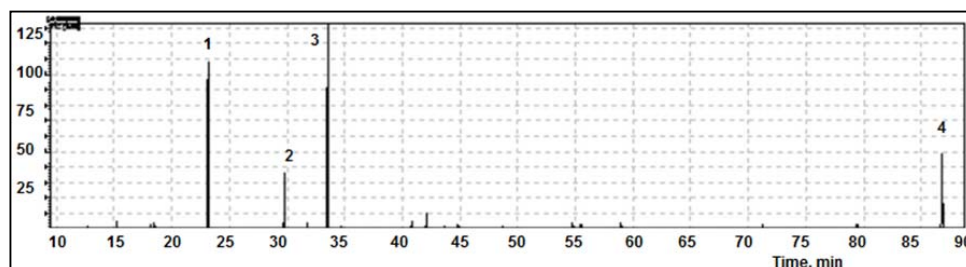


Fig 3: GLC-MS profile of the essential oil from *Salvia sclarea*. 1 - linalool, 2 - α -terpineol, 3 - linalyl acetate, 4 - sclareol.

5. Acknowledgements

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