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SHORT REPORTS

CONSTITUENTS OF THE ESSENTIAL OIL OF *SALVIA STENOPHYLLA*

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Key Word Index—*Salvia stenophylla;* Labiatae; essential oil; IR, ^{1}H and ^{13}C NMR, GC–MS analysis.

Abstract—The composition of the essential oil of *Salvia stenophylla* was investigated by GC–MS. The oil contains a high percentage of α-bisabolol and manool which are mainly responsible for its characteristic smell; in addition, 24 other components were identified.

INTRODUCTION

Salvia stenophylla Burch is an odorous herb widely distributed in the Orange Republic of South Africa, which belongs to the section *Heterosphace* (subgenus *Leonia*) of the genus. Chemically, many species of subgenera *Salvia* and *Sclarea* have had their essential oils analysed [1, 2], but the subgenus *Leonia* has not yet been investigated.

RESULTS AND DISCUSSION

In the present investigation, the essential oil from the plant was obtained by steam distillation of the dried leaf material. To simplify identification, the mono- and sesquiterpene hydrocarbons were separated from the oxygen-containing fraction by fractional distillation. The separate fractions were analysed by GC–MS. Identification was confirmed by comparison of R_t values and the MS of the pure compounds. Among the main components, (+)-α-bisabolol and manool were separated using preparative GLC and identified by IR, MS, ^{1}H and ^{13}C NMR. The results of the analysis of the essential oils are given in Table 1.

The volatile monoterpenes, especially α-phellandren, are present in high concentration (28% of total oil). The oxygenated monoterpenoids constitute 6% of the oil, and the sesquiterpene hydrocarbons 35.5%. Among the oxygenated sesquiterpenoids which constitute the bulk of the oil (46%), α-bisabolol (40, 98%) and manool (4%) are the most abundant. These compounds are mainly responsible for the wood and persistent odor of *Salvia stenophylla* Burch.

Compared with *Salvia sclarea* L., *S. officinalis* L., *S. lavandulaefolia* and *S. triloba* L. [1–3], *S. stenophylla* contains a very low amount of 1,8-cineole and camphor. α-Phellandrene which is the most abundant monoterpene is present as a trace compound in the other species. Like *S. lavandulaefolia*, *S. stenophylla* lacks α- and β-thujone which are the main components of *S. officinalis.* All four *Salvia* species contain the sesquiterpenes farnesene, humulene and caryophyllene. α-Bisabolol has never been identified before in essential oils of *Salvia* species. $\alpha(R)$- and (S)-sinensal are also unique constituents of *S. stenophylla.*

EXPERIMENTAL

Preparation of the essential oil. Salvia stenophylla Burch was collected in the High Weld of the Orange Republic of South Africa. The plant was identified at the Botanical Institute of the Univeristy of Witwatersrand, Transvaal.

Methodology. Steam distillation was carried out by Roland Essential Oils Ltd. in Fouriesburg on 100 kg of the whole plant during 11 hr without cohobation. Yield: 0.5–0.6%. Three fractions, bp 25–30°/0.45 mmHg, 60–90°/0.45 mmHg and 90–100°/0.30 mmHg, were obtained by distillation. The GLC analysis was carried out on a GC with FID detector. The most complete chromatograms were obtained on a 30 m × 0.5 mm i.d. Carbowax 20 M metal capillary (SCOT) column and a 50 m × 0.25 mm i.d. PPG (UCON) metal capillary (WCOT) column. GC–MS were obtained at 70 eV on a single focusing instrument (Hitachi-RMU-6L) equipped with a Bieman–Watson He-separator. Preparative. Separations for IR, ^{1}H and ^{13}C NMR were made on a Perkin–Elmer F21 instrument equipped with 2.7 m × 8 mm i.d. stainless steel columns packed with 5% carbowax 20 M or 5% SE30 on 60–80 mesh Chromosorb G. The ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ with a Bruker spectrometer operating in the FT mode.

(+)-*α-Bisabolol* [4]. MS *m/e*: 222 M^+ (6%), 207 (21), 205 (68), 204 (100), 189 (35), 161 (79), 148 (41), 139 (68), 135 (59), 134 (68), 133 (47), 127 (62), 122 (74), 121 (88),

Table 1. Constituents of the essential oil of *Salvia stenophylla*

Peak No.	Compound	% of total oil	Peak No.	Compound	% of total oil
1	α-Pinene	2.60	18	α-Humulene	2.12
2	Camphene	2.45	19	*trans*-β-Farnesene	
3	β-Pinene	0.38	20	β-Humulene	1.18
4	α-Phellandrene	14.90	21	α-Bisabolene	0.60
5	β-Myrcene	8.01	22	δ-Cadinene	0.24
6	α-Terpinene		23	β-Bisabolene	0.14
7	1,8-Cineole		24	Nerolidol (E)	1.94
8	Limonene	7.44	25	Oxygenated sesquiterpene	1.20
9	γ-Terpinene	0.41	26	(+)-α-Bisabolol	40.99
10	Monoterpene	1.43	27	Oxygenated sesquiterpene	0.81
11	Linalool	0.015	28	α-Sinensal (*R*)	0.39
12	Oxygenated monoterpene	0.41	29	α-Sinensal (*S*)	0.62
13	Camphor	2.96	30	Sesquiterpene alcool	1.12
14	Isoborneol				
15	Borneol	0.46	31	Manool	3.89
16	β-Caryophyllene	2.40		Total	99.00
17	Bergamotene				

119 (100), 109 (94), 95 (88), 93 (88), 91 (59), 69 (94), 55 (82), 43 (94), 41 (82). ^{1}H NMR (270 MHz): δ 1.13 (*s*, Me-1), 1.25 (*m*, CH$_2$-7), 1.5 (*t*, CH$_2$-2), 1.5 (*m*, CH-6), 1.62 (*s*, Me-5 *cis*), 1.65 (*s*, Me-5 *trans*), 1.69 (*s*, Me-9), 1.85 (*m*, CH$_2$-8), 1.85 (*m*, CH$_2$-11), 2.03 (*m*, CH$_2$-3), 5.13 (*m*, CH-4), 5.4 (*m*, CH-10). ^{13}C NMR (22.64 MHz): δ 17.63 (5-Me *cis*), 22.48 (C-11), 23.31 (9-Me), 23.95 (5-Me *trans*), 24.22 (C-3), 25.69 (1-Me), 26.28 (C-7), 31.28 (C-8), 39.68 (C-2), 43.62 (C-6), 74.16 (C-1), 121.11 (C-10), 124.99 (C-4), 131.2 (C-5), 133.52 (C-9).

Manool [5]. MS *m/e*: 272 M$^+$ (25.4%), 257 (45), 137 (100), 123 (39), 121 (38), 119 (30), 109 (50), 107 (46), 105 (30), 95 (80), 93 (69), 91 (35), 81 (98), 79 (50), 69 (82), 55 (67), 43 (60), 41 (76). ^{1}H NMR (400 MHz): δ 0.69 (*s*, Me-10), 0.81 (*s*, Me-19), 0.87 (*s*, Me-18), 1.0–1.87 (*m*, CH and CH$_2$), 1.27 (*s*, Me-16), 1.96 (*txd*, CH$_2$-6), 2.36 (*dxd*, CH-7), 2.37 (*dxd*, CH-7), 4.52 (*d*), 4.81 (*d*), (AX system, $J_{AX} = 1.5$ Hz, 2H-17), 5.04 (*dxd*), 5.19 (*dxd*), 5.9 (*dxd*), (AMX system, $J_{AX} = 17.5$, $J_{MX} = 11.0$, $J_{AM} = 1.0$ Hz, H-15, H-15, H-14). ^{13}C NMR (20.11 MHz): δ 14.37 (Me-20), 14.44 (CH$_2$-11), 17.74 (CH$_2$-2), 19.37 (Me-19), 21.65 (CH$_2$-6), 24.45 (C-16), 27.55 (C-4) and (Me-18), 29.59 (CH$_2$-7), 33.54 (CH$_2$-1), 38.37 (C-10), 39.13 (CH$_2$-12), 39.88 (CH$_2$-3), 41.53 (CH-5), 41.60 (CH-9), 42.26 (C-13), 106.49 (CH$_2$-17), 111.49 (CH$_2$-15), 145.45 (CH-14), 148.70 (CH$_2$-15).

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