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COMPOSITION OF *ELSHOLTZIA POLYSTACHYA* LEAF ESSENTIAL OIL

ATEEQUE AHMAD, MOHAMMAD S. SIDDIQUI and LAXMI N MISRA

Department of Phytochemistry, Central Institute of Medicinal and Aromatic Plants, Lucknow 226016, India

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Abstract—Fragrance components of the leaves of *Elsholtzia polystachya* have been investigated to afford nine monoterpene hydrocarbons, 11 oxygenated monoterpenes, 16 sesquiterpenes, two aliphatic esters, several sesquiterpene alcohols and a phenyl propanoid A chemical grouping of *Elsholtzia* species is discussed briefly.

INTRODUCTION

The genus *Elsholtzia* is an ornamental, usually aromatic herb or undershrub, distributed chiefly in Asia and a few in Africa and Europe [1] The essential oil of 13 species of *Elsholtzia* has been chemically investigated [2–18] *Elsholtzia polystachya* Benth syn. *E fruticosa* D. Don, a pubescent shrub of 3.5 m height, grows in the Himalayas from Kashmir to Sikkim and in Khasi hills at altitudes of 4000–9000 feet where it is often used as a fuel [1]. The essential oil of *E polystachya* has been the subject of a limited earlier investigation [18] A detailed GC-MS analysis of its essential oil is described in this paper.

RESULTS AND DISCUSSION

In our continued effort of searching new sources of aromatic products [19–21], we surveyed the Kumaon hills of Himalayas and collected the leaves of *E. polystachya*, which impart a strong odour reminiscent of Eucalyptus oil. After hydrodistillation it afforded a yellowish oil in 1 4% yield (dry basis). The oil was subjected to GC-MS analysis which showed the presence of 78 well-resolved constituents. Nine were monoterpene hydrocarbons (16.02%), 11 oxygenated monoterpenes (69.03%), 16 sesquiterpenes (6.67%), several sesquiterpene alcohols (2.16%), two aliphatic esters (0.75%), a phenyl propanoid (2.11%) and a few unidentified (see Table 1). The major constituents included 1,4-cineole (20 04%), 1,8-cineole (26 11%), perillaldehyde (7.24%), neryl acetate (10.12%), geranyl acetate (2 14%) and β-caryophyllene (2.56%) The GC-MS spectra indicated the presence of 16 sesquiterpene alcohols including four with $[M]^+$ at *m/z* 220 while the others possess an M^+ at *m/z* 222 Their total percentage has been given in Table 1 The total number of sesquiterpene hydrocarbons was 24 including eight unidentified (0.4%). The other unidentified constituents (15 in number) showed $[M]^+$ at *m/z* 136 and 150 amounting to *ca* 1 02% of the total oil. All constituents were identified by their R_t, Kovats index and MS fragmentation [22] but the chief components, i.e. 1,8-cineole and 1,4-cineole were further confirmed by isolation in pure form and recording their ^{1}H NMR spectra. The presence of five valuable oxygenated monoterpenes in high percentage (*ca* 68%) makes the oil strongly odorous. The oil also contains β-caryophyllene and cadinenes (3 59%) The desirable sesquiterpenes along with sesquiterpene alcohols (2.16%) makes the oil long lasting and thus more attractive.

The occurrence of 1,8-cineole as the major component has earlier been reported from the esssential oils of *Artemisia cina*, *Salvia triloba*, *Eucalyptus globulus*, *Cinnamomum camphora* and Italian laurel leaf oil The co-occurrence of 1,4-cineole with 1,8-cineole has been reported in the oil of *Elletaria cardamomum*, clary sage oil, lime oil and several other essential oils either in traces or in $<5\%$ of total oil. Therefore, it is worth mentioning that the essential oil of *Elsholtzia polystachya* is probably the first source in which 1,4-cineole is found in such a high percentage.

A survey of the literature showed that the essential oil of 13 species of *Elsholtzia* has been chemically investigated [2–18]. These studies suggested that *Elsholtzia* species can be divided into three groups with the following compounds as the main constituents: (i) oxygenated monoterpenoids (*E. pilosa* [6], *E. blanda* [8] and *E. strobilifera* [9, 10]), (ii) furano-monoterpenoids (*E ciliata* [3, 4], *E. densa* [5], *E. cristata* [11], *E. oldhami* [12, 13], *E. argyi* [2], *E. partrinii* [14, 15]) and (iii) phenylpropanoids (*E splendens* [7], *E. incisa* [16], and *E argyi* var. *nipponica* [17]). According to our investigation, the essential oil of *E polystachya* is comprised of monoterpenoids; therefore it may be included in the first category along with *E. strobilifera*, *E. blanda* and *E pilosa* Further work on other *Elsholtzia* species is desirable before chemosystematic conclusions can be drawn.

EXPERIMENTAL

The plant material was collected in the month of March 1983 from Kumaon region of Himalayas. The specimen voucher has been deposited in the herbarium of our institute. Three kg of plant material after hydro-distillation yielded 42 ml of essential oil, d^{35} 0 9461, n_D^{35} 1 4788, α_D^{28} −0 03°, acid value 5 43, ester value 28.54, ester value after acetylation 55.78. Pure 1,8-cineole and 1,4-cineole were obtained after column and preparative TLC on $AgNO_3$ impregnated silica gel, 80 MHz ^{1}H NMR spectra were

Table 1 Constituents of the essential oil of *E polystachya*

Peak No	Compound	Identified by	% of total oil
1	α-Thujene	a, b c	0 56
2	α-Pinene	a, b, c	1 03
3	Camphene	a, b, c	0 07
4	Sabinene	a, b, c	0 07
5	Myrcene	a, b, c	t
6	β-Pinene	a, b, c	2 87
7	δ-3-Carene	a, b, c	6 51
8	1,4-Cineole	a, b, c d	20 04
9	1,8-Cineole	a, b, c, d	26 11
10	cis-Ocimene	a, b, c	1 01
11	γ-Terpinene	a, b, c	3 90
12	Terpinen-4-ol	a, b, c	1 31
13	α-*p*-Dimethyl-styrene	b, c	2 11
14	Linalyl acetate	a, b, c	0 54
15	Perillaldehyde	a, b, c	7 24
16	Myrtenol (t ı)	b, c	0 51
17	Citronellyl acetate	a, b, c	0 38
18	α-Terpinyl acetate	a, b, c	0 41
19	Neryl acetate	a, b, c	10 12
20	Geranyl acetate	a, b, c	2 14
21	Irridomyrmecin (t ı)	b, c	0 23
22	7-Methyl-3-methylene-7-octen-1-yl propionate	b, c	0 65
23	3,7-Dimethyl-2,7-octadien-1 yl propionate	b, c	0 10
24	α-Longipinene (t ı)	b, c	0 10
25	α-Ylangene	b, c	0 10
26	β-Elemene	b, c	0 10
27	β-Farnesene	b, c	0 05
28	α-Gurjunene	b, c	0 38
29	β-Caryophyllene	b, c	2 56
30	Germacrene-D	b, c	0 35
31	α-Humulene	b, c	0 54
32	Santalene (t ı)	b, c	0 25
33	δ-Selinene	b, c	0 25
34	γ-Muurolene	b, c	0 62
35	γ-Bisabolene	b, c	0 20
36	α-Muurolene (t ı)	b, c	0 04
37	δ-Cadinene	b, c	0 38
38	Calamenene	b, c	0 10
39	γ-Cadinene	b, c	0 65
40	Sesqui, alcohols (M^+ 220)	c	0 21
41	Sesqui alcohols (M^+ 222)	c	1 95

t ı Tentative identification

t Trace (< 0 05%)

a co-injection with authentic material, b Kovats index and retention time, c mass fragmentation, d ^{1}H NMR spectrum

recorded on Varian FT 80 A instrument in $CDCl_3$ with TMS as internal reference GC-MS data was obtained with GC Varian model 3700 coupled with MS-Varian MAT model 711 (70 eV direct inlet) using 25 m Chromapack CP sil 5 capillary column programmed as initial temperature, 70° for 4 min then 10°/min to 330° and isothermal for 4 min with He as carrier gas The GC work was carried out with a Perkin-Elmer 3920B GC using a Carbowax 20 m packed column, initially at 60° for 4 min then 4°/min to 180 and isothermal for 16 min using H_2 as carrier gas The spectra of known compounds were compared with the library established by us and with the data available in the literature [22, 23] The identified constituents are listed in Table 1

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