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Chemical composition of the essential oil of *Plectranthus mollis* roots

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The hydro-distilled essential oil of the roots of *Plectranthus mollis* Spreng. (Lamiaceae) was examined for the first time to determine its composition. The oil was analyzed by gas chromatography equipped with a flame ionization detector (GC-FID) and gas chromatography coupled with mass spectrometry (GC/MS). Sixty constituents were identified, representing 98.4% of the total oil. The major constituents were γ-eudesmol (22.5%), bornyl acetate (14.9%), khusinol (11.4%), and *ar*-curcumene (6.8%). Oxygenated sesquiterpenes (46.4%), and oxygenated monoterpenes (25.1%) were the prominent groups of compounds, followed by sesquiterpene hydrocarbons (22.1%), monoterpene hydrocarbons (4.4%), and phenyl derivatives (0.4%) type constituents.

Keywords: *Plectranthus mollis* Spreng., Lamiaceae, essential oil composition, γ-eudesmol, GC-MS.

INTRODUCTION

The genus *Plectranthus* of the family Lamiaceae, containing about 300 species, is found in Tropical Africa, Asia and Australia [1]. *Plectranthus* is a large and widespread genus with a diversity of ethnobotanical uses. The roots of *Plectranthus mollis* (Syn. *Plectranthus incanus* Link.) are used to drive away evil spirits in India, Kenya and Tanzania [2, 3], while the leaves are consumed as a vegetable [4]. In traditional medicine *P. mollis* has been used against snakebites in India, Gabon and Kenya [3]. This plant is also used as a tonic [5], respiratory stimulant and vasoconstrictor, cardiac depressant, cure for haemorrhage [6], treatment of mental retardation [7] and rheumatism [8, 5].

P. mollis is reported to exhibit antimicrobial activity [9], relaxant activity on smooth and skeletal muscles [6]. It has cytotoxic and anti-tumour promoting activities, and can be used in the treatment of cancer [10]. The seeds of *P. mollis* are fried in mustard oil and then massaged all over the body as an insect repellant [3]. The compounds fenchone, α-humulene, piperitenone oxide, *cis*-piperitone oxide, and *E*-*β*-farnesene have been identified in the essential oil of *P. mollis* from South India [9], while fenchone, piperitone oxide, piperitenone, piperitenone oxide [11], *cis*-piperitone oxide and piperitenone oxide [12] have been reported from Northern India. Extensive review of literature revealed that the root oil of *P. mollis* has not been investigated. To the best of the author's knowledge, this is the first report on the essential oil composition of the roots of *P. mollis*.

EXPERIMENTAL

Plant material

The plant was collected in the month of March 2012 from district Belgaum (15º88'66" N - 74º52'35" E) Karnataka, India, at an elevation of 800 m. The plant was identified at the Regional Medical Research Centre, Belgaum (herbarium specimen No RMRC-535).

Isolation of essential oil

The roots (300 g) were chopped to small pieces and subjected to hydro-distillation (2000 mL distilled water + 300 g plant material, in a 3000 mL round-bottom flask) using a Clevenger type apparatus for 3 h [13]. The oil was trapped by adding n-hexane, dried over anhydrous Na_2SO_4, and kept in a sealed vial at -4°C until analysis. The yield of oil was 0.11%, w/w).

Analysis of essential oil

Analysis of the oil was achieved using Varian 450 gas chromatograph (GC) equipped with a fused silica CP-Sil 8 CB capillary column (30 m × 0.25 mm; 0.25 m film thickness) and flame ionization detector. The carrier gas was nitrogen at a flow rate of 1.0 mL/min. The initial oven temperature was 60°C which was increased to 220°C (ramp 3°C/min) and held for 5 min. The injector and detector temperatures were 230 and 240°C, respectively. The injection volume was 1.0 μL diluted in *n*-hexane. The sample was injected using a split ratio of 1:50. The gas chromatography/mass spectrometry (GC-MS) analysis of the oil was

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carried out on a Thermo Scientific Trace Ultra GC interfaced with a Thermo Scientific ITQ 1100 mass spectrometer fitted with TG-5 fused silica capillary column (30 m × 0.25 mm i.d., 0.25 μm film thickness) using the above oven temperature program. The carrier gas was helium at 1.0 mL/min. The injector temperature was 230°C, the injection volume 0.1 μL prepared in *n*-hexane. The sample was injected using a split ratio of 1:50. MS were taken at 70 eV over the mass scan range of 40-450 amu. All parameters of GC and GC/MS applied for analysis of the oil were those literatures reported earlier [14-19].

Identification of the compounds

Identification of constituents was done on the basis of the retention index (RI) determined with reference to homologous series of *n*-alkanes C_8-C_{25}, under identical experimental conditions, MS library search (NIST 08 MS Library (Version 2.0 f; Thermo Fisher Scientific, Austria) and WILEY MS 9th Edition (Thermo Fisher Scientific, Austria), and by comparing with MS literature data [20] and co-injection of authentic samples purchased from Sigma-Aldrich, India. The relative amounts of individual components were calculated based on the GC peak area (FID response) without using a correction factor.

RESULTS AND DISCUSSION

Sixty compounds were characterized and identified according to their mass spectra and their relative retention indices determined on a non-polar stationary phase capillary column, comprising 98.4% of the total oil constituents. The identified compounds are listed in Table 1 in elution order from the TG-5 column, along with the percentage composition of each component and its retention index.

Table 1. Chemical composition of the essential oil of *P. mollis* roots

Compound	RI	%	Identification
Tricyclene	901	0.1	RI, MS
α-Pinene	908	0.4	RI, MS, CI
α-Fenchene	919	0.7	RI, MS
Sabinene	927	0.9	RI, MS
β-Pinene	941	0.9	RI, MS
Myrcene	950	0.1	RI, MS
α-Terpinene	974	0.6	RI, MS
o-Cymene	981	0.3	RI, MS
Limonene	985	0.2	RI, MS
1,8-Cineole	988	0.1	RI, MS,CI
(*Z*)-*β*-Ocimene	992	t	RI, MS
(*E*)-*β*-Ocimene	1003	t	RI, MS
Bergamal	1009	t	RI, MS
γ-Terpinene	1014	0.1	RI, MS
Fenchone	1046	1.2	RI, MS
endo-Fenchol	1073	0.2	RI, MS
trans-Sabinol	1102	1.0	RI, MS
Camphor	1108	0.7	RI, MS, CI
Borneol	1132	1.5	RI, MS
Terpin-4-ol	1146	0.2	RI, MS, CI
α-Terpineol	1162	0.2	RI, MS, CI
Myrtenal	1169	t	RI, MS
endo-Fenchyl acetate	1196	5.1	RI, MS
Neo-iso-dihydro carveol	1206	0.1	RI, MS
Bornyl acetate	1277	14.9	RI, MS
α-Longipinene	1352	0.2	RI, MS
Cyclosativene	1373	0.5	RI, MS
α-Copaene	1384	0.7	RI, MS
β-Patchoulene	1391	0.4	RI, MS
β-Cubebene	1401	0.8	RI, MS
Longifolene	1424	0.5	RI, MS
cis-*α*-Bergamotene	1431	0.9	RI, MS
β-Caryophyllene	1436	0.6	RI, MS, CI
trans-*α*-Bergamotene	1449	0.4	RI, MS
(*E*)-*β*-Farnesene	1479	0.4	RI, MS
β-Acoradiene	1491	0.7	RI, MS
β-Chamigrene	1499	2.9	RI, MS
ar-Curcumene	1510	6.8	RI, MS
α-Zingiberene	1525	0.9	RI, MS
Cuparene	1536	4.7	RI, MS
β-Bisabolene	1540	0.2	RI, MS
γ-Cadinene	1546	0.3	RI, MS
cis-Calamenene	1557	t	RI, MS
Kessane	1528	t	RI, MS
Liguloxide	1565	t	RI, MS
α-Cadinene	1573	0.2	RI, MS
trans-Sesquisabinene hydrate	1620	1.2	RI, MS
β-Copaen-4-*α*-ol	1629	0.5	RI, MS
Khusimone	1637	1.7	RI, MS
10-*epi*-*γ*-Eudesmol	1658	2.1	RI, MS
γ-Eudesmol	1688	22.5	RI, MS
α-Eudesmol	1698	3.1	RI, MS
Khusinol	1722	11.4	RI, MS
(*Z*)-*α*-Santalol	1729	0.4	RI, MS
α-Bisabolol	1734	1.8	RI, MS
(*Z*)-*α*-*trans*-Bergamotol	1748	0.2	RI, MS
Cedroxyde	1758	0.7	RI, MS
(*Z*)-*α*-Atlantone	1767	0.3	RI, MS
14-oxy-*α*-Muurolene	1815	0.5	RI, MS
2-hexyl-(*Z*)-Cinnamaldehyde	1825	0.4	RI, MS
Monoterpene hydrocarbons		4.4	
Oxygenated monoterpenes		25.1	
Sesquiterpene hydrocarbons		22.1	
Oxygenated sesquiterpenes		46.4	
Phenyl derivatives		0.4	
Total identified		98.4	

RI=Retention index relative to C_8-C_{25}*n*-alkanes on TG-5 column, MS=NIST and Wiley library and the literature, CI=Co-injection of authentic samples, t=trace (<0.1%).

The main constituents were identified as *γ*-eudesmol (22.5%), bornyl acetate (14.9%), khusinol (11.4%), *ar*-curcumene (6.8%). The oil was rich in oxygenated sesquiterpenes (46.4%), followed by oxygenated monoterpenes (25.1%), sesquiterpene hydrocarbons (22.1%), monoterpene hydrocarbons (4.4%), and phenyl derivatives (0.4%). This is the first report on the chemical composition of the essential oil of roots of *P. mollis*. Further studies are required to investigate biological activities of roots essential oil of this plant.

It is interesting that constituents identified in the essential oil of the roots of *P. mollis* were found somehow contrary to those in the aerial parts [9, 11, 12] oil. Myrcene, limonene, fenchone, camphor, borneol, terpin-4-ol, *α*-terpineol, *β*-cubebene, *β*-caryophyllene, trans *α*-bergamotene and (*E*)-*β*-farnesene were detected as common constituents in roots and aerial parts [9] oils. The overall quantitative contribution of these common compounds in roots and aerial parts [9] was found to be 6.3% and 50.3%, respectively. Moreover, the quantity of the compound fenchone was reported to be 32.3% in the aerial parts [9] oil, while 1.2% in the roots oil. Furthermore, the major compounds *α*-humulene, piperitenone oxide, and *cis*-piperitone oxide which were reported in significant quantities in the aerial parts oil of *P. mollis* [9, 11, 12] could not be detected even in trace amounts in the roots oil. In addition, the aerial parts oil was reported to be rich in oxygenated monoterpenes type constituents [9, 11, 12], while in this report the roots oil was found to be affluent oxygenated sesquiterpenes type constituents.

The composition of the essential oil often varies between different plant parts [21]. It is noteworthy that the complex composition of essential oils in the same plant parts can differ. The formation of essential oils depends on the tissue differentiation (secretory cells, excretion cavities, etc.) and on the ontogenetic phase of the respective plant [22]. Individual plants also showed variation in the percentage of chemical components depending on the part of the plant from which the oil was extracted [23]. The secondary volatile metabolites from different parts of the same plant virtually showed quantitative differences of compounds reported in the essential oil composition from aerial parts and flowers [24-26] but derived different chemotypes from the roots of same plant [27-29]. Nevertheless, there is an almost uncountable number of single substances and a tremendous variation is observed in the composition of essential oils of aromatic plants.

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ХИМИЧЕН СЪСТАВ НА ЕТЕРИЧНО МАСЛО ОТ КОРЕНИ НА *PLECTRANTHUS MOLLIS*

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(Резюме)

Изследвано е етерично масло, получено от корените на *Plectranthus mollis* Spreng. (Lamiaceae), получено чрез дестилация с водна пара. За първи път е установен химичният му състав. Маслото е анализирано чрез газ-хроматография с FID-детектор, съчетана с мас-спектрометрия (GC/MS). Идентифицирани са 60 компоненти, представляващи 98.4% от цялото масло. Главните съставки са *γ*-евдесмол (22.5%), борнил-ацетат (14.9%), хусинол (11.4%) и *ar*-куркумен (6.8%). Окислените сески-терпени (46.4%) и окислените монотерпени (25.1%) са главната група от съединенията, следвани от сески-терпенови въглеводороди (22.1%), монотерпенови въглеводороди (4.4%) и фенилови производни (0.4%).