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GC-FID and GC-MS analysis of the sesquiterpene rich essential oil of *Nepeta govaniana* (Wall. ex Benth.) Benth. from Jammu and Kashmir.

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Abstract: The chemical profile of the hydrodistilled essential oil obtained from the aerial parts of *N. govaniana* growing in Jammu and Kashmir (India) is reported in the current study. Capillary GC-FID and GC-MS analysis led to the identification of 17 components accounting for 87.3% of the total oil composition. The oil contains a high percentage of sesquiterpene hydrocarbons (80.5%) followed by oxygenated sesquiterpenes (6.4%). Pregeijerene (56.9%), germacrene D (9.4%) and β -caryophyllene (6.1%) were the principal components of sesquiterpene hydrocarbons. No nepetalactone isomers were identified in the essential oil.

Keywords: Nepeta govaniana, essential oil, GC-FID, GC-MS, Pregeijerene, germacrene D, β-caryophyllene.

1. INTRODUCTION

The genus *Nepeta*, also called catmint, is a multiregional genus of the family Lamiaceae consisting of about 250 species distributed in central and southern parts of Europe, Asia and Middle East. In India about 30 species are found, mostly distributed in temperate Himalayas and few on foothills and plains (1-3). Several species of *Nepeta* are used as laxative to treat dysentery, kidney and liver diseases and tooth troubles (4). They are also used as antispasmodic, expectorant, diuretic, antiseptic, antiasthmatic and febrifuge (5-7). Some species are also used to reduce serum lipids and have anti-inflammatory effects (8,9).

Various biologically active iridoids present in several *Nepeta* species possess diverse biological activities like feline attractant, canine attractant and insect repellant (10,11). *Nepeta govaniana* commonly known as yellow catmint is a tall, erect aromatic and sticky perennial herb with pale-yellow tubular flowers throughout summer. The leaves have a sweet aromatic fragrance when crushed. It grows upto 2-4 feet with stem sturdy, 4-angled, very finely velvety or hairy leafs. It is found in the Himalayas from Pakistan to Uttarakhand; at altitudes of 2400-3300 m. Literature survey reveals that *N. govaniana* has been the focus of earlier studies especially with respect to its essential

oil from the aerial parts (12). However, there are no reports on the essential oil composition of N. *govaniana* from the high Himalayas of Jammu and Kashmir. As part of the Institute's programme to screen the rich aromatic flora of the region for new essential oils and aroma chemicals, the objective behind the current study was to characterize the chemical constituents of the essential oil of N. *govaniana* growing in Jammu and Kashmir (India) using a combination of capillary GC-FID and GC-MS analytical techniques.

2. EXPERIMENTAL

2.1. Plant Material

The plant material of *Nepeta govaniana* was collected from Gulmarg region of Kashmir valley during July 2010 and identified in the department of plant taxonomy, University of Kashmir, Srinagar (India). A voucher specimen has been deposited in the herbarium of the department (voucher No. KASH-2729).

2.2. Isolation of Essential oil

The fresh plant material was finely chopped and then subjected to hydro-distillation using Clevenger-type apparatus for 3 hours. The oil yield was found to be 0.2% calculated on fresh weight basis. The oil was dried over anhydrous Na_2SO_4 and stored at $4^{\circ}C$ in a sealed vial prior to analysis.

2.3. Gas Chromatography (GC-FID)

Gas chromatography was carried out on Perkin Elmer auto system XL Gas Chromatograph 8500 series equipped with flame ionization detector (FID) and head space analyzer using a fused silica capillary RTX-5 column ($30m \times 0.32 mm$, film thickness 0.25μ m) coated with dimethyl polysiloxane. Oven temperature was programmed from 60 to $230 \,^{0}$ C, with injector temperature $230 \,^{0}$ C and detector temperat ure $250 \,^{0}$ C. Injection volume 0.9μ l, nitrogen was used as a carrier gas ($1.0 \,$ ml/min).

2.4. Gas Chromatography-Mass Spectrometry (GC-MS)

GC-MS analysis was carried on a Varian Gas Chromat ograph series 3800 fitted with a VF-5 ms fused silica c apillary column ($60m \ge 0.25mm$, film thickness 0.25μ

m) coupled with a 4000 series mass detector under the following conditions: injection volume 1 μ l with split r atio 60, helium as carrier gas at 1 ml/min constant flow mode, injector temperature 230 °C, oven temperature 40 °C to 250 °C at 3 °C/min. The MS operating parame ters were as follows: electron impact (EI+) mode, 70 e v and ion source temperature 250 °C. Mass spectra wer e recorded over 50-500 a.m.u range.

2.5. Identification of components

Identification of the essential oil constituents was based on Retention Index (RI, determined with respect to homologous series of n-alkanes (C_9 - C_{24} , Polyscience Corp., Niles IL) under the same experimental conditions), co-injection with standards (Sigma Aldrich and standard isolates), MS Library search (NIST 98 and WILEY), by comparing with the MS literature data [13,14]. The percentage composition of the individual components was computed from the GC-FID peak areas without using correction factors.

3. RESULTS AND DISCUSSION

The chemical constituents of the essential oil were analyzed by capillary GC-FID and GC-MS. The various essential oil components of N. govaniana are listed in Table-1, with their percentage and relative retention indices (RRI). The average oil yield was 0.2% calculated on fresh weight basis of the plant material. GC-FID and GC-MS analysis led to the identification of 17 components accounting for 87.3% of the total oil composition. The total ion (TIC) chromatogram of the essential oil is shown in figure 1, the chemical structures and their corresponding mass spectra are shown in figures 2-7. The oil contains a high percentage of sesquiterpene hydrocarbons constituting 80.5% followed by oxygenated sesquiterpenes constituting 6.4% of the total oil composition. Pregeijerene (56.9%), germacrene D (9.4%), β -caryophyllene (6.1%) and β -bourbonene (3.6%) were the principal components of the sesquiterpene hydrocarbons. Torreyol (5.1%) was the main component of oxygenated sesquiterpenes. Some minor components were elemol, germacrene-D-4-ol, αcadinol and α -eudesmol.

Compound	Peak Area %	RRI
β-Pinene	0.1	974
1,8-Cineole	0.5	1026
γ-Terpinene	0.1	1058
Geranyl acetate	0.2	1356
β-Bourbonene	3.6	1383
β-Caryophyllene	6.1	1418
α-Farnesene	0.2	1451
Germacrene-D	9.4	1484
α-Muurolene	3.6	1497
γ-Cadinene	0.1	1515
δ-Cadinene	0.1	1527
Elemol	0.3	1552
Germacrene-D-4-ol	0.4	1578
Pregeijerene	56.9	1628
Torreyol	5.1	1641
α-Eudesmol	0.3	1653
α-Cadinol	0.3	1660
Monoterpene hydrocarbons	0.2	
Oxygenated monoterpenes	0.2	
Sesquiterpene hydrocarbons	80.5	
Oxygenated sesquiterpenes	6.4	
Total	87.3	

Table 1: Chemical constituents of the essential oil from the aerial parts of *N. govaniana*.





Figure 1: GC-MS Total ion chromatogram (TIC) of the essential oil of *Nepeta govaniana* growing in the Kashmir Himalayas showing three major chemical constituents of the essential oil.



Figure 2:- Structure and mass spectrum of Pregeijerene.



Figure 3:- Structure and mass spectrum of β-caryophyllene.



Figure 4:- Structure and mass spectrum of β-bourbonene.



Figure 5:- Structure and mass spectrum of germacrene D.



Figure 6:- Structure and mass spectrum of α-muurolene.



Figure 7:-Structure and mass spectrum of Torreyol.

No nepetalactone isomers were identified in the essential oil of *N. govaniana* which have been reported in several *Nepeta* species like *N. santenisii* Bornm. (15), *N. racemosa* (16), *N. crassifolia* (5), *N. cephalotes*, *N. denudata* (17) and *N. nuda* (18,19). These nepetalactone isomers have been labeled as the biochemical markers for the *Nepeta* essential oils and are very useful in chemotaxonomic studies. Literature survey reveals that the essential oil of *N. govaniana* has been the focus of earlier studies which have revealed the presence of 4a α , 7 α , 7 α -nepetalactone, β -elemene, germacrene D, allo-aromadendrene and α -

pinene as the major constituents from the aerial parts of *N. govaniana* growing in Western Himalayan region of Himachal Pradesh, India (12). In yet another study from the Himalayan region of Uttarakhand, the essential oil from the flowering aerial parts of *N. govaniana* have been reported to contain two major constituents viz. isoiridomyrmecin (35.2%) and pregeijerene (20.75%). The research article also reported the antifungal activity of the essential oil of *N. govaniana* against *Candida albicans* and *Trichophyton rubrum* (20). On comparative analysis of the present study with the previous reports, it is obvious that our results are comparable to those of Bisht *et al* who also reported pregeijerene as a major constituent of the essential oil of *N. govaniana*. Our results differ to those of Thappa *at al* who reported $4a\alpha$, 7α , $7a\alpha$ -nepetalactone, β -elemene, germacrene D, allo-aromadendrene and α -pinene as the major essential oil constituents from the aerial parts of *N. govaniana*. These compositional differences in the essential oils of the same plant species from different geographical regions can be attributed to different

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environmental and geographical conditions such as temperature, humidity, altitude etc.

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