Research Article

Chemical Composition of the Essential oil of *Chromolaena odorata* (L.) R. M. King & H. Rob. Roots from India

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The hydrodistilled essential oil of the roots of *Chromolaena odorata* (L.) R. M. King & H. Rob. was analysed by gas chromatography equipped with flame ionization detector (GC-FID) and gas chromatography coupled with mass spectrometry (GC/MS). A total of twenty-nine compounds have been identified, accounting 97.6% of the total oil. The main constituents were himachalol (24.2%), 7-isopropyl-1,4-dimethyl-2-azulenol (17.6%), androencecalinol (14.1%), and 2-methoxy-6-(1-methoxy-2-propenyl) naphthalene (5.6%). The essential oil consists mainly of phenyl derivatives (41.6%), followed by oxygenated sesquiterpenes ((26.6%), long-chain hydrocarbons (18.9%), sesquiterpene hydrocarbons (6.8%), oxygenated monoterpenes (2.8%), and monoterpene hydrocarbons (0.9%). This study revealed that the roots of *C. odorata* produced different chemotypes other than leaves oil. This is the first report on the essential oil composition of the roots of *C. odorata*.

1. Introduction

Chromolaena odorata (L.) R. M. King & H. Rob. (Syn: *Eupatorium odoratum* L.) (Asteraceae) is a perennial herb and distributed throughout India, tropical Asia, and Mexico [1, 2]. In traditional medicine this plant is used in the treatment of coughs, colds, and skin diseases [3], wound healing, and as a local antiseptic agent [4]. *C. odorata* is a medicinal plant having diverse pharmacological properties, namely, anti-inflammatory [5, 6], antimicrobial [7, 8], antigonorrhoeal [9], antipyretic, antispasmodic [6], diuretic [10], analgesic [11], and wound healing [12] activities. The chemical compositions of the essential oils of *C. odorata* that have been reported from different countries [13–20] are summarized in Table 1. The essential oil constituents of the leaves of *C. odorata* from Benin reported as α -pinene, pregeijerene, geijerene, β -pinene, and germacrene D [13] as the major compounds. In a report from Cameroon and Congo, α -pinene and p-cymene [14], while, from India, pregeijerene, epi-cubebol, cubebol, cis-sabinene hydrate, 10-epi- γ -eudesmol, germacrene-D-4-ol, δ -cadinene, germacrene D, geijerene, cyperene, 10-epi- γ -eudesmol, α -muurolol and khusimone [15] have been

identified as the major constituents. The major compounds such as α -pinene, geijerene, and pregeijerene from Ivory Coast [16, 17] and α -pinene, β -pinene, germacrene D, β -copaen-4 α -ol, β -caryophyllene, geijerene, pregeijerene [18], α -pinene, cadinene, camphor, limonene, β -caryophyllene and cadinol isomer [8] from Nigeria have been identified. In another report from Thailand, pregeijerene, germacrene D, α -pinene, β -caryophyllene, vestitenone, β -pinene, δ -cadinene, geijerene, bulnesol, and trans-ocimene [19] have been reported as the major constituents. Review of literature revealed that the essential oil composition of the roots of *C. odorata* has not been examined. Thus the aim of this work is to present the volatile constituents from the roots of *C. odorata*. To the best of the author's knowledge, this is the first report on the essential oil composition of the roots of *C. odorata*.

2. Experimental

2.1. Plant Material. The roots of *C. odorata* were collected in June 2011, at a height of 800 m from the district Belgaum (N 15.88668; E 74.52353), Karnataka, India. The plant was identified by Dr. Harsha Hegde, Research Scientist, Regional

TABLE 1: Chemical composition of the essential oil of *C. odorata* from various countries.

Country name	Major constituents from essential oil of <i>C. odorata</i>
Benin	α -pinene, pregeijerene, geijerene, β -pinene, and germacrene-D [13]
Cameroon and Congo	α -Pinene and p-cymene [14]
India	Pregeijerene, epi-cubebol, cubebol, cis-sabinene hydrate, 10-epi- γ -eudesmol, germacrene-D-4-ol, δ -cadinene, germacrene D, geijerene, cyperene, 10-epi- γ -eudesmol, α -muurolol, and khusimone [15]
Ivory Coast	α -pinene, geijerene, and pregeijerene [16, 17]
Nigeria	α -pinene, β -pinene, germacrene D, β -copaen-4 α -ol, β -caryophyllene, geijerene and pregeijerene [18], α -pinene, cadinene, camphor, limonene, β -caryophyllene, and cadinol isomer [8]
Thailand	pregeijerene, germacrene D, α -pinene, β -caryophyllene, vestitenone, β -pinene, δ -cadinene, geijerene, bulnesol, and trans-ocimene [19]

Medical Research Centre (ICMR), Belgaum (voucher specimen no. RMRC-410).

2.2. Isolation of Essential Oil. The fresh plant material (250 g) was chopped in small pieces and subjected to hydrodistillation using Clevenger-type apparatus for 3 h. The oil was collected and dried over anhydrous sodium sulfate and stored in sealed vials at -4°C until analysis. The oil yield was 0.3% v/w.

2.3. Gas Chromatography. The GC analysis of the oil was carried out on Varian 450 gas chromatograph equipped with FID, using stationary phase CP Sil-8-CB (30 m $\times$ 0.25 mm i.d., 0.25 μm film thickness) column under the experimental conditions reported earlier [20]. Nitrogen was a carrier gas at 1.0 mL/min flow rate. Temperature programming was set to 60–220 $^{\circ}\text{C}$ at 3 $^{\circ}\text{C}/\text{min}$ and the injector and detector temperatures were 230 and 250 $^{\circ}\text{C}$, respectively. The injection volume was 1.0 mL of 1% solution diluted in n-hexane; split ratio was 1 : 50.

2.4. Gas Chromatography-Mass Spectrometry. The GC-MS analysis of the oil was carried out on Thermo Scientific Trace Ultra GC (Thermo Fisher Scientific Austria, Vienna, Austria) interfaced with a Thermo Scientific ITQ 1100 Mass Spectrometer (Thermo Fisher Scientific Austria) fitted with TG-5 (30 m $\times$ 0.25 mm i.d., 0.25 μm film thickness) column. The oven temperature was programmed from 60 to 220 $^{\circ}\text{C}$ at 3 $^{\circ}\text{C}/\text{min}$ using helium as a carrier gas at 1.0 mL/min. The injector temperature was 230 $^{\circ}\text{C}$, injection volume was 0.1 mL of 1% solution prepared in n-hexane; split ratio was 1 : 50. MS were taken at 70 eV with mass scan range of 40–450 amu.

2.5. Identification of the Components. Identification of the constituents was done on the basis of 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 the MS literature data [21]. The relative amounts of individual components

were calculated based on the GC peak area (FID response) without using a correction factor.

3. Results and Discussion

Twenty-nine compounds were characterized and identified by GC-MS, comprising 97.6% of the total oil. The identified compounds are listed in Table 1 in elution order from the TG-5 MS column, along with the percentage composition of each component and its retention index. The main constituents were himachalol (24.2%), 7-isopropyl-1,4-dimethyl-2-azulenol (17.6%), androencecalinol (14.1%), and 2-methoxy-6-(1-methoxy-2-propenyl) naphthalene (5.6%). The essential oil consists mainly of 5 phenyl derivatives (41.6%), followed by 5 oxygenated sesquiterpenes (26.6%), 6 long-chain hydrocarbons (18.9%), 6 sesquiterpene hydrocarbons (6.8%), 4 oxygenated monoterpenes (2.8%), and 3 monoterpene hydrocarbons (0.9%). It is interesting that constituents identified in the essential oil of the roots of *C. odorata* were found contrary (see Table 2). The signature compounds from the leaves oil of this plant reported from different countries were almost the same with quantitative differences. The major constituents, pregeijerene, epi-cubebol, cubebol, cis-sabinene hydrate, germacrene-D-4-ol, germacrene D, geijerene, cyperene, α -muurolol, khusimone, β -copaen-4 α -ol, camphor, limonene, vestitenone, bulnesol, and trans-ocimene (Table 1) were reported from the leaves oil of *C. odorata*, which could not identified even in trace amount from the roots oil of this plant. Moreover, the majority of the oil composition from other plant parts, namely, aerial parts and flowers of *C. odorata* were dominated by monoterpene and sesquiterpene hydrocarbons [13–20]. In this report, it is found that long-chain hydrocarbons and high contents of phenyl derivative compounds are present. The composition of the essential oil often changes between different plant parts [22]. The difference in the complex composition of essential oils of one kind may sometimes be difficult to assign to specific chemotypes. The formation of essential oils depends on the tissue differentiation (secretory cells and excretion cavities, etc.) and on ontogenetic phase of the respective plant [23]. The conclusion of this study revealed that the roots of *C. odorata* produced

TABLE 2: Chemical composition of the essential oil of the roots of *C. odorata*.

Compound	RI	%	Identification
α -Pinene	908	0.2	RI, MS
Camphene	920	0.4	RI, MS
β -Pinene	941	0.3	RI, MS
n-Decane	957	1.1	RI, MS
<i>trans</i> -Decalin	1011	0.8	RI, MS
n-Undecane	1055	4.9	RI, MS
<i>cis</i> -Thujone	1102	0.8	RI, MS
<i>trans</i> -Thujone	1114	0.7	RI, MS
(<i>E</i>)-Tagetone	1110	0.4	RI, MS
Tetrahydrolavandulol	1117	0.9	RI, MS
n-Dodecane	1170	5.1	RI, MS
n-Tridecane	1291	3.3	RI, MS
α -Longipinene	1353	2.5	RI, MS
n-Tetradecane	1412	4.3	RI, MS
β -Caryophyllene	1436	0.2	RI, MS
<i>E</i> - β -Farnesene	1479	0.2	RI, MS
γ -Muurolene	1507	3.3	RI, MS
β -Selinene	1511	t	RI, MS
α -Bulnesene	1540	0.5	RI, MS
δ -Cadinene	1557	0.3	RI, MS
Guaiol	1647	0.7	RI, MS
10- <i>epi</i> - γ -Eudesmol	1670	0.8	RI, MS
α -Acorenol	1679	0.9	RI, MS
Himachalol	1693	24.2	RI, MS
Androencecalinol	1717	14.1	RI, MS
Cedr-8- <i>en</i> -14-ol	1735	t	RI, MS
2-Methoxy-6-(1-methoxy-2-propenyl) naphthalene	1786	5.6	RI, MS
9,10-Dimethyl-1,2,3,4,5,6,7,8-octahydroanthracene	1801	3.5	RI, MS
7-Isopropyl-1,4-dimethyl-2-azulenol	1825	17.6	RI, MS
Total identified			97.6
Monoterpene hydrocarbons			0.9
Oxygenated monoterpenes			2.8
Sesquiterpene hydrocarbons			6.8
Oxygenated sesquiterpenes			26.6
Phenyl derivatives			41.6
Long chain hydrocarbons			18.9

RI: Retention index relative to C₈–C₂₅ *n*-alkanes on TG-5 column, MS: NIST and Wiley library, and the literature, t: trace (<0.1%).

different chemotypes, namely, himachalol, 7-isopropyl-1,4-dimethyl-2-azulenol, androencecalinol, and 2-methoxy-6-(1-methoxy-2-propenyl) naphthalene, other than reported from the leaves oil.

Conflict of Interests

The author reports no conflict of interests. The author alone is responsible for the content and writing of this paper.

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