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## The essential oil compositions of *Centratherum punctatum* growing wild in Vietnam

**Prabodh Satyal, Ho Viet Hieu, Do Thi Lai, Nguyen Thi Bich Ngoc, Nguyen Huy Hung and William N Setzer**

### Abstract

The essential oils from the aerial parts, leaves, flowers, and stems, of *Centratherum punctatum*, growing wild in Da Nang, Vietnam, were obtained by hydrodistillation and analyzed by gas chromatography – mass spectrometry. The essential oils were dominated by sesquiterpene hydrocarbons (86.1-92.7%), including  $\beta$ -caryophyllene (25.4-28.3%), cyclosativene (3.6-4.6%),  $\alpha$ -copaene (5.5-6.8%), *trans*- $\alpha$ -bergamotene (4.6-5.6%), (*Z*)- $\beta$ -farnesene (6.8-8.4%),  $\alpha$ -humulene (6.2-6.9%), germacrene D (5.8-9.7%), bicyclogermacrene (2.2-4.2%), and  $\delta$ -cadinene (3.3-7.0%).

**Keywords:** *Centratherum intermedium*; essential oil; chemical composition;  $\beta$ -caryophyllene

### 1. Introduction

*Centratherum punctatum* Cass. (syn. *C. intermedium* (Link) Less.) is native to the Neotropics, from Mexico [1] through Paraguay [2] and northern Argentina [3]. The plant has been introduced as an ornamental to tropical regions worldwide, but has escaped cultivation and is considered an invasive pest in Hawaii [4], the Galápagos [5], Australia [6], and Vietnam [7]. In Vietnam, *C. punctatum* is found throughout the country, from urban to mountainous areas, for example, Nui Coc Lake (Thai Nguyen province), and Bach Ma National Park (Thua Thien-Hue province) [8]. This species is also found in Thailand and Indonesia.

This species is used by Nùng and Tày ethnic minorities in Thai Nguyen province to treat flu-like illness and to treat jaundice. A bath prepared from a decoction of *C. punctatum* is used to bathe the women after childbirth. The purpose of this research is to compare the chemical compositions of essential oil of *C. punctatum* in Vietnam's natural environment with the results with other published studies on this species growing in other geographical locations. In addition, the study also aims to assess the potential use of *C. punctatum* essential oil as a natural fragrance or flavoring agent.

### 2. Materials and Methods

#### 2.1 Plant Material

The plant sample was collected at Da Nang, Vietnam. Voucher specimens have been deposited at the Center for Advanced Chemistry Institute of Research & Development, Duy Tan University. The collected material was air-dried at room temperature ( $\approx 25^\circ\text{C}$ ) in the shade and subjected to hydrodistillation, using a Clevenger-type apparatus for 3 h until total recovery of oil. The obtained oils were stored at  $4^\circ\text{C}$  until use. The dry weight of the leaves, stems, and flowers were 0.5, 0.5, and 0.2 g, respectively.

#### 2.2 Gas chromatographic – Mass spectral analysis

Each of the essential oils of *Centratherum punctatum* was analyzed by GC-MS using a Shimadzu GCMS-QP2010 Ultra operated in the electron impact (EI) mode (electron energy = 70 eV), scan range = 40–400 atomic mass units, scan rate = 3.0 scans/s, and GC-MS solution software. The GC column was a ZB-5 fused silica capillary column with a (5% phenyl)-polymethylsiloxane stationary phase and a film thickness of 0.25  $\mu\text{m}$ . The carrier gas was helium with a column head pressure of 552 kPa and flow rate of 1.37 mL/min. Injector temperature was  $250^\circ\text{C}$  and the ion source temperature was  $200^\circ\text{C}$ . The GC oven temperature program was programmed for  $50^\circ\text{C}$  initial temperature, temperature increased at a rate of  $2^\circ\text{C}/\text{min}$  to  $260^\circ\text{C}$ . A 5% w/v solution of the sample in  $\text{CH}_2\text{Cl}_2$  was prepared and 0.1  $\mu\text{L}$

was injected with a splitting mode (30:1). Identification of the oil components was based on their retention indices determined by reference to a homologous series of *n*-alkanes, and by comparison of their mass spectral fragmentation patterns with those reported in the literature [9], and stored in our in-house Sat-Set library [10].

### 3. Results and Discussion

The essential oils, obtained as colorless, with mild pleasant aromas, were obtained in yields of 0.43% (v/w; aerial parts); 0.52% (v/w; leaves), 0.17% (v/w; stems), and 0.23% (v/w; flowers), calculated on a dry weight basis.

The chemical compositions from the aerial parts, the leaves, flowers, and stems of *C. punctatum* are compiled in Table 1. A total of 115 compounds were identified in the essential oils accounting for 99.8, 99.7, 98.7, and 98.7% of the compositions, respectively. Sesquiterpene hydrocarbons dominated all essential oil samples from this plant species. The most abundant component was  $\beta$ -caryophyllene (25.4-28.3%), but cyclosativene (3.6-4.6%),  $\alpha$ -copaene (5.5-6.8%), *trans*- $\alpha$ -bergamotene (4.6-5.6%), (*Z*)- $\beta$ -farnesene (6.8-8.4%),  $\alpha$ -humulene (6.2-6.9%), germacrene D (5.8-9.7%), bicyclogermacrene (2.2-4.2%), and  $\delta$ -cadinene (3.3-7.0%), were also abundant.

**Table 1:** Chemical compositions of essential oils from *Centratherum punctatum* growing wild in Vietnam.

RI <sup>a</sup>	Compound	aerial parts	leaves	flowers	stems
931	$\alpha$ -Pinene	0.1	0.1	---	---
970	Sabinene	0.1	0.1	---	tr <sup>b</sup>
976	$\beta$ -Pinene	0.1	0.1	---	tr
987	Myrcene	0.1	0.1	---	---
1023	<i>p</i> -Cymene	---	tr	---	---
1028	Limonene	---	---	---	tr
1044	( <i>E</i> )- $\beta$ -Ocimene	0.2	0.2	---	tr
1098	Isopentyl 2-methyl butanoate	tr	tr	---	tr
1103	Nonanal	---	---	tr	---
1205	Decanal	---	---	tr	---
1229	(3 <i>Z</i> )-Hexenyl 2-methylbutanoate	tr	0.1	tr	tr
1234	(3 <i>Z</i> )-Hexenyl 3-methylbutanoate	---	tr	---	---
1287	Dihydroedulan IA	---	---	tr	---
1330	Bicycloelemene	0.2	0.3	0.2	0.1
1333	Silphiperfol-5-ene	---	---	0.1	0.1
1334	$\delta$ -Elemene	0.2	0.2	---	---
1342	7- <i>epi</i> -Silphiperfol-5-ene	---	tr	tr	---
1345	$\alpha$ -Cubebene	0.1	0.1	0.1	0.1
1369	Cyclosativene	4.5	4.5	3.6	4.6
1375	$\alpha$ -Copaene	6.7	6.8	5.5	6.7
1382	$\beta$ -Bourbonene	1.0	0.7	0.6	0.7
1386	7- <i>epi</i> -Sesquithujene	0.5	0.5	0.4	0.5
1388	$\beta$ -Elemene	0.8	0.8	0.7	0.7
1391	Sativene	0.1	0.1	---	0.1
1401	Cyperene	0.1	---	tr	---
1401	Sesquithujene	---	tr	---	tr
1404	Ylanga-2,4(15)-diene	0.1	0.1	0.1	0.1
1405	$\beta$ -Maaliene	0.8	0.9	0.6	0.7
1410	$\alpha$ -Gurjunene	tr	tr	---	---
1411	<i>cis</i> - $\alpha$ -Bergamotene	0.1	0.1	0.1	0.1
1419	$\beta$ -Caryophyllene	25.0	25.6	25.4	28.3
1429	$\beta$ -Gurjunene	0.9	0.8	0.7	0.7
1432	<i>trans</i> - $\alpha$ -Bergamotene	4.6	5.2	4.6	5.6
1434	$\alpha$ -Guaiene	0.4	0.4	0.4	0.5
1437	Aromadendrene	0.1	0.2	0.1	---
1440	( <i>Z</i> )- $\beta$ -Farnesene	6.9	8.1	6.8	8.4
1443	<i>cis</i> -Muurolo-3,5-diene	0.1	---	0.1	---
1444	Mylytayl-4(12)-ene + Isopentyl octanoate	tr	0.1	0.2	0.2
1448	<i>trans</i> -Muurolo-3,5-diene	0.2	0.2	0.2	0.2
1451	( <i>E</i> )- $\beta$ -Farnesene	1.5	2.0	0.7	1.5
1451	Sesquisabinene	---	---	0.7	---
1454	$\alpha$ -Humulene	6.8	6.8	6.2	6.9
1459	Alloaromadendrene	0.6	0.5	0.7	0.4
1461	<i>cis</i> -Cadina-1(6),4-diene	0.1	0.1	0.1	tr
1467	9- <i>epi</i> -( <i>E</i> )-Caryophyllene	0.1	---	---	---
1471	Dauca-5,8-diene	0.3	0.2	---	---
1471	$\gamma$ -Gurjunene	---	---	0.2	0.2
1474	<i>trans</i> -Cadina-1(6),4-diene	0.7	0.6	0.7	0.6
1476	$\gamma$ -Curcumene	0.4	0.4	0.3	0.2
1481	Germacrene D	8.6	9.7	6.4	5.8
1483	( <i>Z,Z</i> )- $\alpha$ -Farnesene	2.7	2.8	2.9	3.1
1485	$\delta$ -Selinene	0.1	0.1	0.1	---
1488	$\beta$ -Selinene	1.8	1.5	1.8	1.6
1490	$\alpha$ -Selinene	---	0.3	---	0.2
1491	<i>trans</i> -Muurolo-4(14),5-diene	0.8	0.5	0.6	0.3

1494	Bicyclogermacrene	3.9	4.2	3.0	2.2
1497	$\alpha$ -Muurolene	1.3	1.1	1.2	1.0
1500	$\alpha$ -Bulnesene	0.2	0.2	0.3	0.1
1505	$\beta$ -Bisabolene	0.1	0.1	0.2	0.1
1507	$\beta$ -Curcumene	0.6	0.5	0.3	0.2
1511	$\delta$ -Amorphene	0.6	0.4	0.6	0.5
1513	Cubebol	0.1	0.1	0.1	0.1
1517	$\delta$ -Cadinene	5.6	4.0	7.0	3.3
1520	<i>trans</i> -Calamenene	0.2	0.2	0.3	0.3
1522	$\beta$ -Sesquiphellandrene	0.5	0.4	0.5	0.4
1525	( <i>E</i> )- $\gamma$ -Bisabolene	tr	tr	---	---
1531	<i>trans</i> -Cadina-1,4-diene	0.1	0.1	0.1	---
1535	$\alpha$ -Cadinene	0.1	0.1	0.1	0.1
1539	$\alpha$ -Calacorene	0.3	0.2	0.4	0.3
1541	<i>cis</i> -Sesquisabinene-hydrate	0.2	0.2	0.3	0.2
1546	Elemol	tr	tr	---	---
1549	Isocaryophyllene oxide	---	---	0.1	0.2
1553	Humulene epoxide I	0.1	---	---	---
1557	Germacrene B	tr	---	---	---
1559	( <i>E</i> )-Nerolidol	tr	0.2	0.2	0.2
1560	$\beta$ -Calcorene	0.1	0.1	0.2	0.3
1566	1,5-Epoxy-salvial-4(14)-ene	---	---	---	0.1
1568	Caryophyllenol	---	---	0.1	0.1
1569	Palustrol	tr	tr	---	---
1571	Sesquirosefuran	0.1	---	0.1	---
1575	Spathulenol	0.7	0.6	0.9	1.2
1577	<i>trans</i> -Sesquisabinene hydrate	0.1	0.1	---	---
1581	Caryophyllene oxide	2.0	1.4	3.1	3.3
1584	Globulol	0.1	0.4	0.4	0.4
1592	Viridiflorol	1.3	1.2	1.9	1.2
1594	Guaiol	0.1	---	0.1	---
1594	Cubeban-11-ol	---	---	---	0.1
1597	<i>cis</i> -Bisabol-11-ol	tr	---	---	---
1602	Ledol	0.3	0.2	0.4	0.3
1605	5- <i>epi</i> -7- <i>epi</i> - $\alpha$ -Eudesmol + $\beta$ -Oplopenone	tr	tr	0.1	0.1
1608	Humulene epoxide II	0.3	0.2	0.4	0.4
1611	5- <i>epi</i> -7- <i>epi</i> - $\beta$ -Eudesmol	0.1	0.1	0.2	0.1
1613	1,10-di- <i>epi</i> -Cubenol	0.1	---	---	---
1624	Muurola-4,10(14)-dien-1 $\beta$ -ol	0.2	0.1	0.3	0.1
1626	1- <i>epi</i> -Cubenol	0.2	0.2	0.2	0.2
1630	<i>iso</i> -Spathulenol	0.3	0.2	0.4	0.3
1635	Caryophylla-4(12),8(13)-dien-5 $\beta$ -ol	0.3	0.2	0.4	0.2
1640	<i>epi</i> - $\alpha$ -Cadinol	0.1	0.1	0.2	0.1
1642	<i>epi</i> - $\alpha$ -Muurolol	0.1	0.1	0.2	0.1
1644	$\delta$ -Cadinol	0.1	0.1	0.2	0.2
1653	$\alpha$ -Cadinol	0.4	0.3	0.6	0.5
1656	Pogostol	0.1	0.1	0.2	0.2
1663	<i>cis</i> -Calamenen-10-ol	---	---	tr	---
1663	Selin-11-en-4 $\beta$ -ol	tr	tr	tr	---
1668	14-Hydroxy-9- <i>epi</i> -( <i>E</i> )-caryophyllene	---	---	0.5	0.2
1669	<i>epi</i> - $\beta$ -Bisabolol	0.3	0.3	---	---
1683	$\alpha$ -Bisabolol	0.1	0.1	0.1	0.1
1688	Eudesma-4(15),7-dien-1 $\beta$ -ol	tr	---	---	---
1713	Pentadecanal	0.1	---	0.2	---
1739	Aromadendrane-4,10-diol	---	tr	0.1	0.2
1822	Methandrostenolone	---	tr	0.1	0.2
1838	Phytone	---	---	0.2	---
1838	$\alpha$ -Chenopodiol	---	---	---	0.1
1859	Platambin	---	tr	0.1	0.2
2104	Phytol	---	tr	0.1	---
	Monoterpene hydrocarbons	0.6	0.7	0.0	0.0
	Oxygenated monoterpenoids	0.0	0.0	0.0	0.0
	Sesquiterpene hydrocarbons	91.3	92.7	86.1	87.9
	Oxygenated sesquiterpenoids	7.9	6.3	12.2	10.4
	Others	0.1	0.1	0.6	0.4
	Total identified	99.8	99.7	98.7	98.7

<sup>a</sup>RI = Retention Index determined with reference to a homologous series of alkanes on a ZB-5 capillary column. <sup>b</sup>tr = trace (< 0.05%).

The high concentration of sesquiterpene hydrocarbons is consistent with previously published reports from Brazil and from Nigeria. The essential oil from the flowering parts of *C.*

*punctatum* from Fortaleza, Ceará, northeastern Brazil, was composed largely of sesquiterpenes, including  $\delta$ -cadinene (17.9%),  $\beta$ -caryophyllene (11.1%),  $\gamma$ -cadinene (8.6%),

germacrene D (5.7%), and  $\alpha$ -copaene (5.6%), in addition to the monoterpene  $\beta$ -pinene (9.1%) [11]. A sesquiterpene-rich essential oil from the leaves and flowering tops of *C. punctatum* from Araraquara, São Paulo, Brazil, has also been reported [12], but unfortunately, too few components were identified for useful comparison. The major components in the leaf essential oil of *C. punctatum* growing in Nigeria were  $\beta$ -caryophyllene (16.6%), globulol (5.7%), germacrene D (6.4%),  $\alpha$ -copaene (5.3%), (Z)- $\beta$ -farnesene (reported as sesquisabinene, but the RI is more consistent with (Z)- $\beta$ -farnesene),  $\delta$ -cadinene (4.7%), and  $\alpha$ -humulene (4.1%) [13]. In another report, the essential oil from the aerial parts (herb) of *C. punctatum* from Nigeria was also dominated by sesquiterpene hydrocarbons,  $\beta$ -caryophyllene (27.4%),  $\alpha$ -humulene (7.0%),  $\delta$ -cadinene (6.6%), germacrene D (5.9%), and  $\alpha$ -copaene (5.0%) [14].

#### 4. Conflict of interest statement

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