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Research Article

Chemical composition of the essential oil of *Vernonia gracilis* Kunth from Venezuela

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Abstract

The essential oil from the *Vernonia gracilis* Kunth (Asteraceae) leaves collected in San Juan de Lagunillas, Venezuela was obtained by hydrodistillation and its composition was determined by GC/MS. The yield of the essential oil was 0.001 % (v/w), calculated on a dry weight basis. Twenty four compounds were identified, representing 93.19 % of the oil. The most abundant components were β-caryophyllene (23.15 %), germacrene-D (18.68 %), bicyclogermacrene (18.31 %), α-humulene (6.38 %), caryophyllene epoxide (4.84 %) and spathulenol (4.53 %).

1. Introduction

Vernonia (family Asteraceae, tribe Vernonieae) is a genus of about 1300 species, it's widely distributed in tropical and sub-tropical areas, especially in South America, Asia and Africa [1]. Several *Vernonia* species have been used in traditional medicine to treat reproductive problems, including urinary tract infections, diabetes mellitus, bacterial infections and malaria [2-6]. Various studies have reported antioxidant, anthelminthic, antimicrobial, anti-diabetes, anti-inflammatory, antitumor, analgesic, anti-plasmodial, anticancer and neuroprotective activities [7-11].

Numerous phytochemical studies of the genus *Vernonia* have revealed the presence of diterpenes, triterpenes, steroids, and the most frequently isolated chemical constituents are flavonoids and sesquiterpene lactones, which have been used as taxonomic markers [12-16]. Despite this extensive investigation, little is known about the composition of the genus *Vernonia* essential oils.

Vernonia gracilis Kunth is a synonym for *Lepidaploa gracilis* [17,18]. Literature surveys reveal that no phytochemical investigations have been previously conducted on the essential oil of *V. gracilis*, the present study was undertaken to obtain knowledge of their chemical composition.

2. Materials and methods

2.1 Plant Material

Leaves of *V. gracilis* were collected in May 2016 at San Juan de Lagunillas, Mérida State, Venezuela. A voucher specimen (LCGM01) has been deposited at

the MERF Herbarium (Herbarium of the Faculty of Pharmacy and Bioanalysis in Mérida, Venezuela). The botanical identification was made by Dr. Pablo Meléndez.

2.2 Extraction and analysis of the essential oil

Fresh leaves (1000 g) were cut into small pieces and submitted to hydrodistillation for 3 hours using a Clevenger-type apparatus. A volume of 0.1 mL of essential oil was obtained (0.001 %, v/w). The composition of the essential oil was determined by comparison of the mass spectrum of each component with Wiley GC/MS library data and also from RI data.

2.3 Gas chromatography – mass spectrometry

Gas chromatography – mass spectrometry (GC-MS) analyses were conducted on a Model 5973 Hewlett-Packard GC-MS system fitted with a HP- 5MS fused silica column (30 m x 0.25 mm i.d., film thickness 0.25 µm, Hewlett-Packard). The oven temperature program was the same as the one used for the HP-5 column for GC analysis; the transfer line temperature was programmed from 150 °C to 180 °C; source temperature, 230 °C; quadrupole temperature 150 °C; carrier gas, helium adjusted to a linear velocity of 34 cm/s; ionization energy, 70 eV; scan range, 40 to 500 amu; 3.9 scans/s. A sample of a 2 % solution of the essential oil (1.0 µL) was injected using a Hewlett-Packard ALS injector with a split ratio of 50:1. The identity of the oil components was established from their GC retention indices, by comparing their MS and those of standard components available in the laboratory, and through library search (Nist 05 and Wiley MS Data Library, 6th edn) [19, 20].

3. Results and discussion

The hydrodistillation from the leaves of *V. gracilis* produced 0.1 mL yellow oil with a yield of 0.001 %. The chemical composition of the oil was investigated using GC-MS technique. Twenty-four components were identified in the leaves' oil, which represent 93.19 % of the total oil. These compounds and their retention indices (RI) and relative percentage concentrations are listed in Table 1 and Fig. 1, according to the elution order on HP-5 column. The identified products may be divided into four different groups: monoterpenes (0.62 %), oxygenated monoterpenes (0.19 %), sesquiterpenes (76.89 %) and oxygenated sesquiterpenes (15.49 %). The main components of the leaves' oil were β-caryophyllene (23.15 %), germacrene-D (18.68 %), bicyclogermacrene (18.31 %), α-humulene (6.38 %), caryophyllene epoxide (4.84 %) and spathulenol (4.53 %). This is the first report on the volatile compounds of *V. gracilis*, the present data could not be compared with other analysis of the same species.

There are several reports on the oil composition of the plants of the genus *Vernonia* described in other parts of the world (Vietnam, Brazil, India and Nigeria) [21]. Most of them are characterized by the presence of monoterpenoids and sesquiterpenoids. The preliminary chemical analysis of the essential oils of *Vernonia* has been performed earlier the major components were β-caryophyllene (28.50 %), caryophyllene oxide (16.60 %), α-copaene (9.00 %) and α-humulene (7.10 %) from the leaves of *V. patula* [21] and the essential oil was obtained from *V. chalybaea* showing it was rich in β-caryophyllene (39.06 %) and bicyclogermacrene (19.69 %) [22]. The major components found in the essential oil from aerial parts of *V. scorpiodes* were β -caryophyllene (30.60 %), germacrene D (27.30 %), and bicyclogermacrene (8.50 %) [23]. On the other hand, the major components of the essential oils from the aerial parts of *V. amygdalina* and from the roots of *V. cinerea* were α-muurolol (45.70 %) and α-muurolene (30.70 %), respectively [24, 25]. The principal components of the essential oil analysis of *V. crotonoides* were α-cadinol (14.10 %), spathulenol (9.80 %), caryophyllene oxide (5.90 %), and epi-α-cadinol (5.30 %) [26].

The major constituents reported in the essential oils from different organs of *V. condensata* were the leaf oil β-caryophyllene (18.35 %), γ-muurolene (16.41 %) and α-humulene (6.03). Linalol (12.13 %), 10-epi-italicene ether (8.88 %), myrcene (7.68 %), and 2-δ-carene (6.86 %) were in the stem oil. The monoterpenes 1,8-cineole (11.03 %), thymol (7.68 %) and linalool (6.30 %) were the major constituents reported in the flower oil [27]. It is well known that sesquiterpenes compounds, as identified in the present study, predominate in the essential oils of the genus *Vernonia*. These differences are mainly due to variations in the ecological conditions, genetic and environmental factors, such as temperature, moisture, the soil, the harvest period, geographical position, seasonal variations and the vegetative cycle are important [28, 29].

Table 1. Percentage composition of the essential oil from leaves of *Vernonia gracilis* Kunth.

No.	Compounds	Composition of essential oil (%)	[a]RI	[b]RI
1	*β*-Pinene	0.46	965	979
2	Limonene	0.16	1032	1029
3	*Cis*-3-hexenyl 3-methylbutanoato	0.19	1231	1235
4	*β*-Copaene	2.18	1382	1387
5	*β*- Bourbonene	0.74	1385	1388
6	*β*-Elemene	0.98	1396	1390
7	*β* -Gurjunene	0.35	1428	1433
8	***β*-Caryophyllene**	**23.15**	1440	1433
9	Epi-Bicyclosesquiphellandrene	0.34	1448	1463
10	***α*-Humulene**	**6.38**	1457	1465
11	Alloaromadendrene	2.10	1471	1460
12	*α*-Amorphene	0.75	1482	1484
13	**Germacrene-D**	**18.68**	1492	1485
14	**Bicyclogermacrene**	**18.31**	1502	1500
15	Germacreno A	0.77	1503	1509
16	*γ*-Cadinene	0.60	1513	1528
17	*δ*-Cadineno	1.56	1526	1530
18	**Spathulenol**	**4.53**	1575	1578
19	**Caryophyllene epoxide**	**4.84**	1603	1588
20	Viridiflorol	1.45	1611	1610
21	Humulene epoxide	0.63	1609	1608
22	Isospathulenol	1.27	1624	1626
23	*α*-Cadinol	1.68	1661	1672
24	T-Muurolol	1.09	1658	1659
	Total Identified	**93.19**		

[a]**RI**: Retention index this work. [b]**RI**: Theoretical Retention index.

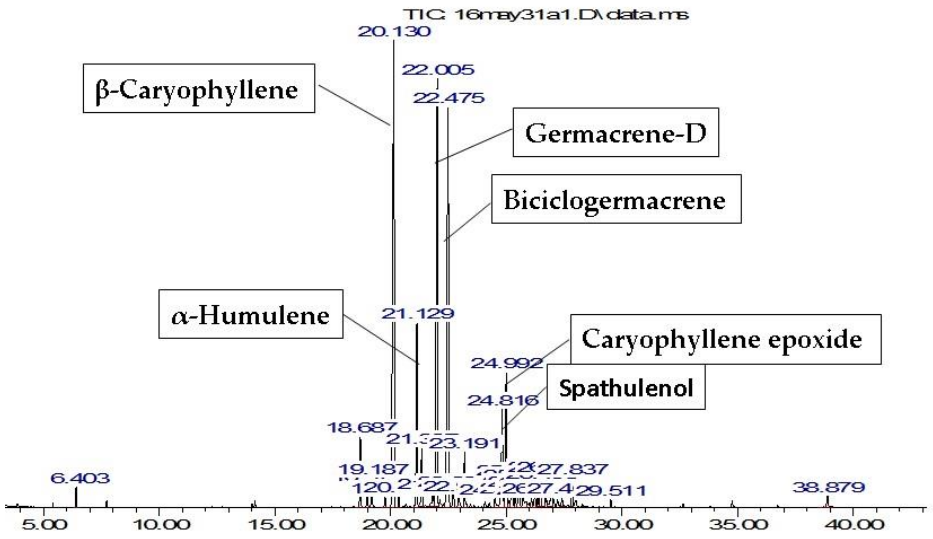

Figure. 1. GC chromatogram (HP-5 column) and representative compounds of leaves of *Vernonia gracilis* Kunth.

4. Conclusions

In the current investigation, the chemical composition of essential oil of fresh leaves of *Vernonia gracilis* (Asteraceae) collected in Mérida, Venezuela was evaluated. The essential oil is dominated by the presence of sesquiterpenes (76.89 %) and oxygenated sesquiterpenes (15.49 %). The main components were *β*-caryophyllene (23.15 %), germacrene-D (18.68 %) and bicyclogermacrene (18.31 %). To our knowledge, this is the first time that the chemical composition of the essential oil of the leaves *V. gracilis* of has been reported and this compounds may also aid in future chemotaxonomic research of this species.

Authors' contributions

Conceptualization, L.R.F.; Methodology, L.R.F.; Software, L.R.F.; Validation, A.P.C., Formal Analysis, A.P.C. and Y.O.D.; Investigation, A.P.C., R.A.Z. and Y.O.D.; Resources, A.P.C., R.A.Z. and Y.O.D; Data Curation, R.A.Z.; Writing – Original Draft Preparation, A.P.C. and Y.O.D.; Writing – Review & Editing, A.P.C., R.A.Z. and Y.O.D.

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Conflicts of interest

The authors declare no conflict of interest.

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