Original Article

CHEMICAL DIVERSITY OF ESSENTIAL OILS FROM *Hyptis pectinata* (L.) Poit

DIVERSIDADE QUÍMICA DE ÓLEOS ESSENCIAIS DE Hyptis pectinata *(L.) Poit*

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ABSTRACT: The essential oils are secondary metabolites formed by several chemical compounds that confer to these substances great social and economic importance. This diversity of compounds is generally determined by the genetic constitution of the plant, although environmental factors may also influence the type, amount, and concentrations of the compounds present in the essential oil. The aim of this work was to analyze the chemical diversity of the essential oils of native *Hyptis pectinata* plants collected in the state of Sergipe. The essential oils of 24 plants were obtained by hydrodistillation and analyzed by GC-MS/FID, revealing 30 compounds. Two clusters were formed by the cluster analysis. Cluster I consisted of 18 plants, and presented β-elemene (2.46-25.77%), β-caryophyllene (16.20-60.95%), germacrene D (0.00-21.59%), and caryophyllene oxide (5.38-42.21%) as major compounds. Cluster II consisted of six plants, and presented β-caryophyllene (5.68-15.57%), (*Z*)-β-guaiene (2.18-7.31%), caryophyllene oxide (1.58-22.89%), and calamusenone (23.12-64.36%) as major compounds. Strong correlation was observed between *p*-cymene and γ-terpinene (r=0.94), and between (*E*)-β-guaiene and lepidozene (r=0.95). Results of the present study indicate variation in the essential oil content, and show that the compounds β-elemene, β-caryophyllene, germacrene D, (*Z*)-β-guaiene, caryophyllene oxide and calamusenone were detected in greater proportions in native plants of *H. pectinata* of the state of Sergipe. The knowledge of the chemical diversity found in *H. pectinata* plants can assist in the selection of plants of specific interest.

KEYWORDS: Medicinal plant. Germplasm. Volatile oil. Chemical compounds.

INTRODUCTION

The Lamiaceae family has about 300 genera and approximately 7500 species. In Brazil, approximately 350 species are distributed in 26 genera (SOUZA; LORENZI, 2008). The family is known for the chemical variability of its essential oils, and its plants are widely used by the population for therapeutic purposes (RAYMUNDO et al., 2011).

The genus *Hyptis* is composed of several medicinal and aromatic species of great economic interest. Among these species, *H. pectinata,* popularly known in the Brazilian Northeast as "sambacaitá" or "canudinho", is extensively used in folk medicine in the treatment of bacterial infections and inflammation (ARRIGONI-BLANK et al., 2005). In addition, several biological properties of its essential oils or extracts have already been proved, such as its antidematogenic, antinociceptive (ARRIGONI-BLANK et al., 2008), antimicrobial (NASCIMENTO et al., 2008), insecticide (SILVA et al., 2008), anti-inflammatory (RAYMUNDO et al., 2011), and leishmanicide activities (FALCAO et al., 2013).

The essential oils are products of secondary metabolism, characterized as complex chemical mixtures extracted from different parts of the plant, and confer adaptive advantages to the different environments in which they are inserted (OUSSALAH et al., 2007).

The genetic constitution is usually the main determinant of plant adaptive responses, allowing for differences in the synthesis of secondary metabolites related to the types, amounts, and concentrations of the compounds. However, these variations can also be influenced by environmental factors, such as luminosity, temperature, water availability, soil conditions, among others (MARTINS et al., 2006).

The characterization of the chemical composition of the essential oils of plants of the same species allows generating information for the obtainment of the most suitable plants for therapeutic use, and for the obtainment of plants with higher essential oil content, allowing selection and insertion in genetic improvement programs (VELOSO et al., 2014).

Several studies have found great chemical diversity in the essential oil of medicinal and aromatic species, such as *Ocimum basilicum* L. (VELOSO et al., 2014; COSTA et al., 2015), *Lippia alba* (Mill.) N. E. Brown (NETO et al., 2012; BLANK et al., 2015), *Varronia curassavica* Jacq. (NIZIO et al., 2015), *Lippia sidoides* Cham. (SANTOS et al., 2015), and *Hyptis pectinata*

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(TCHOUMBOUGNANG et al., 2005; NASCIMENTO et al., 2008; SANTOS et al., 2008; ARRIGONI-BLANK et al., 2008; RAYMUNDO et al., 2011).

Thus, the objective of the present study was to evaluate the chemical diversity and the essential oil content of native plants of *Hyptis pectinata* of the state of Sergipe.

MATERIAL AND METHODS

Plant material

Leaves of 24 native plants of *H. pectinata* were collected from 21 municipalities of the state of Sergipe, Brazil (Table 1).

Table 1. Identification and origin of *H. pectinata* plants collected in Sergipe, Brazil.

Plants	Origin (municipality)	Georeferenced information
Plant-01	Poço Redondo	9º58'23.01'S; 37°52'05.0"W
Plant-02	Poço Redondo	9°57'45.2"S; 37°51'51.2"W
Plant-03	Canindé do São Francisco	9°42'06.7"S; 37°51'06.1''W
Plant-04	Nossa Senhora da Glória	10°08'41.0"S; 37°31.17'05"W
Plant-05	São Cristóvão	11°00'00.0''S; 37°12'00.0''W
Plant-06	São Cristóvão	10°54'44.9"S; 37°11'45.9"W
Plant-07	São Cristóvão	10°53'33.4"S; 37°10'50.9"W
Plant-08	Capela	10°35'29.8"S; 36°59'08.5"W
Plant-09	Graccho Cardoso	10°17'11.8"S; 37°16'58.3"W
Plant-10	Itabaiana	10°35'06.6"S; 37°28'21.4"W
Plant-11	Itaporanga	10°59'44.8"S; 37°20' 04.2"W
Plant-12	Japaratuba	10°35'01.6"S; 36°57'50.3"W
Plant-13	Barra dos Coqueiros	10°48'22.6"S; 36°55'56.6"W
Plant-14	Lagarto	10°58'19.5"S; 37°24'44.1"W
Plant-15	Malhador	10°39'40.3"S; 37°18'43.8"W
Plant-16	Moita Bonita	10°37'47.2"S; 37°21'48.2"W
Plant-17	Muribeca	10°24'34.6"S; 36°57'27.2"W
Plant-18	Neopólis	10°20'11.3"S; 36°41'16.5"W
Plant-19	Pirambú	10°17'19.1"S; 36°51'42.4"W
Plant-20	Porto da Folha	9°58'11.2"S; 37°27'12.0"W
Plant-21	Riachão do Dantas	10°05'46.8"S; 37°43'28.5"W
Plant-22	Riachuelo	10°43'04.8"S; 37°12'41.6"W
Plant-23	Ribeirópolis	10°33'34.1"S; 37°22'23.7"W
Plant-24	Santana do São Francisco	10°16'04.8"S; 36°36'53.3"W

Extraction, content and chemical analyses of essential oils

The essential oils were extracted and analyzed in the Phytotechnology Laboratory and Laboratory of Chromatography respectively, both in the Federal University of Sergipe.

The collected leaves were dried in a forced air circulation oven, at 40ºC, for five days. The essential oils of *H. pectinata* were extracted using 70g, in triplicate, by the hydrodistillation method, in a modified Clevenger apparatus, for 150 minutes (EHLERT et al., 2006). The essential oils were stored in amber flasks, and kept in freezer at -20 °C until chemical composition analysis.

The analyses of the chemical composition of the essential oils of *H. pectinata* were performed using a GC-MS/FID (QP2010 Ultra, Shimadzu Corporation, Kyoto, Japan), equipped with an autosampler AOC-20i (Shimadzu). Separations were accomplished using an Rtx®-5MS Restek fused silica capillary column (5%-diphenyl–95%-dimethyl polysiloxane) of 30 m × 0.25 mm i.d., 0.25µm film thickness, at a constant helium (99.999%) flow rate of 1.2 mL/min. Injection volume of 0.5 µL (5 mg/mL) was employed, with a split ratio of 1:10. The oven temperature was programmed from 50 °C (isothermal for 1.5 min), with an increase of 4 °C/min, to 200 °C, then 10 °C/min to 250 °C, ending with a 5 min isothermal at 250 °C.

The MS and FID data were simultaneously acquired employing a Detector Splitting System; the split flow ratio was 4:1 (MS:FID). A 0.62 m x 0.15 mm i.d. restrictor tube (capillary column) was used to connect the splitter to the MS detector; a 0.74 m x 0.22 mm i.d. restrictor tube was used to connect the splitter to the FID detector. The MS data (total ion chromatogram, TIC) were acquired in the full scan mode (*m/z* of 40–350) at a scan rate of 0.3 scan/s using the electron ionization (EI) with an electron energy of 70 eV. The injector temperature was 250 °C and the ion-source

temperature was 250°C. The FID temperature was set to 250 ºC, and the gas supplies for the FID were hydrogen, air, and helium at flow rates of 30, 300, and 30 mL/min, respectively. Quantification of each constituent was estimated by FID peak-area normalization (%). Compound concentrations were calculated from the GC peak areas and they were arranged in order of GC elution.

The retention index (Van den Dool and Kratz 1963) was obtained by injecting a C_7-C_{30} linear hydrocarbon mixture under these same conditions, and identification of constituents was made on the basis of comparison of retention index and MS with those in the literature (ADAMS, 2007), as well as by computerized matching of the acquired mass spectra with those stored in NIST21, NIST107, and WILEY8 mass spectral libraries of the GC-MS data system.

Statistical analyses

Two multivariate analysis techniques were used for the chemical diversity analysis (cluster analysis and principal component analysis - PCA), using the Statistica software version 7.0. A dendrogram was generated using the Ward clustering method, based on a dissimilarity matrix constructed using the Euclidean distances of the chemical composition of each sampled plant and the correlation analysis between the chemical compounds of the essential oil of the sampled plants.

The results of the essential oils contents were subject to analysis of variance. Means were compared by the Scott-Knott test ($P \leq 0.05$), using the Sisvar® software, when significant.

The graph with the means of the chemical compounds and standard deviations for each chemical cluster was obtained using the Graph Pad Prism® software.

RESULTS AND DISCUSSION

The diversity of the chemical compounds of the essential oils was significant among the native plants of *H. pectinata* of the state of Sergipe. Thirty compounds were detected in the chemical analyses of the 24 plants (Table 2, Figure 1). Essential oil content varied between the plants, and a higher percentage (0.90) was obtained in the plant from the municipality of Porto da Folha (Table 2).

The plant kingdom presents wide chemical diversity. Variation in chemical compounds is usually observed among plants of the same species (KLEINE and MULLER, 2011). The number of compounds and the concentrations of each compound in the essential oil of the plants and the oil content can be influenced by genetic, climatic, and/or edaphic factors (OLIVEIRA et al., 2012; TEIXEIRA et al., 2013; BLANK et al., 2015; COSTA et al., 2015; PINTO et al., 2015).

These factors can redirect the metabolic pathway, and thus form other compounds that help plants adapt to the conditions to which they are subject (KLEINE and MULLER, 2011). This redirection is possibly related to the catalytic flexibility of the terpene-synthase enzymes, which often produce multiple products from a single substrate. The monoterpenes are synthesized from geranyl diphosphate (GDP), farnesyl diphosphate (FDP) sesquiterpenes, and geranylgeranyl diphosphate diterpenes (GGDP) (ARIMURA et al., 2009).

Considering the similarities of the chemical compounds of the essential oils of the *H. pectinata* plants, two main clusters were characterized by the cluster analysis (Figure 2). The first cluster consisted of the following compounds: β-elemene (2.46-25.77%), β-caryophyllene (16.20-60.95%), germacrene (0.00-21.59%), and caryophyllene oxide (5.38-42.21%). This cluster was divided into subcluster I (Plant-01, Plant-02, Plant-04, Plant-08, Plant-11, Plant-14, Plant-21 and Plant-22), and subcluster II (Plant-06, Plant-07, Plant-12, Plant-13, Plant-15, Plant-16, Plant-17, Plant-19, Plant-23, Plant-24). The mean values of β-caryophyllene and caryoplyllene oxide were the main determinant factor for the subdivision of these plants.

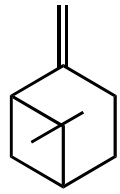
The second cluster consisted of the following compounds: β-caryophyllene (5.68-15.57%), (*Z*)-β-guaiene (2.18-7.31%), caryophyllene oxide (1.58-22.89%), and calamusenone (23.12-64.36%); and was subdivided into subcluster I (Plant-03, Plant-05, Plant-09 and Plant-10), and subcluster II (Plant-18 and Plant-20) (Figures 2 and 3). The compound calamusenone was the determinant for this subdivision.

Results showed that some plants collected in the same municipality or in neighboring municipalities, with similar climatic and edaphic factors, such as Canindé do São Francisco and Poço Redondo, were clustered according to their chemical composition.

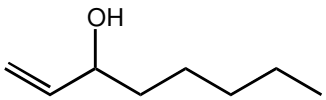
Table 2. Content (%) of the chemical compounds of the essential oil *H. pectinata* collected in Sergipe, Brazil.

COMPOUNDS	**Plants (*H. pectinata*)**																								
	IRRl	01	02	03	04	05	06	07	08	09	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
β-pinene	974	2.26	-	1.57	0.30	-	-	-	-	-	0.97	-	0.35	-	0.59	-	1.27	-	2.20	-	0.55	-	-	-	-
1-octen-3-ol	974	-	-	4.07	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
p-cymene	1020	1.32	-	0.74	0.31	-	-	-	-	-	-	-	5.47	-	-	-	0.58	-	-	-	-	-	-	0.62	-
γ-terpinene	1054	-	-	-	-	-	-	-	-	-	-	-	2.63	-	-	-	0.70	-	-	-	-	-	-	0.56	-
δ-elemene	1335	3.92	0.58	-	2.85	-	0.53	0.83	0.43	-	1.45	2.75	-	1.57	5.11	1.00	2.28	0.98	-	1.02	-	4.29	2.40	1.02	0.28
α-copaene	1374	4.85	4.02	2.08	4.56	1.12	0.96	1.91	5.33	3.25	1.81	3.72	1.90	2.02	2.61	1.97	2.28	2.76	1.74	2.25	1.02	2.47	3.04	2.59	2.71
β-elemene	1389	7.79	11.38	-	9.87	2.05	6.70	12.32	25.77	8.53	7.78	9.35	2.46	9.42	11.93	3.59	10.50	7.16	1.42	3.28	2.27	20.83	15.46	2.94	3.14
β-caryophyllene	1417	17.66	16.20	11.68	18.37	9.42	27.28	43.06	24.47	15.57	12.53	30.97	27.63	38.68	28.69	36.97	35.89	39.00	5.68	27.51	8.34	22.29	25.34	31.63	60.95
γ-elemene	1434	-	2.64	-	-	0.63	-	-	-	1.71	-	-	-	-	-	-	0.75	1.02	0.81	0.45	0.66	0.99	1.35	-	-
(Z)-muurola-3,5-diene	1448	-	-	-	1.08	0.56	-	-	1.72	-	0.47	-	0.67	-	0.14	-	0.66	0.59	-	0.42	-	0.62	-	0.78	1.09
α-humulene	1452	1.66	1.86	0.92	1.37	0.81	1.55	2.71	2.83	1.66	1.26	1.48	1.18	2.02	1.48	1.19	1.64	1.56	0.56	0.90	0.47	1.91	1.72	1.17	1.85
γ-muurolene	1478	5.66	-	1.34	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
germacrene D	1484	0.00	5.68	-	9.58	1.87	4.81	10.11	17.48	5.09	9.08	14.88	12.97	14.34	14.00	4.62	8.06	12.27	2.71	17.86	3.49	12.62	21.59	14.09	15.41
(Z)- β-guaiene	1492	0.00	7.46	2.18	-	4.77	0.57	2.35	0.40	7.31	4.38	1.06	-	-	0.40	0.18	0.22	0.30	6.23	-	6.07	0.56	-	-	-
bicyclogermacrene	1500	4.57	3.14	-	-	-	1.95	1.22	1.39	2.04	2.44	7.94	1.17	5.27	2.32	1.88	1.54	2.21	0.41	4.66	0.82	5.20	1.72	1.15	-
(E)- β-guaiene	1502	-	0.52	-	2.47	-	-	-	-	-	0.25	-	-	-	0.28	-	-	-	-	-	-	-	-	-	-
Lepidozene	1502	-	-	-	4.38	0.68	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
γ-cadinene	1513	-	1.37	1.88	0.77	2.72	0.91	-	0.69	1.57	0.94	0.32	-	-	1.04	0.69	1.44	1.23	1.44	1.65	0.87	1.87	-	-	1.26
(E)-calamenene	1521	5.76	3.11	1.93	-	1.81	-	-	-	1.76	-	-	1.84	1.76	-	-	-	-	-	-	-	-	-	2.92	-
δ-cadinene	1522	-	1.06	-	2.58	-	1.16	0.72	2.34	-	1.74	2.59	-	-	0.08	-	0.67	-	1.32	-	-	0.37	2.14	-	0.52
spathulenol	1577	10.09	5.91	5.83	3.63	-	1.44	1.38	0.23	4.51	0.81	3.69	1.47	2.04	1.50	1.93	2.09	0.75	-	3.51	2.19	2.32	1.67	1.21	-
Caryophyllene oxide	1582	11.52	11.22	12.78	10.86	22.89	42.21	19.78	5.38	13.62	6.27	10.27	25.41	17.23	16.52	37.18	17.65	21.21	1.58	29.23	8.03	10.64	17.71	27.64	9.63
1,10-di-epi-cubenol	1618	-	1.58	1.91	-	-	-	-	-	2.38	1.37	-	-	-	-	-	-	-	-	-	-	-	-	-	-
1-epi-cubenol	1627	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.68	-	2.53	-	-	-	-
α -acorenol	1632	-	-	-	-	0.15	0.29	-	-	-	0.93	0.71	-	0.37	2.58	0.28	1.75	0.25	-	-	-	1.50	-	0.97	-
epi-α-cadinol	1638	4.88	1.74	-	-	-	0.00	-	0.62	-	0.54	1.40	1.14	0.67	0.91	0.18	1.12	0.62	0.21	1.11	0.49	1.63	-	1.02	-
epi-α-muurolol	1640	-	2.81	-	-	-	0.58	-	-	-	0.55	0.83	0.33	-	-	-	-	-	-	-	-	-	1.31	0.58	-
Cubenol	1645	-	-	-	-	3.29	-	-	-	-	-	-	-	-	-	-	-	-	0.38	-	0.49	-	-	-	-
α-cadinol	1652	2.22	-	2.12	1.41	1.59	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Calamusenone	-	-	10.05	23.12	11.02	36.08	-	-	0.72	28.97	38.88	-	-	-	-	-	-	0.43	64.36	-	53.56	-	-	-	-
Essential oil content (%)		0.67c	0.52d	0.62c	0.76b	0.52d	0.48d	0.67c	0.52d	0.62c	0.62c	0.57d	0.43d	0.57d	0.62c	0.62c	0.62c	0.38d	0.67c	0.44d	0.90a	0.52d	0.52d	0.48d	0.66c

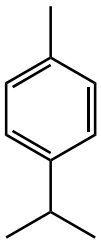
IRRo: Relative Retention Index - observed; IRRl: Relative Retention Index – literature. Means followed by the same letter in the line did not significantly differ from each other by the Scott-Knott test, $p<0.05$.



β-pinene



1-octen-3-ol



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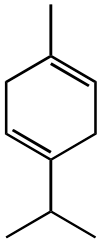
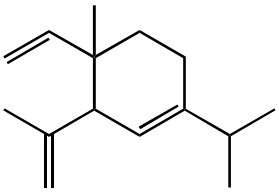
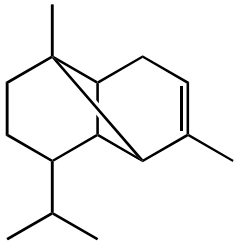


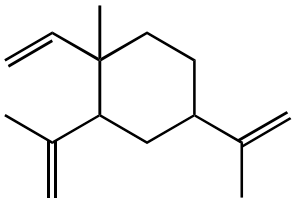
γ-terpinene



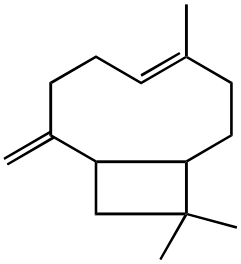
δ-elemene



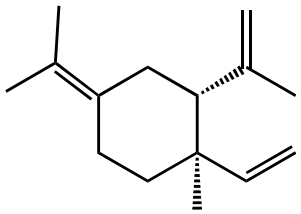
α-copaene



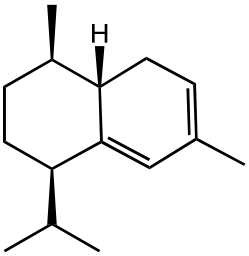
β-elemene



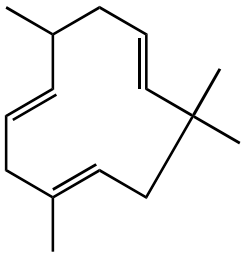
β-caryophyllene



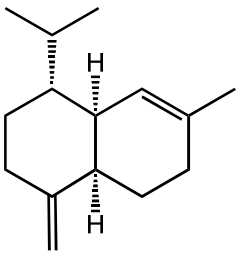
γ-elemene



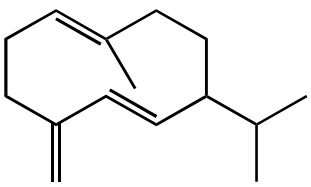
(Z)-muurola-3,5-diene



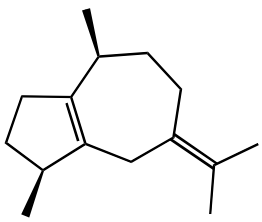
α-humulene



γ-muurolene



germacrene D



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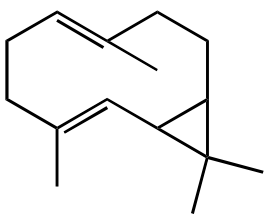
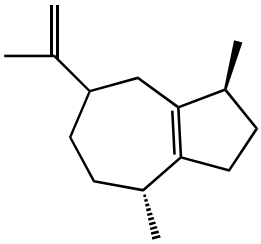
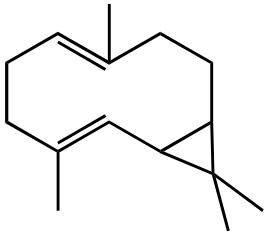


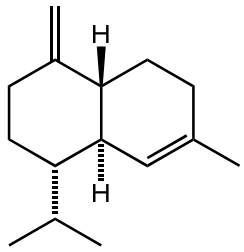
bicyclogermacrene



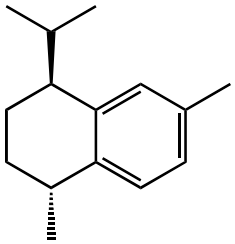
(E)- β-guaiene



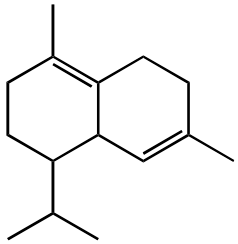
Lepidozene



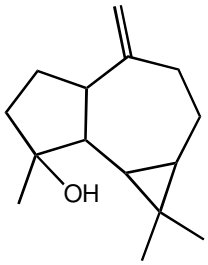
γ-cadinene



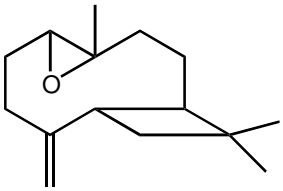
(E)-calamenene



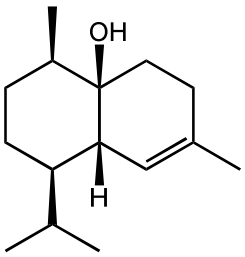
δ-cadinene



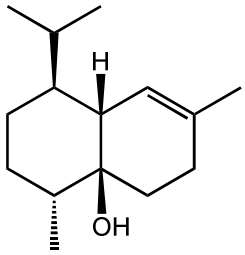
Spathulenol



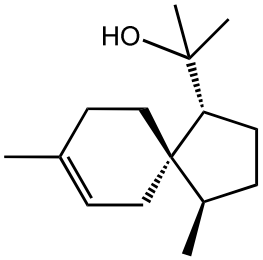
Caryophyllene oxide



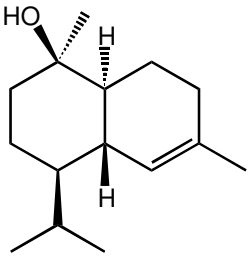
1,10-di-epi-cubenol



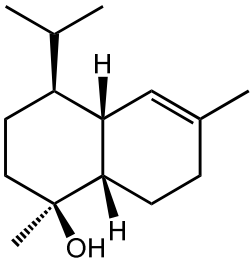
1-epi-cubenol



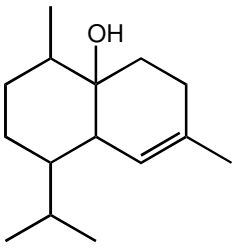
α-acorenol



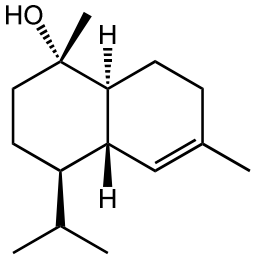
epi- α-cadinol



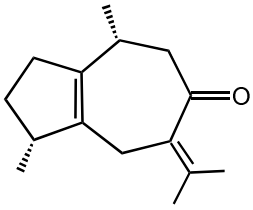
epi- α-muurolol



Cubenol



α-cadinol



Calamusenone

Figure 1. Chemical structure of compounds identified in the essential oils of *H. pectinata* collected in Sergipe, Brazil.

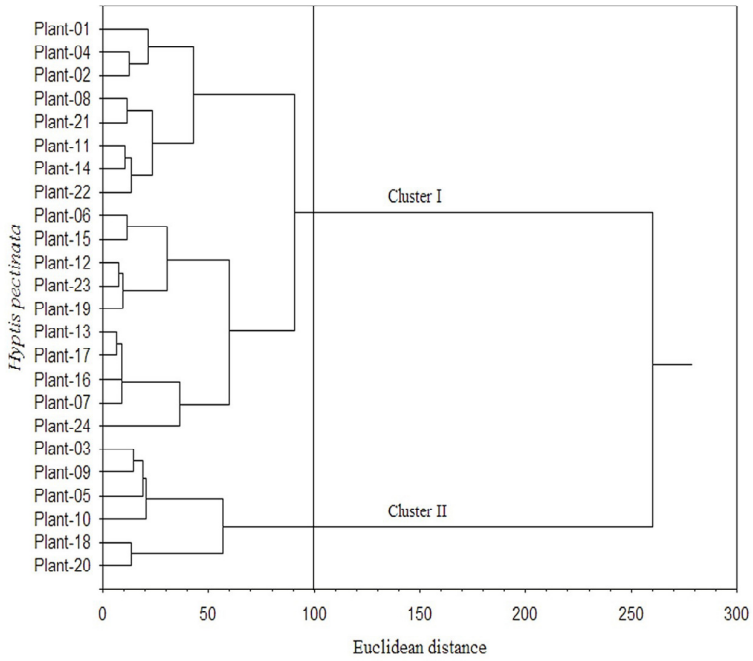


Figure 2. Bidimensional dendrogram representing the similarity between 24 *H. pectinata* plants for the chemical composition of essential oils.

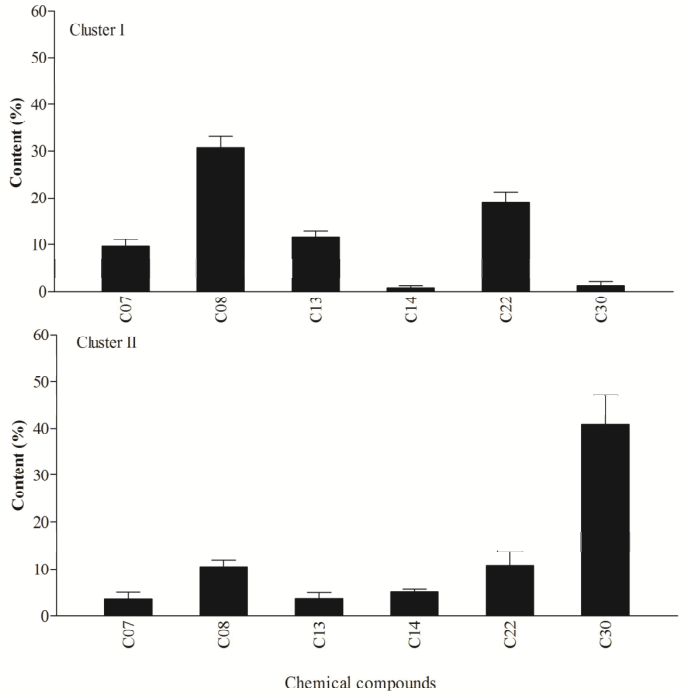


Figure 3. Means of the chemical compounds of the essential oils of *H. pectinate* plants, clusters I and II. (C7) β-elemene, (C8) β-caryophyllene, (C13) germacrene-D, (C14) (Z)-β-guaiene, (C22), caryophyllene oxide, and (C30) calamusenone.

The conventional propagation process of the genus *Hyptis* is through seeds, which may allow great genetic variability (WULFF, 1973). This suggests that the differences found may be related mainly to genetic factors, since such plants were subject to the same or very similar environmental conditions. Similar results were found in studies on *Varronia curassavica*, in which some plants collected in the same municipality were also classified into different clusters (NIZIO et al., 2015).

The major compounds reported in this study corroborate other works involving the essential oil of *H. pectinata*, in which the main chemical compounds commonly detected were: *p*-cymene (33.7%), β-pinene (6.95%), β-caryophyllene (7.00-54.07%), caryophyllene oxide (1.98-38.05%), calamusenone (1.85-48.00%),

germacrene D (3.07-28.00%) (TCHOUMBOUGNANG et al., 2005, ARRIGONI-BLANK et al., 2008, NASCIMENTO et al., 2008, SANTOS et al., 2008, ARRIGONI-BLANK et al., 2010, RAYMUNDO et al., 2011, MENEZES et al., 2015).

The bioactive compounds α-copaene, β-caryophyllene, α-humulene and caryophyllene oxide were detected in all plants, with levels ranging from 0.96% (SC-2) to 5.33% (CA); 5.68% (NE) to 60.95% (SF); 0.47% (FP) to 2.83% (CA); and 1.58% (NE) to 42.21% (SC-2) (Table 2), respectively.

According to the principal component analysis (Figure 4), the first principal component represented 20.31% of the total variance, and was positively related to the compound (*Z*)-β-guaiene (r =-0.70), and calamusenone (r=-0.79); and negatively related to germacrene D (r =-0.84) and β-caryophyllene (r=-0.73). The second principal component represented 16.33% of the total variance, and was positively related to the compounds γ-muurolene (r = 0.85), (*E*)-calamenene (r = 0.71), spathulenol (r = 0.84), and *epi*-α-cadinol (r = 0.86) (Figure 4).

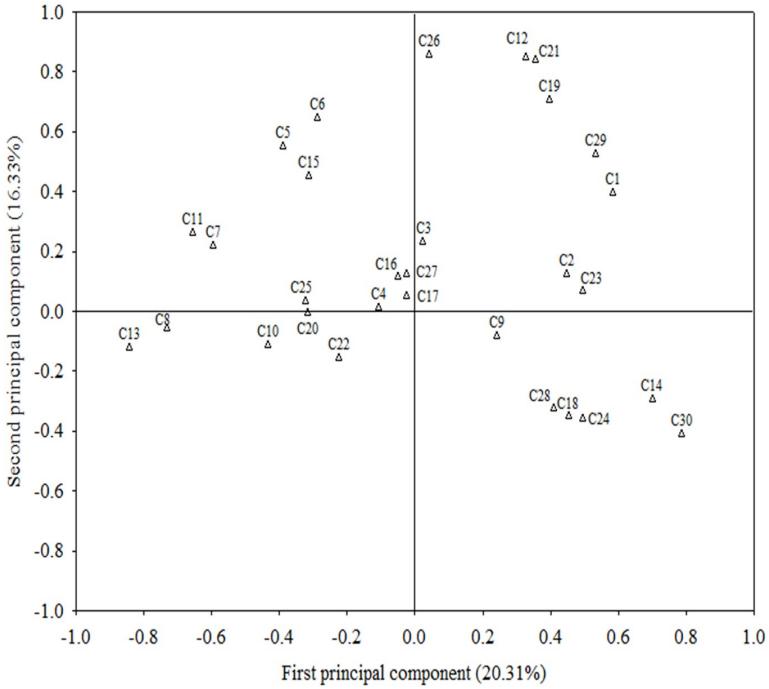


Figure 4. Distribution of the chemical compounds of the essential oil of 24 *H. pectinate* plants in relation to the two principal components, by means of the principal component analysis (PCA). C1: β-pinene. C2:1-octen-3-ol. C3: p-cymene. C4: γ-terpinene. C5: δ-elemene. C6:α-copaene. C7:β-elemene. C8: β-caryophyllene. C9: γ-elemene. C10: (Z)-muurola-3.5-diene. C11: α-humulene. C12: γ-muurolene. C13: germacrene D. C14: (Z)-β-guaiene. C15: bicyclogermacrene. C16: (E)-β-guaiene. C17: lepidozene. C18: γ-cadinene. C19: (E)-calamenene. C20: δ-cadinene. C21: spathulenol. C22: caryophyllene oxide. C23: 1.10-di-epi-cubenol. C24: 1-epi-cubenol. C25: α-acorenol. C26: epi-α-cadinol. C27: epi-α-muurolol. C28: cubenol. C29:α-cadinol. C30: calamusenone.

The principal components of this study explained only about 36% of the total variance. According to Sampaio et al (2016), the use of many variables for the analysis may generate this low explanation of the principal components.

High positive correlation was observed between some constituents of the essential oil of the studied plants (Table 3). Very strong correlation was observed between p-cymene and γ-terpinene (r= 0.94); and between (*E*)-β-guaine and lepidozene (r=0.95). The compound γ-muurolene presented positive correlation with (*E*)-calamenene (0.73), spathulenol (r=0.76), and *epi*-α-cadinol (0.79). Positive correlation coefficient (0.79) was observed between β-elemene and α-humulene, and between calamusenone and (*Z*)-β-guaiene. The compound β-caryophyllene presented negative correlation with calamusenone (-0,72) and (*Z*)-β-guaiene (-0,62). The compound α-cubenene presented positive correlation between α-copaene (0.66) and epi-α-cadinol (0.65). Epi-α-cadinol positively correlated to spathulenol (0.69) and (*E*)-calamenene (0.68) (Table 3).

Table 3. Correlation coefficients for the chemical compounds of the essential oils of *H. pectinata* plants in Sergipe, Brazil.

Compostos	**C02**	**C03**	**C04**	**C05**	**C06**	**C07**	**C08**	**C09**	**C10**	**C11**	**C12**	**C13**	**C14**	**C15**	**C16**	**C17**	**C18**	**C19**	**C20**	**C21**	**C22**	**C23**	**C24**	**C25**	**C26**	**C27**	**C28**	**C29**	**C30**
C01	0.35	0.17	0.02	0.13	0.02	-0.28	-0.44	-0.13	-0.23	-0.35	0.62	-0.56	0.15	-0.14	-0.04	-0.05	0.06	0.33	-0.06	0.39	-0.41	0.11	0.33	0.05	0.41	-0.22	-0.06	0.49	0.43
C02		0.07	-0.06	-0.20	-0.10	-0.28	-0.23	-0.14	-0.17	-0.21	0.19	-0.34	0.03	-0.23	-0.06	-0.05	0.27	0.15	-0.17	0.31	-0.09	0.48	-0.06	-0.13	-0.16	-0.10	-0.05	0.54	0.13
C03			0.94	-0.12	-0.03	-0.24	-0.01	-0.21	0.13	-0.14	0.19	-0.00	-0.22	-0.11	-0.04	-0.02	-0.31	0.34	-0.22	0.11	0.16	-0.07	-0.10	-0.12	0.26	-0.03	-0.09	0.12	-0.16
C04				-0.17	-0.15	-0.20	0.09	-0.14	0.20	-0.12	-0.08	0.13	-0.21	-0.15	-0.09	-0.07	-0.28	0.16	-0.20	-0.12	0.23	-0.13	-0.09	0.02	0.10	0.01	-0.08	-0.13	-0.18
C05					0.36	0.47	0.09	-0.13	-0.04	0.22	0.31	0.25	-0.45	0.50	0.24	0.18	-0.19	0.02	0.15	0.29	-0.13	-0.30	-0.28	0.67	0.50	-0.04	-0.25	0.10	-0.42
C06						0.56	0.02	0.12	0.38	0.51	0.38	0.24	-0.18	0.24	0.39	0.31	-0.26	0.30	0.46	0.47	-0.41	0.08	-0.34	-0.11	0.46	0.22	-0.34	0.22	-0.36
C07							0.10	0.17	0.34	0.79	-0.08	0.47	-0.20	0.30	0.09	0.03	-0.16	-0.20	0.48	-0.04	-0.28	-0.10	-0.30	0.26	0.14	0.15	-0.26	-0.25	-0.40
C08								-0.30	0.23	0.50	-0.18	0.54	-0.62	0.11	-0.17	-0.16	-0.34	-0.24	-0.11	-0.29	0.33	-0.40	-0.43	0.14	-0.10	-0.13	-0.35	-0.39	-0.72
C09									-0.24	0.01	-0.17	-0.09	0.60	0.04	-0.03	-0.13	0.37	0.12	-0.02	0.18	-0.19	0.44	0.11	-0.12	0.02	0.59	0.07	-0.21	0.21
C10										0.29	-0.20	0.41	-0.36	-0.29	0.28	0.34	0.09	-0.20	0.26	-0.39	-0.17	-0.26	-0.24	0.04	-0.10	-0.24	0.05	-0.04	-0.22
C11											0.01	0.42	-0.29	0.21	-0.02	-0.08	-0.35	-0.03	0.28	-0.01	-0.10	-0.05	-0.52	0.04	0.10	0.11	-0.35	-0.22	-0.60
C12												-0.42	-0.14	0.19	-0.07	-0.06	-0.20	0.73	-0.20	0.76	-0.13	0.02	-0.07	-0.15	0.79	-0.12	-0.07	0.69	-0.09
C13													-0.54	0.28	-0.02	-0.05	-0.37	-0.40	0.31	-0.40	0.03	-0.37	-0.32	0.19	-0.13	0.10	-0.33	-0.55	-0.56
C14														-0.19	-0.05	-0.11	0.42	0.12	-0.03	0.07	-0.39	0.61	0.49	-0.25	-0.17	0.30	0.33	-0.03	0.79
C15															-0.21	-0.27	-0.22	0.12	0.09	0.37	-0.02	-0.09	-0.23	0.24	0.55	0.20	-0.28	-0.18	-0.38
C16																0.95	-0.02	-0.08	0.45	0.15	-0.18	0.01	-0.09	-0.06	-0.11	0.08	-0.08	0.29	0.01
C17																	0.03	-0.10	0.40	0.08	-0.11	-0.10	-0.07	-0.14	-0.18	-0.11	0.10	0.39	0.04
C18																		-0.17	-0.22	-0.10	-0.10	0.33	0.06	0.09	-0.25	-0.13	0.52	0.20	0.41
C19																			-0.38	0.69	-0.01	0.27	-0.18	-0.21	0.68	0.23	0.10	0.55	-0.06
C20																				-0.13	-0.37	-0.08	-0.06	-0.09	-0.16	0.33	-0.17	-0.11	0.00
C21																					-0.12	0.39	-0.14	-0.17	0.69	0.22	-0.25	0.58	-0.13
C22																						-0.24	-0.35	0.01	-0.15	-0.02	0.06	-0.12	-0.45
C23																							-0.13	-0.15	-0.12	0.30	-0.11	0.16	0.33
C24																								-0.18	-0.11	-0.14	0.12	-0.13	0.74
C25																									0.14	-0.10	-0.11	-0.25	-0.22
C26																										0.13	-0.18	0.31	-0.27
C27																											-0.12	-0.20	-0.10
C28																												0.36	0.41
C29																													0.13
C30																													

C1: β-pinene. C2:1-octen-3-ol. C3: p-cymene. C4: γ-terpinene. C5: δ-elemene. C6:α-copaene. C7:β-elemene. C8: β-caryophyllene. C9: γ-elemene. C10: (Z)-muurola-3,5-diene. C11: α-humulene. C12: γ-muurolene. C13: germacrene D. C14: (Z)-β-guaiene. C15: bicyclogermacrene. C16: (E)-β-guaiene. C17: lepidozene. C18: γ-cadinene. C19: (E)-calamenene. C20: δ-cadinene. C21: spathulenol. C22: caryophyllene oxide. C23: 1.10-di-epi-cubenol. C24: 1-epi-cubenol. C25: α-acorenol. C26: epi-α-cadinol. C27: epi-α-muurolol. C28: cubenol. C29:α-cadinol. C30:calamusenone

The high correlation between compounds indicates that a plant with high content of the first compound will probably present high content of the second compound. This information can assist in the selection process of breeding programs (NIZIO et al., 2015). Possibly, this correlation can be explained by the ability of a single enzyme to synthesize different products, due to the similarity between the biosynthetic pathways of the compounds (DEGENHARDT et al., 2009).

Results of the present study indicate variation in the essential oil content, and show that the compounds β-elemene, β-caryophyllene, germacrene D, (*Z*)-β-guaiene, caryophyllene oxide and calamusenone were detected in greater proportions in native plants of *H. pectinate* of the state of Sergipe. The knowledge of the chemical diversity found in *H. pectinata* plants can assist in the selection of plants of specific interest. It also assists in the correct use and conservation of these genetic resources and in the discovery of new biological properties from the exploration and study of the different compounds present in the species.

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RESUMO: Os óleos essenciais são metabólitos secundários formados por diversos compostos químicos que atrelam a estas substâncias grande importância social e econômica. Essa diversidade de compostos geralmente é determinada pela constituição genética da planta, embora fatores ambientais também possam influenciar quanto ao tipo, quantidade e concentrações dos compostos presentes no óleo essencial. O objetivo deste trabalho foi analisar a diversidade química dos óleos essenciais de plantas nativas de *H. pectinata* coletadas no Estado de Sergipe. O óleo essencial de 24 plantas foi obtido por hidrodestilação e analisados por GC/MS-FID. Foram detectados 30 compostos no óleo essencial. Pela análise de agrupamento, foi observada a formação de dois grupos. Grupo 1 foi constituído por 18 plantas, e apresentou o β-elemeno (2,46-25,77%), β-cariofileno (16,20-60,95%), germacreno-D (0,00-21,59%) e óxido de cariofileno (5,38-42,21%) como compostos majoritários. Grupo 2 foi constituído por 6 plantas com β-cariofileno (5,68-15,57%), Z-β-guaieno (2,18-7,31%), óxido de cariofileno (1,58-22,89%) e calamusenona (23,12-64,36%) como compostos majoritários. Uma forte correlação foi observada entre os compostos p-cimeno e γ-terpineno (r=0,94) e entre (E)-β-guaieno e lepidozeno (r=0,95). Os resultados do presente estudo indicam que existe variação no teor do óleo essencial, e que os compostos β-elemeno, β-cariofileno, germacreno-D, (Z)-β-guaieno, óxido de cariofileno e calamusenona, foram detectados em maiores proporções nas plantas nativas de *H. pectinata* do Estado de Sergipe. O conhecimento da diversidade química encontrada nas plantas de *H. pectinata* pode auxiliar na seleção de plantas de interesse específico.

PALAVRAS-CHAVE: Planta medicinal. Germoplasma. Óleo volátil. Compostos químicos.

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