

# Chemical composition of the essential oil and fixed oil *Bauhinia pentandra* (Bong.) D. Dietr

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## ABSTRACT

**Background:** *Bauhinia pentandra* is popularly known as “mororó” and inhabits the Caatinga and Savannah biomes. **Objective:** This paper reports the chemical composition of the essential and fatty oils of the leaves from *B. pentandra*. **Materials and Methods:** The essential oil was obtained by hydrodistillation and the fixed oil by extraction with hexane, followed by saponification with KOH/MeOH, and methylation using MeOH/HCl. The constituents were analyzed by gas chromatography-mass spectrometry. **Results:** The major constituent of the essential oil was the phytol (58.78% ± 8.51%), and of the fatty oil were palmitic (29.03%), stearic (28.58%) and linolenic (10.53%) acids. **Conclusion:** Of the compounds identified in the essential oil, three are first reported in this species, and this is the first record of the chemical composition of the fixed oil.

**Key words:** *Bauhinia pentandra* (Bong.) D. Dietr, essential oil, fixed oil, gas chromatography-mass spectrometry, Leguminosae

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## INTRODUCTION

The genus *Bauhinia* (Leguminosae) consists of about 300 species, distributed in most tropical countries, including Africa, Asia, and America.<sup>[1]</sup> Species of the genus *Bauhinia* are present as trees, shrubs and vines, and in Brazil are used by the population as hypoglycemic agents.<sup>[2]</sup> Multiple biological activities are allocated to *Bauhinia* species such as antidiabetic, diuretic, hypocholesterolemic, antimicrobial, analgesic, antioxidant, larvicidal, acetylcholinesterase, anti-inflammatory,<sup>[2-7]</sup> among others. Chemical compositions of essential oils of *Bauhinias* are cited in the literature, among them *Bauhinia aculeata*, *B. brevipes*, *B. forficata*, *B. longifolia*, *B. pentandra*, *B. rufa*, *B. variegata*, *B. unguilata* and *B. acuruana*.<sup>[8-11]</sup> The *B. pentandra* species inhabits the Caatinga and Savannah biomes and is known in the Northeast region of Brazil as “mororó”. Literature reports the chemical composition of its essential oil from Rio de Janeiro-Brazil.<sup>[8]</sup> Therefore, the aim of this work is to identify the chemical composition of the essential and fatty oils from the leaves of *B. pentandra* species collected in the Medicinal Garden of Plants-Federal University of Ceará (UFC)-Brazil, whose composition was different from already reported.

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## MATERIALS AND METHODS

### Plant material

*Bauhinia pentandra* (Bong.) D. Dietr. leaves were collected at Medicinal Plants Garden, UFC. A voucher specimen (number 53444) is deposited in the Herbarium Prisco Bezerra of the Department of Biology, UFC.

### Essential oil extraction

The fresh leaves (162 g) were subjected to hydrodistillation process in Clevenger-type apparatus for 5 h. The hydrodistilled volatiles were dried over anhydrous sodium sulfate and stored in a freezer at 4°C until the analysis procedure. The experiment was performed in triplicate.

### Fixed oil extraction

The air-dried leaves (55 g) were extracted with hexane at room temperature for 5 days, followed by filtration and concentration under reduced pressure to yield a crude extract (0.924 g; 1.7%).

### Saponification

To the crude hexane extract (923 mg) was added MeOH (15 mL) and KOH (923 mg), which reacted for 1 h under reflux. After cooling, the mixture was diluted with H<sub>2</sub>O (40 mL) and extracted with hexane (2 mL × 50 mL). The aqueous phase was acidified to pH 3 with concentrated

HCl and extracted with EtOAc (2 mL × 50 mL). The combined EtOAc fractions were dried (Na<sub>2</sub>SO<sub>4</sub>) and concentrated under reduced pressure to give fatty acids (344 mg).

### Methylation

Fatty acids (344 mg) were refluxed for 1 h in MeOH (10 mL) in the presence concentrated HCl (1 mL). After cooling, the mixture was diluted with H<sub>2</sub>O (30 mL) and extracted with CH<sub>2</sub>Cl<sub>2</sub> (3 mL × 30 mL). The combined CH<sub>2</sub>Cl<sub>2</sub> fractions were dried (Na<sub>2</sub>SO<sub>4</sub>) and concentrated under reduced pressure to give methyl esters (221 mg). The crude reaction was chromatographed on a column Si gel, eluted with hexane, followed by CH<sub>2</sub>Cl<sub>2</sub>, and fractions were analyzed by thin-layer chromatography and gas chromatography-mass spectrometry (GC/MS).

### Gas chromatography-mass spectrometry

Analysis of the oils was performed on a Shimadzu/QP2010 GC/MS instrument employing the following conditions: RTX-5 (5% phenyl e 95% dimethylpolysiloxane) capillary column (30 mm × 0.25 mm, 0.25 μm film thickness); carrier gas: Helium (1 mL/min); column temperature: 40°C–180°C at 4°C/min then of 180°C–280°C at 20°C/min and held at 280°C for 10 min, for essential oil and RTX-5 (5% phenyl e 95% dimethylpolysiloxane) capillary column (30 mm × 0.25 mm, 0.25 μm film thickness); carrier gas:

Helium (1.46 mL/min); column temperature: 80°C–280°C at 5°C/min then of 280°C–300°C at 20°C/min and held at 300°C for 5 min, for fatty oil. The retention indices Kovat's were calculated using a series of standard n-alkane (C7–C30). The identification of compounds was performed by comparing their mass spectra with those of NIST08 library, retention indices, and published data.<sup>[12]</sup>

## RESULTS AND DISCUSSION

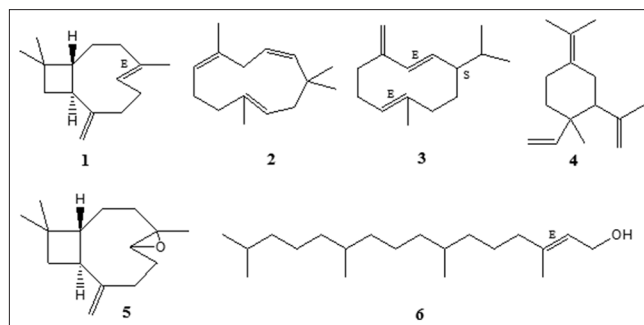
The essential oil yield from fresh leaves was 0.01%. The results of GC/MS analysis Table 1 shows the presence of 6 components [Figure 1], which 5 were sesquiterpenes (1–5, 37.17%) and 1 diterpene (6, 58.78%), representing 95.95 ± 1.02% of the total composition. The main constituent was phytol (6, 58.78% ± 8.51%), which was not reported in the previous study.<sup>[9]</sup> Beyond of phytol, germacrene D (3, 8.40 ± 1.04%) and elixene (4, 11.73 ± 1.52%) are first recorded in *B. pentandra*. Germacrene is an important component identified in the essential oil with significant biological activities.<sup>[13]</sup>

From the fatty oil, 11 components were identified, representing 85.53% of the total composition. The results of GC/MS analysis [Table 2] from methylated derivatives showed that the major components were methyl hexadecanoate (29.03%),

**Table 1: Chemical composition of the essential oil from the leaves of *B. pentandra***

Constituents	R.T. (min)	KI*	Area (%)
β-caryophyllene (1)	25.960	1428	13.64±5.37
α-humulene (2)	27.068	1463	2.66±0.61
Germacrene D (3)	27.977	1492	8.40±1.04
Elixene (4)	28.499	1509	11.73±1.52
Caryophyllene oxide (5)	31.201	1594	0.74±0.68
Phytol (6)	39.847	2123	58.78±8.51
Total			95.95±1.02

\*KI on RTX-5 capillary column. R.T.: Retention time; KI: Kovats index



**Figure 1:** Terpenoids identified in the essential oil extracted from *B. pentandra* (leaves fresh)

**Table 2: Chemical composition of the fixed oil from the leaves of *B. pentandra***

Constituents	R.T. (min)	KI*	Area (%)
Methyl dodecanoate	15.118	1498	4.13
Methyl tetradecanoate	19.797	1725	5.72
Methyl 9(Z)-9-hexadecenoate	23.620	1904	1.46
Methyl hexadecanoate	24.225	1931	29.03
Methyl heptadecanoate	26.030	2023	0.78
Methyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate	27.800	2117	28.93
Methyl octadecanoate	28.089	2132	10.58
Methyl (9Z,12Z)-9,12-octadecadienoate	28.510	2152	0.91
Methyl 18-methylnonadecanoate	31.546	2327	2.04
Methyl docosanoate	34.842	2529	1.39
Methyl tetracosanoate	37.893	2730	0.56
Total			85.53

\*KI on RTX-5 capillary column. R.T.: Retention time; KI: Kovats index

methyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate (28.93%) and methyl octadecanoate (10.58%), or palmitic, linolenic and stearic acids, respectively. The major compounds identified in the fatty acids are considered healthy for the human consumption.<sup>[14]</sup> This is the first report in the literature component of the fixed oil of this species.

Analysis of chemical constituents of less polar fraction of this species revealed the presence of components without toxicity. This species is used in the form of infusion in folk medicine, therefore, is important to know the chemical constituents, especially of leaves.

## CONCLUSION

Analysis of essential oil allowed the identification of six compounds, being the phytol (6, 58.78 ± 8.51%) the major constituent. Of the identified compounds, three are being reported for the first time in the species: germacrene D (3), elixene (4) and phytol (6).

The study of fatty acid profile in the hexane extract from leaves presented as major components the palmitic (29.03%), linolenic (28.93%) and stearic (10.58%) acids. To the best of our knowledge, this is the first report on the chemical composition of the fixed oil this species.

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