BJPS

Brazilian Journal of Pharmaceutical Sciences

http://dx.doi.org/10.1590/s2175-97902022e21609

Article

# Preliminary prospection of phytotherapic compounds from the essential oils from barks and leaves of Umburana (*Commiphora Leptophloeos*)

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The potential of the biome caatinga (exclusive from northeastern Brazil) has been evaluated in recent research for application in the pharmaceutical industry. Among the species of medicinal plants from caatinga, one can highlight the *Commiphora leptophloeos* (umburana), which has been used as infusions and syrups by the regional population for inflammatory and infectious diseases. Essential oils from umburana leaves and barks were obtained in a Clevenger apparatus and analyzed by gas chromatography/mass spectrometry, and total phenolic and flavonoids were determined by spectrophotometric analysis. It was observed that a large part of the major compounds present in the essential oil is described as having antitumor activity, enabling research in investigational oncology with umburana (*C. leptophloeos*). In addition, some little explored components have been identified, such as cadinene, alpha-selinene, and elemenone. Despite being easily found in several plants, there are no clinical trials involving their biological activity in a well-defined isolated form, which could make exploring new studies possible. Furthermore, the presence of phenolic compounds and flavonoids allows future studies about the potential antimicrobial and antioxidant activity.

**Keywords:** *Commiphora leptophloeos*. Medicinal plant. Gas chromatography. Essential oil.

## INTRODUCTION

Plants are used as a therapeutic resource by a large part of the population due to the great variety of chemical substances with antimicrobial, expectorant, antiseptic, anti-inflammatory, and hepatoprotective properties (Dutra *et al*., 2016). However, popular culture often induces the use of plants without any scientific evidence, in the form of essential oil, extracts, infusions, or patches to treat common infections. Bioprospecting studies involving various aspects of plant biology and phytochemistry are proving the traditional uses of several plants for therapeutic purposes (Trentin *et al*., 2011; Dutra *et al*., 2016).

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Brazil has one of the greatest biodiversity on the planet with the potential to provide products of natural origin, by the extraction of plants, and their respective active principles, for application in foods and drugs. The biome caatinga (exclusive from northeastern Brazil, with an area of around 735,000 km$^2$) has a great diversity of plants with high biological potential and great interest in the pharmaceutical industry, being a key point for the development of prospecting studies of plants, aiming to use as phytotherapics (Trentin *et al*., 2011).

Among the species of medicinal plants of the caatinga, *Commiphora leptophloeos (Mart.) J.B. Gillett* is a resinous angiosperm adapted to semi-arid and desert climates that survive in total sun exposure. It has been used in the form of infusions and syrups, by indigenous populations, for inflammatory and infectious diseases (Pereira *et al*., 2017; Silva *et al*., 2017). Some studies have demonstrated its anti-inflammatory and healing potential,

as too against gastritis, ulcers, bronchitis, coughs, inflammation of the urinary tract, and anesthetic and cytotoxic activities (Dong *et al*., 2017).

The literature register that secondary metabolites found in these species and other plants of the same genus are condensed tannins, anthocyanins, flavonoids, saponins, alkaloids, albumins, and sesquiterpenes (Dong *et al*., 2017; Fang *et al*., 2018).

Few studies on the detailed chemical composition of its essential oil have been reported. Most of the published studies on the chemical composition (by gas chromatographic analyzes) are related to other similar species such as C. *guidottii* (Yeo *et al*., 2016), *C. myrrha* (Ahamad *et al*., 2017), and *C. mukull* (Rhourrhi-Frih *et al*., 2012).

Because of the above, this work aims to evaluate in more detail the chemical composition of the essential oils of the Umburana bark and leaves and to indicate the potential phytotherapy application.

## MATERIAL AND METHODS

### Samples and Reagents

Samples of bark and leaves of *Commiphora leptophloeos* were collected in the "Barra da Onça Settlement" located in the city of Poço Redondo, Sergipe, Northeast Brazil (GPS 9 ° 48 '23 "S 37 ° 41' 08W"). The exsiccate of the plant material was deposited in the herbarium of Tiradentes University - Aracaju/SE.

The collection of biological material was according to the SISBio (Biodiversity Authorization and Information System), linked to the Chico Mendes Institute for Biodiversity Conservation (ICMBio), under registry number 62387-5. It was also registered in the National System management of Genetic heritage and Traditional Associated Knowledge (SISGEN) under number AD82169.

The plant materials (barks and leaves) were sanitized with deionized water, dried in an oven at 50 ºC for 48 hours, and ground in a stainless-steel knife mill. A mixture of n-alkanes (C7-C37) (Supelco Park, PA, USA) was used in the gas chromatograph coupled to quadrupole mass spectrometry (GC/qMS) to calculate the retention index. The carrier gas used was Helium (He) with purities higher than 99.999%, obtained from White Martins (Aracaju, SE).

### Essential oil extraction

The essential oil of *C. leptophloeos* was obtained by hydrodistillation in a graduated Clevenger apparatus using a method adapted from Hou *et al.* (2019). 50 g of plant material (leaves and bark) and 500 mL of distilled water was used for the extraction. The temperature was raised to 100 °C until boiling, then reduced to 75 °C and held for 2 hours. After extraction, the oil was collected and filtered in anhydrous sodium sulfate and stored in a vial protected from light with aluminum foil for further chromatographic analysis.

### GC/qMS analysis

The chromatographic analysis was performed by GC/qMS (SHIMADZU-GCMS-QP2010-Ultra, Japan), with automatic injector AOC- 20 (SHIMADZU, AOC-20i, Japan), capillary column SLB-5 (equivalent to 5% phenyl methyl silicone) with 60 m x 0.25 mm x 0.25 μm. Helium (99.999%) was used as carrier gas with a linear velocity of 31 cm $s^{-1}$.

Initially, 1 μL of the sample (1.000 mg $L^{-1}$ in dichloromethane) was injected in splitless mode. The temperatures of the injector, the interface, and the ion source were 280 ºC, ionization energy by electron impact (70 eV), and spectra scanning in masses in the range of 35 to 450 Daltons. The analysis was performed in the temperature ramp, with the initial temperature of 40 °C for 2 min, heating at 4 °C $min^{-1}$ until reaching the temperature of 300 °C, holding for 40 min.

Chromatography data were handled by the GCMS solution software, version 4.3. The identification of the compounds was performed by comparing the fragmentation profile of each compound with those present in the NIST 14 library (National Institute of Standards and Technology). Spectral similarity ≥ 80%, and Linear Temperature Programmed Retention Indices (LPTRI) with a maximum difference of 15 units for columns with similar polarities, were used as criteria for considering the

compound tentatively identified. The retention index was automatically calculated by the software of the equipment, using a mixture of linear alkanes from seven to thirty-seven carbon atoms in the chain.

### Total phenolic and flavonoids

The spectrophotometric analysis was performed in an equipment Shimadzu (model - 1900 UV-VIS, Japan) measured in triplicate in quartz cuvettes.

The total phenolic compounds of the essential oil were determined using the Folin-Ciocalteau reagent according to the methodology described by Djeridane *et al*. (2006). Five milligrams of each essential oil were weighed separately and transferred to volumetric flasks of 5 mL and completed their volume with methanol. After, 0.5 mL of this solution were added to test tubes, previously prepared with 2.5 mL of reagent Folin-Ciocalteau, distilled water (1:10) (v/v), and 2 mL of $Na_2CO_3$ solution 7.5 % (m/v). Subsequently, the test tubes with the samples were kept in a low-light environment and externally protected with aluminum foil for 2 hours. The absorbance was measured at 760 nm.

The flavonoid content was determined using the aluminum nitrate colorimetric method. as(Barbosa *et al*., 2019).

## RESULTS AND DISCUSSION

### Gas Chromatographic Analysis

The essential oil yield for the bark was 3.13% ± 0.30, while for the leaves it was 2.05% ± 0.24. These results may be justified by the resinous character of the plant. In addition, the extraction of the essential oil from leaves was more efficient when compared to the extraction performed by Da Silva *et al*. (2015) (Da Silva *et al*., 2015), which obtained only 0.08% oil using the same technique, but a higher amount of sample (150 g) and higher extraction time (4 h).

The chromatograms of the essential oils of barks and leaves of C. *Leptophloeos* can be viewed in Figure 1. It is possible to observe a different profile for each sample. In bark, the essential oil has highlighted the presence of compounds with lower boiling points, compared with the leaves essential oil.

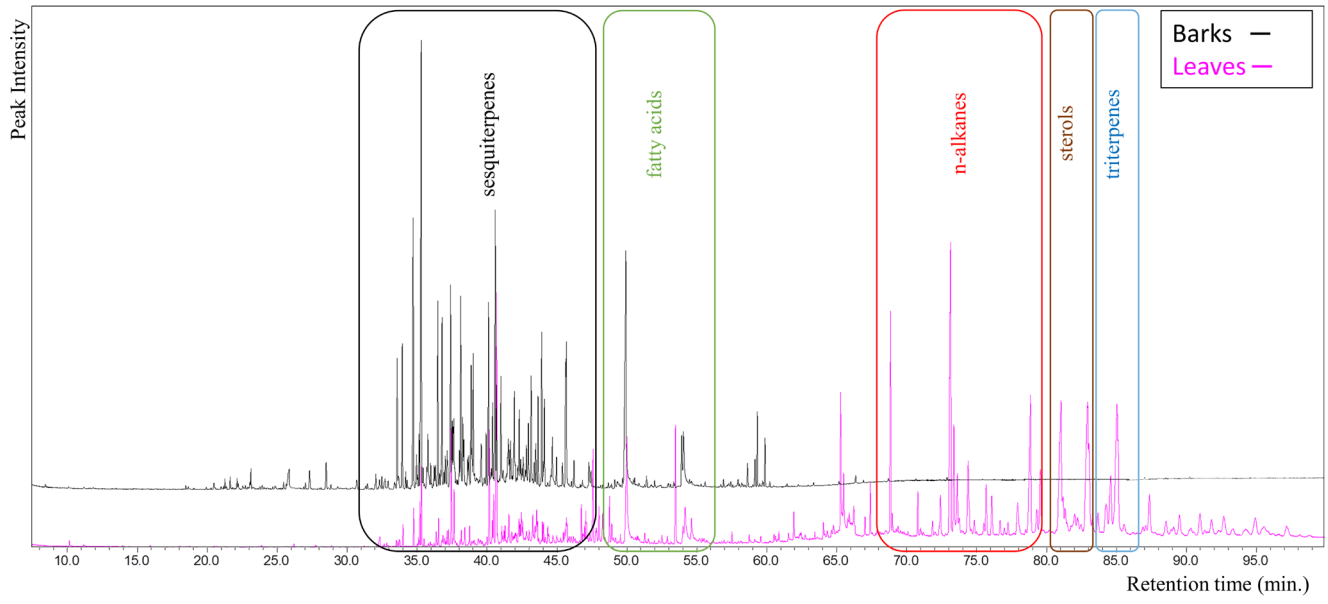


**FIGURE 1 -** Chromatogram analysis of the essential oil from *C. leptophloeos* barks (black) and leaves (pink) analyzed by GC/qMS.

The complete identification of compounds can be found in the Supplementary Electronic Material (Table SI). This Table shows the tentatively identified compounds, retention time, chemical class of compounds, relative area (%), and retention index.

Figure 2 shows the distribution of relative area for each identified chemical class of compounds in both samples, while the main compounds (area % > 3 %) for at least one of the samples are presented in Figure 3.

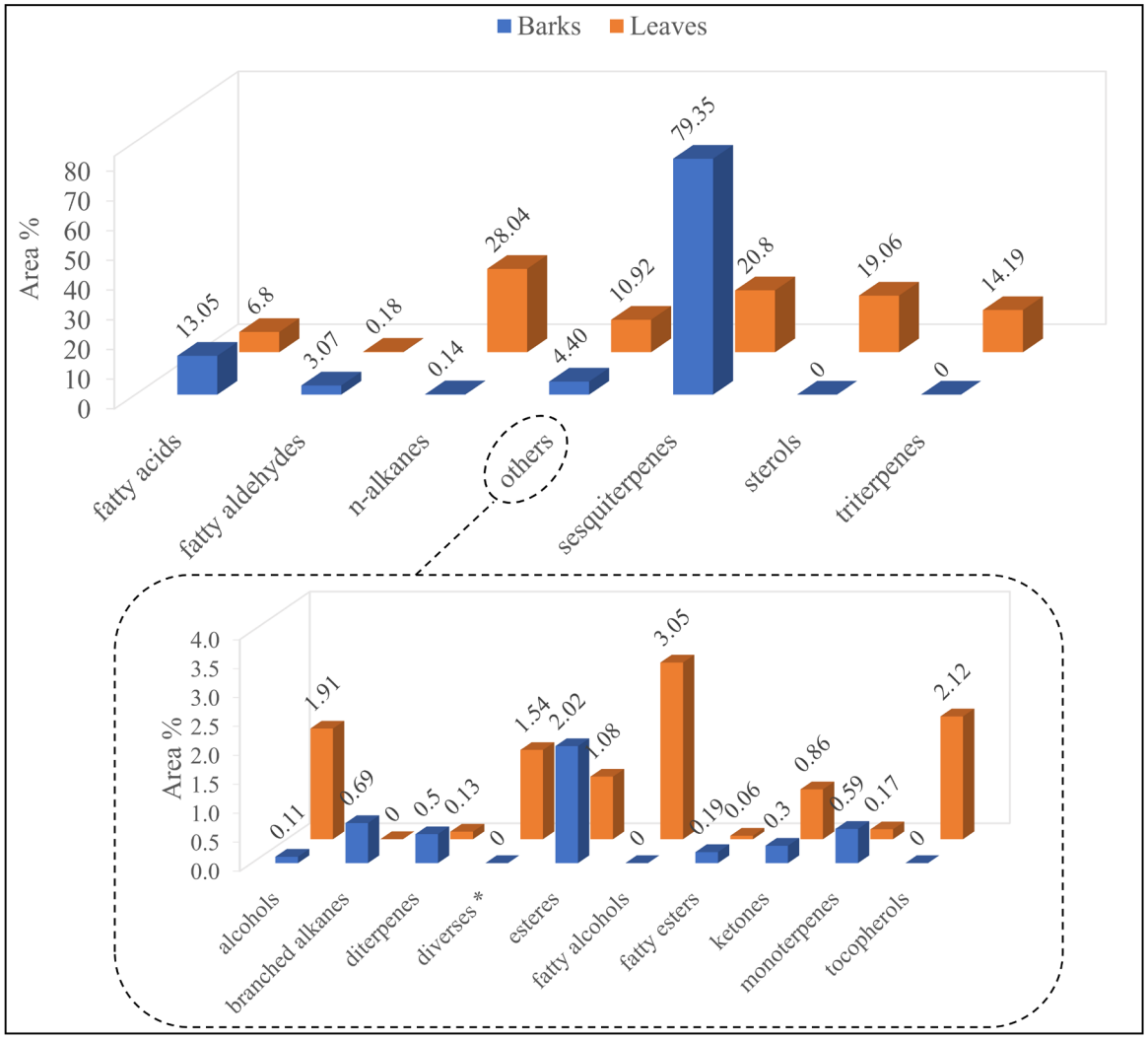


**FIGURE 2 -** Distribution of relative area for each identified chemical class of compounds.

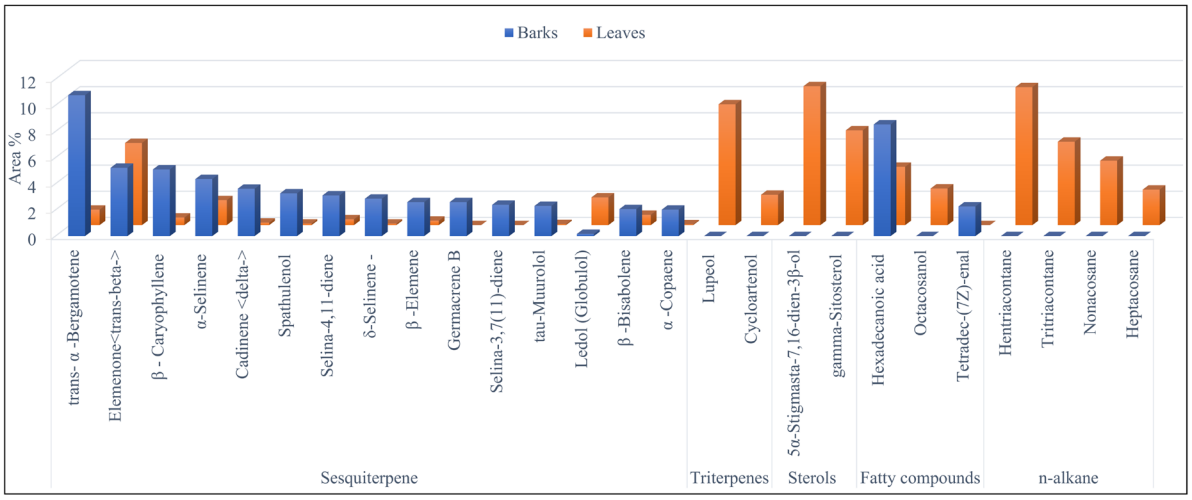


**FIGURE 3 -** Percentage area of the terpenes identified in the essential oil of barks and leaves from *C. leptophloeos*.

In the bark essential oil, 127 peaks were found, of which it was possible to identify 94 compounds (84.3%) and 29 remained without identification (15.7%). In the sample, sesquiterpenes present a larger percentage area (79.4%), followed by fatty acids (13.1%), aldehydes (3.1%), and esters (2.2%). Among the major compounds are β-caryophyllene, trans-α-bergamotene, α-selinene, δ-cadinene, β-elemenone, and hexadecenoic acid.

In the essential oil obtained from the leaves, 95 peaks were found, of which 83 compounds (87.3%) were tentatively identified and 12 were not identified (12.7%). In this sample, hydrocarbons correspond to 28.0%, sesquiterpenes 20.8%, and other classes are also present, such as sterols (19.1%), triterpenes (14.2%), fatty acids (6.3%), fatty alcohols (3.1%). Among the major compounds of leaf essential oil are β-elemenone, nonacosane, hentriacontane, γ-sitosterol, tritriacontane, lupeol, hexadecanoic acid, 5α-Stigmasta-7,16-dien-3β-ol.

Only one study was found in the literature (Da Silva *et al*., 2015), approaching the GC-MS analysis of essential oil of the C. *leptophloeos* leaves. In that work was observed the presence of only 55 compounds, with 46 tentatively identified compounds, being α-phellandrene, trans -caryophyllene, and β-phellandrene, the majors (Da Silva *et al*., 2015).

The antioxidant activity has been described in the literature for fatty acids (Elagbar *et al*., 2016) and gamma-sitosterol (Yoshida, Niki, 2003), a triterpene phytosterol present in the essential oil. Phytosterols have a well-known activity, being that one of the main, is the reduction of serum cholesterol and lipid levels (Styrczewska *et al*., 2015). In addition, triterpenes have been described as compounds that improve the quality of healing by regulating pro-and anti-inflammatory mediators, chemokines, growth factors, inducing granulation formation, re-epithelization, and wound contraction (Kim *et al*., 2013). Styrczewska *et al*. (2015) (Styrczewska *et al*., 2015). demonstrated the synergistic activity of cannabidiol with β-sitosterol inducing anti-inflammatory and collagen production activities, being phytosterol responsible for the matrix remodeling effect.

The essential oil of the leaves also presented lupeol as one of its major compounds, which presents involvement in the healing of cutaneous wounds by stimulating the migration of keratinocytes and increasing the contraction of fibroblasts in a collagen matrix (Beserra *et al*., 2018). Lupeol is a triterpene widely found in medicinal plants and has a varied pharmacological potency with anti-inflammatory, antioxidant, anti-infectious, antihyperglycemic, antiasthmatic, antiarthritic, cardioprotective, neuroprotective, hepatoprotective, and chemosensitizing effects (Badshah *et al*., 2016).

Wang *et al*. (2018) demonstrated the *in vitro* anti-cancer effect of lupeol by modifying cell viability, induction of apoptosis, migration, cell cycle arrest, and inactivation of Wnt-β-catenin signaling activity in human

colorectal cancer cells. Other authors further suggest that this compound may be used in the future as an inhibitor of human osteosarcoma cell metastases (Hsu *et al*., 2019).

The γ-sitosterol, another phytosterol presented in leaves, has been described by its ability to increase the secretion of insulin in the presence of glucose (Sirikhansaeng *et al*., 2017) and anti-cancer activities interrupting the cell cycle causing apoptosis of cancer cells, being cytotoxic to cell lines the colon and liver (Endrini *et al*., 2014). Suttiarporn *et al*. (2015) also claim that phytosterol concentrations in the blood may increase the proliferation of antileukemic cells and suggest extraction of the compound for addition at higher doses in other foods and dietary supplements.

The identification and isolation of plant-derived antioxidant compounds may be a solution to treat a variety of lesions and diseases caused by oxidative stress, such as depression and hepatotoxicity (Mhalla *et al*., 2018).

Sesquiterpenes are the chemical class with the highest number of compounds in the essential oils of barks of *C. Leptophloeos*, being were found 63 sesquiterpenes (Table SI) corresponding to 67% of the total area of the chromatogram (considering the identified and unknown peaks).

As can be seen in Figures 1 and 3 the major compounds in sesquiterpenes were trans-α-bergamotene (10.8%), followed by trans-β-elemenone (5.3%), β-caryophyllene (5.1%) and α-selinene (4.4%). Already in the essential oil of leaves, 42 sesquiterpenes were found (Table SI) corresponding to only 18.5% (Figure 2) of the total area of the chromatogram. Although the essential oil of leaves of C. *Leptophloeos* presents many peaks of sesquiterpenes, the total percentual area was inferior when compared to the essential oil of the bark. The sesquiterpene that presented the highest relative area (Figure 4) was trans-β- Elemenone (6.3%).

Govindarajan *et al*. (2018) identified the trans-β-elemenone compound as a major component in the essential oil of the pitanga leaves (Eugenia uniflora) and demonstrated efficacy against *Anopheles subpictus*, *Aedes albopictus,* and *Culex tritaeniorhynchus* larvae, as well as low toxicity for humans.

Another important compound of the essential oil, β-caryophyllene, is a bicyclic sesquiterpene with a cyclobutene ring also found in several plants, which has biological importance, anticonvulsive, antimalarial, antileishmanial, local anesthetic, spasmolytic and antimicrobial activities have been described (Fidyt *et al*., 2016). In addition, this compound has potential for the treatment of inflammatory diseases, atherosclerosis, ischemia, and cerebral inflammation (Viveros-Paredes *et al*., 2017; Hammad *et al*., 2018), as well as ischemic heart and liver lesions (Hammad *et al*., 2018).

As well as other compounds present in essential oil from *C. leptophloeos* that present anti-cancer activities, studies have already demonstrated that β-caryophyllene has chemo-preventive or antimutagenic properties, besides having an antioxidant role, being able to be desensitized chemo-resistant cancer cells when combined with other drugs (Di Giacomo *et al*., 2017 and 2018).

The trans-α-bergamotene compound has been identified as an active compound that can attract ectoparasites such as *Melittobia digitata* (wasps), serving as a trapping strategy, where pests are attracted away from the main crop (Yin, Wong 2019).

Li *et al*. (2017) found trans-α-bergamotene as one of the main compounds in the distilled fraction of basil oil and associated its presence with the ability of this oil in reducing inflammatory cytokines.

Several studies have identified the compounds α-selinene, cadinene, and elemenone, however, there is a deficiency of clinical trials demonstrating its isolated properties. Cadinene has recently been identified in the study by Zhu *et al*. (2019) which demonstrated its cytotoxicity and selectivity for the human liver cancer cell line. In general, studies have described such compounds as part of the class of sesquiterpenes with anti-inflammatory, bactericidal, antioxidant, and antitumor activities (Dutra *et al*., 2016; Fidyt *et al*., 2016; Viveros-Paredes *et al*., 2017).

## Determination of phenolic and flavonoids compounds

The phenolic compounds have in their structure one or more hydroxyls directly connected to an aromatic ring. Flavonoids, inserted within phenolic compounds, are subdivided into flavonols, flavones, flavanones,

anthocyanidins, and isoflavones according to their chemical structure (Singh *et al*., 2017; Gandhi *et al*., 2018).

For the analysis of phenolics compounds and flavonoids was constructed analytical curves which can be viewed in Figure 4.

The analytical curve for the quantification of the phenolic compounds showed a coefficient of determination of 0.9954 (Figure 4a), which reflects a high degree of linearity. The obtained polyphenols content, measured in mg GAE $g^{-1}$, was 60.02 ± 0.19 for barks and 62.56 ± 0.2 for leaves.

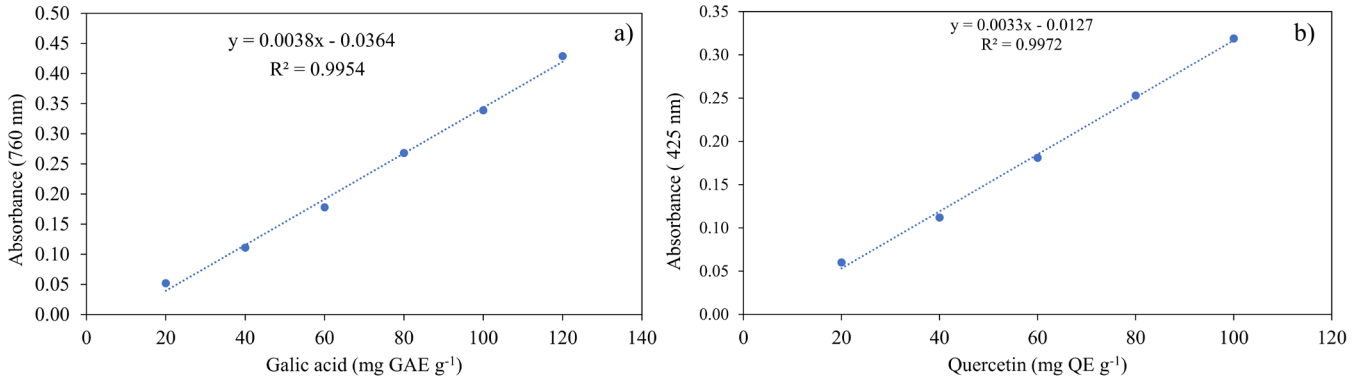


**FIGURE 4 -** Analytical curve for the analysis of phenols and flavonoids. a) Gallic acid with concentrations of 20, 40, 60, 80, 100 and 120 mg GAE $g^{-1}$ analyzed at 765 nm, b) Quercitina with concentrations of 20, 40, 60, 80, 100 mg QE $g^{-1}$ analyzed at 420 nm.

These values were higher than those presented by Pereira *et al*. (2017) (Pereira *et al*., 2017), which obtained 20.3 ± 0.78 mg GAE $g^{-1}$ in its aqueous extract from barks obtained in Catimbau National Park (Pernambuco/ Brazil). Phenolic substances have a higher affinity for polar solvents such as ethyl alcohol (Tiwari *et al*., 2011), but high concentrations of these compounds were found in essential oil too.

The coefficient of determination obtained from the analytical curve for flavonoids was 0.9972 (Figure 4b). The total flavonoids of samples varied from 64.56 ± 0.2 mg QE $g^{-1}$ in essential oil from barks, slightly higher than the leaves, 57.18 ± 0.17 mg QE $g^{-1}$.

The phenolic compounds tentatively identified by GC/qMS in the leaves correspond to only 2.15% of the area (eugenol, gamma-tocopherol, and α-tocopherol). In the bark sample, no phenolic compounds were identified. About flavonoids, no component was tentatively identified in the samples by GC/qMS. The difficulty in identifying these classes of molecules is associated with the complexity of the sample since more than 10% of the area in both samples refers to unidentified compounds. For a more complete elucidation of these components, it is necessary to employ a methodology with greater separation power, such as comprehensive two-dimensional gas chromatography.

Phenolic compounds and flavonoids are described in the literature as they have important biological activities such as antioxidant (Rufino *et al*., 2009), immunomodulating (Talhaoui *et al*., 2016; Jarger, Parylak, Gage, 2018), anti-inflammatory (Oteiza *et al*., 2018), gastroprotective (Yousefian *et al*., 2018) and antimicrobial activity (Santos *et al*., 2015; Silva *et al*., 2016). The plant is responsible for the bactericidal activity against gram-positive bacteria *E. faecalis*, *B. subtilis*, *M. luteus,* and *S. aureus*, according to Pereira *et al.* (2017) (Pereira *et al*., 2017). This result may be promising for the evaluation of the bactericidal and bacteriostatic activity of these and other strains using the essential oil of *Commiphora leptophloeos* collected in the state of Sergipe.

## CONCLUSIONS

In this work, several constituents of the essential oil of umburana (*Commiphora leptophloeos*) were tentatively identified, which present new biotechnological possibilities, indicating the beginning of great research involving plants of the caatinga biome of northeastern Brazil.

It was observed that the major compounds on the essential oil are known by their antitumor activity, creating the possibility of investigations in investigational oncology with the essential oil of umburana. Still, compounds little exploited, like cadinene, alpha-selinene, and elemenone, despite being easily found in several plants, have no clinical trials involving their biological activity in a well-defined isolated form, which could make possible the exploration in new studies.

The presence of phenolic compounds and flavonoids allows the exploration of studies with bactericidal activity investigation with strains of various bacteria, which helps in the possibility of new therapies against microbial resistance.

## ACKNOWLEDGMENT

The author thanks CAPES and CNPq for the financial support.

## CONFLICT OF INTEREST

The authors declare that there is no conflict of interest associated with this work.

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## SUPPLEMENTARY ELECTRONIC MATERIAL

**TABLE SI -** Tentatively identified compounds in Essential Oils from barks and leaves of *Commiphora Leptophloeos* by GC/qMS

| Compound name | Chemical Classes | R.T. | Area % | | LTPRI | | | Reference (NIST WEB BOOK) |
|---|---|---|---|---|---|---|---|---|
| | | | Barks | Leaves | Exp | Lit. | Diff | |
| 1-Hexanol, 3,5,5-trimethyl | Alcohol | 20.57 | 0.04 | 0.00 | 1039 | 1049 | -10 | Begnaud, Pérès, et al., 2003 |
| Geraniol (2,6-Octadien-1-ol, 3,7-dimethyl) | Alcohol | 28.85 | 0.07 | 0.00 | 1252 | 1260 | -8 | Cao, Li, et al., 2011 |
| Isophytol | Alcohol | 49.53 | 0.00 | 0.07 | 1947 | 1947 | 0 | Todua, 2011 |
| Phytol | Alcohol | 53.47 | 0.00 | 1.84 | 2114 | 2114 | 0 | Skaltsa, Mavrommati, et al., 2001 |
| **alcohols** | | | **0.11** | **1.91** | | | | |
| Benzoic acid, octyl ester | Esters | 44.54 | 0.13 | 0.00 | 1754 | 1757 | -3 | Korhonen, 1986, |
| abd-7,13(E)-dien-15-yl acetate | Esters | 59.32 | 1.16 | 0.00 | 2387 | 2393 | -6 | Anastasaki, Demetzos, et al., 1999 |
| Kolavenol acetate | Esters | 59.88 | 0.72 | 0.00 | 2415 | 2412 | 3 | Andriamaharavo, 2014 |
| Octacosyl acetate | Esters | 76.09 | 0.00 | 1.08 | 3215 | 3215 | 0 | Zheng and White, 2008 |
| **esteres** | | | **2.02** | **1.08** | | | | |
| Octanoic acid | Fatty acid | 25.87 | 0.81 | 0.00 | 1172 | 1170 | 2 | Andriamaharavo, 2014 |
| Geranic acid | Fatty acid | 32.27 | 0.02 | 0.30 | 1350 | 1355 | -5 | Andriamaharavo, 2014 |
| Decanoic acid | Fatty acid | 32.72 | 0.36 | 0.00 | 1363 | 1373 | -10 | Engel and Ratel, 2007 |
| Tetradecanoic acid | Fatty acid | 44.69 | 1.24 | 0.19 | 1760 | 1759 | 1 | Lalel, Singh, et al., 2003 |
| Pentadecanoic acid | Fatty acid | 47.28 | 0.50 | 0.00 | 1858 | 1867 | -9 | Tret'yakov, 2008 |
| 9-Hexadecenoic acid | Fatty acid | 49.35 | 0.25 | 0.00 | 1949 | 1957 | -8 | Tret'yakov, 2007 |
| Hexadecanoic acid | Fatty acid | 49.97 | 8.54 | 4.46 | 1966 | 1963 | 3 | Yu, Liao, et al., 2007 |
| Linolenic acid, methyl ester | Fatty acid | 53.35 | 0.06 | 0.00 | 2109 | 2108 | 1 | Rout, Rao, et al., 2007 |
| 9,12-Octadecadienoic acid | Fatty acid | 53.92 | 1.27 | 0.00 | 2134 | 2133 | 1 | Radulovic, Dordevic, et al., 2010 |
| Linoleic acid | Fatty acid | 54.17 | 0.00 | 0.72 | 2145 | 2144 | 1 | Saroglou, Dorizas, et al., 2006 |
| Octadecanoic acid | Fatty acid | 54.62 | 0.00 | 0.59 | 2165 | 2166 | -1 | bin Jantan, Yalvema, et al., 2005 |
| Palmitic acid β-monoglyceride | Fatty acid | 61.93 | 0.00 | 0.54 | 2520 | 2519 | 1 | Andriamaharavo, 2014 |

**TABLE SI -** Tentatively identified compounds in Essential Oils from barks and leaves of *Commiphora Leptophloeos* by GC/qMS

| Compound name | Chemical Classes | R.T. | Area % | | LTPRI | | | Reference (NIST WEB BOOK) |
|---|---|---|---|---|---|---|---|---|
| | | | Barks | Leaves | Exp | Lit. | Diff | |
| **fatty acids** | | | **13.05** | **6.80** | | | | |
| 1-Hexacosanol | Fatty Alcohol | 68.97 | 0.00 | 0.26 | 2907 | 2906 | 1 | Andriamaharavo, 2014 |
| Octacosanol | Fatty Alcohol | 73.38 | 0.00 | 2.80 | 3113 | 3110 | 3 | Andriamaharavo, 2014 |
| **fatty alcohols** | | | **0.00** | **3.05** | | | | |
| Pentadecanal | Fatty Aldehyde | 43.49 | 0.80 | 0.00 | 1715 | 1717 | -2 | Flamini, Tebano, et al., 2006 |
| Heptadecanal | Fatty Aldehyde | 48.92 | 0.00 | 0.18 | 1922 | 1922 | 0 | Tkachev, Dobrotvorsky, et al., 2000 |
| Tetradec-(7Z)-enal | Fatty Aldehyde | 54.05 | 2.27 | 0.00 | 2140 | 2141 | -1 | Radulovic, Blagojevic, et al., 2009 |
| **fatty aldehydes** | | | **3.07** | **0.18** | | | | |
| Hexadecanoic acid, methyl ester | Fatty Esters | 49.14 | 0.19 | 0.00 | 1931 | 1926 | 5 | Quijano, Salamanca, et al., 2007 |
| Hexadecanoic acid, ethyl ester | Fatty Esters | 50.63 | 0.00 | 0.06 | 1992 | 1992 | 0 | Rout, Rao, et al., 2007 |
| **fatty esters** | | | **0.19** | **0.06** | | | | |
| Decane, 4- methyl- | branched-alkane | 21.17 | 0.05 | 0.00 | 1052 | 1054 | -2 | Oruna-Concha, Ames, et al., 2002 |
| Decane, 5- methyl- | branched-alkane | 21.27 | 0.15 | 0.00 | 1054 | 1057 | -3 | Rembold, Wallner, et al., 1989 |
| Decane, 3- methyl- | branched-alkane | 21.64 | 0.19 | 0.00 | 1068 | 1069 | -1 | Zaikin and Borisov, 2002 |
| Decane, 2- methyl- | branched-alkane | 22.13 | 0.13 | 0.00 | 1075 | 1076 | -1 | Saroglou, Marin, et al., 2007 |
| Undecane, 5- methyl- | branched-alkane | 25.46 | 0.08 | 0.00 | 1161 | 1159 | 2 | Kallio, Jussila, et al., 2006 |
| Undecane, 2- methyl- | branched-alkane | 25.65 | 0.08 | 0.00 | 1166 | 1164 | 2 | Kallio, Jussila, et al., 2006 |
| **branched alkanes** | | | **0.69** | **0.00** | | | | |
| Undecane | n-alkane | 23.06 | 0.11 | 0.00 | 1099 | 1100 | -1 | Standard |
| Dodecane | n-alkane | 26.89 | 0.04 | 0.00 | 1200 | 1200 | 0 | Standard |
| Tetracosane | n-alkane | 59.58 | 0.00 | 0.10 | 2400 | 2400 | 0 | Standard |
| Heptacosane | n-alkane | 65.29 | 0.00 | 2.71 | 2700 | 2700 | 0 | Standard |
| Octacosane | n-alkane | 67.02 | 0.00 | 0.25 | 2799 | 2800 | -1 | Standard |
| Nonacosane | n-alkane | 68.85 | 0.00 | 4.93 | 2901 | 2900 | 1 | Standard |
| Triacontane | n-alkane | 70.80 | 0.00 | 0.91 | 2999 | 3000 | -1 | Standard |
| Hentriacontane | n-alkane | 73.14 | 0.00 | 10.55 | 3104 | 3100 | 4 | Standard |
| Dotriacontane | n-alkane | 75.69 | 0.00 | 1.31 | 3202 | 3200 | 2 | Standard |
| Tritriacontane | n-alkane | 78.85 | 0.00 | 6.38 | 3304 | 3300 | 4 | Standard |
| Hexatriacontane | n-alkane | 92.67 | 0.00 | 0.91 | 3607 | 3600 | 7 | Standard |
| **n-alkanes** | | | **0.14** | **28.04** | | | | |
| 6-Methyl-2-heptene-5-one | Ketone | 18.47 | 0.06 | 0.00 | 985 | 982 | 3 | Bastos, Ishimoto, et al., 2006 |
| 5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)- | Ketone | 35.55 | 0.05 | 0.00 | 1449 | 1456 | -7 | Xian Q., Chen H., et al., 2006 |
| Phytone | Ketone | 46.90 | 0.10 | 0.11 | 1843 | 1842 | 1 | Bendiabdellah, El Amine Dib, et al., 2012 |
| Farnesyl acetone | Ketone | 48.72 | 0.10 | 0.75 | 1915 | 1913 | 2 | Mondello, 2012 |
| **ketones** | | | **0.30** | **0.86** | | | | |
| Hinokinin | Lignan | 73.63 | 0.00 | 1.28 | 3103 | 3096 | 7 | Andriamaharavo, 2014 |

**TABLE SI -** Tentatively identified compounds in Essential Oils from barks and leaves of *Commiphora Leptophloeos* by GC/qMS

| Compound name | Chemical Classes | R.T. | Area % | | LTPRI | | | Reference (NIST WEB BOOK) |
|---|---|---|---|---|---|---|---|---|
| | | | Barks | Leaves | Exp | Lit. | Diff | |
| Loliolide | ketone | 45.57 | 0.00 | 0.22 | 1792 | 1784 | 8 | Andriamaharavo, 2014 |
| Eugenol | Phenols | 32.66 | 0.00 | 0.03 | 1361 | 1365 | -4 | Mondello, Sciarrone, et al., 2007 |
| **others** | | | **0.00** | **1.54** | | | | |
| Myrcene | Monoterpene | 18.65 | 0.05 | 0.00 | 989 | 989 | 0 | Dharmawan, Kasapis, et al., 2007 |
| Ocimene (1,3,6-Octatriene, 3,7-dimethyl) | Monoterpene | 20.98 | 0.05 | 0.00 | 1047 | 1048 | -1 | Dob, Dahmane, et al., 2006, |
| Linalool | Monoterpene | 23.13 | 0.29 | 0.00 | 1100 | 1100 | 0 | Cho, Namgung, et al., 2008 |
| Linalool oxide <trans-> | Monoterpene | 26.21 | 0.00 | 0.03 | 1180 | 1176 | 4 | Adams, 2017 |
| Terpineol, cis-ß- | Monoterpene | 27.03 | 0.11 | 0.00 | 1202 | 1207 | -5 | Cho, Namgung, et al., 2008 |
| Myrtenyl acetate | Monoterpene | 31.45 | 0.11 | 0.00 | 1326 | 1326 | 0 | Houël., 2015 |
| 8-Hydroxylinalool | Monoterpene | 32.84 | 0.00 | 0.04 | 1367 | 1367 | 0 | Andriamaharavo, 2014 |
| Isogermacrene D | Monoterpene | 35.11 | 0.00 | 0.09 | 1435 | 1439 | -4 | Radulovic, Lazarevic, et al., 2007 |
| **monoterpenes** | | | **0.59** | **0.17** | | | | |
| 4,8,12,16-Tetramethylheptadecan-4-olide | Diterpenes | 58.75 | 0.00 | 0.13 | 2359 | 2364 | -5 | Andriamaharavo, 2014 |
| Methyl kolavenate | Diterpenes | 59.16 | 0.50 | 0.00 | 2379 | 2372 | 7 | Andriamaharavo, 2014 |
| **diterpenes** | | | **0.50** | **0.13** | | | | |
| Supraene | Triterpene | 67.40 | 0.00 | 0.80 | 2820 | 2822 | -2 | Steiner, Steidle, et al., 2005 |
| Lup-20(29)-en-3-one | Triterpene | 82.01 | 0.00 | 0.36 | 3390 | 3384 | 6 | Andriamaharavo, 2014 |
| Cycloartenol | Triterpene | 84.59 | 0.00 | 2.32 | 3454 | 3466 | -12 | Andriamaharavo, 2014 |
| Lupeol | Triterpene | 85.04 | 0.00 | 9.24 | 3459 | 3450 | 9 | Leite, 2018 |
| Friedelan-3-one | Triterpene | 87.36 | 0.00 | 1.47 | 3510 | 3511 | -1 | Andriamaharavo, 2014 |
| **triterpenes** | | | **0.00** | **14.19** | | | | |
| Bicycloelemene | Sesquiterpene | 32.06 | 0.23 | 0.00 | 1344 | 1338 | 6 | Houël., 2015 |
| α -Cubebene | Sesquiterpene | 32.49 | 0.18 | 0.00 | 1357 | 1356 | 1 | Cardeal, da Silva, et al., 2006 |
| α -Copaene | Sesquiterpene | 33.61 | 2.02 | 0.06 | 1389 | 1393 | -4 | Carasek and Pawliszyn, 2006 |
| β -Elemene | Sesquiterpene | 33.97 | 2.60 | 0.34 | 1400 | 1396 | 4 | Gauvin-Bialecki and Marodon, 2009 |
| β - Caryophyllene | Sesquiterpene | 34.74 | 5.10 | 0.58 | 1424 | 1423 | 1 | Houël., 2015 |
| γ-Elemene | Sesquiterpene | 34.97 | 0.53 | 0.00 | 1431 | 1432 | -1 | Houël., 2015 |
| β -Ylangene | Sesquiterpene | 35.03 | 0.21 | 0.04 | 1433 | 1431 | 2 | Mosayebi, Amin, et al., 2008 |
| Caryophyllene | Sesquiterpene | 35.18 | 0.83 | 0.62 | 1438 | 1440 | -3 | Cardeal, da Silva, et al., 2006 |
| trans- α -Bergamotene | Sesquiterpene | 35.31 | 10.77 | 1.18 | 1442 | 1441 | 1 | Benkaci-Ali, Baaliouamer, et al., 2007 |
| β -Copaene | Sesquiterpene | 35.46 | 0.34 | 0.11 | 1447 | 1437 | 10 | Andriamaharavo, 2014 |
| α -Guaiene | Sesquiterpene | 35.50 | 0.04 | 0.00 | 1448 | 1446 | 2 | Cardeal, da Silva, et al., 2006 |
| β -Farmesene | Sesquiterpene | 35.70 | 0.34 | 0.00 | 1454 | 1459 | -5 | Flamini, Cioni, et al., 2007 |
| Aromandendrene | Sesquiterpene | 35.77 | 1.50 | 0.00 | 1456 | 1447 | 9 | Elias, Simoneit, et al., 1997 |
| epi-β-Caryophylleno | Sesquiterpene | 35.83 | 0.00 | 0.03 | 1458 | 1463 | -5 | Yu, Liao, et al., 2007 |

**TABLE SI -** Tentatively identified compounds in Essential Oils from barks and leaves of *Commiphora Leptophloeos* by GC/qMS

| Compound name | Chemical Classes | R.T. | Area % | | LTPRI | | | Reference (NIST WEB BOOK) |
|---|---|---|---|---|---|---|---|---|
| | | | Barks | Leaves | Exp | Lit. | Diff | |
| Valerena-4,7(11)-diene | Sesquiterpene | 35.97 | 0.40 | 0.04 | 1462 | 1465 | -3 | Andriamaharavo, 2014 |
| Cadina-3,5-diene | Sesquiterpene | 36.05 | 0.06 | 0.00 | 1465 | 1457 | 8 | Dickschat, Martens, et al., 2005 |
| Alloaromadendrene | Sesquiterpene | 36.22 | 0.37 | 0.00 | 1470 | 1464 | 6 | Houël., 2015 |
| Humulene < α -> | Sesquiterpene | 36.34 | 0.48 | 0.25 | 1474 | 1467 | 7 | Dharmawan, Kasapis, et al., 2007 |
| Selina-4,11-diene | Sesquiterpene | 36.51 | 3.11 | 0.45 | 1479 | 1476 | 3 | Houël., 2015 |
| ε-Cadinene - | Sesquiterpene | 36.60 | 0.27 | 0.00 | 1482 | 1482 | 0 | Houël., 2015 |
| Germacrene D | Sesquiterpene | 36.70 | 0.32 | 0.00 | 1485 | 1484 | 1 | Houël., 2015 |
| δ-Selinene - | Sesquiterpene | 36.82 | 2.86 | 0.12 | 1489 | 1489 | 0 | Houël., 2015 |
| β-Selinene | Sesquiterpene | 36.93 | 0.32 | 0.00 | 1492 | 1493 | -1 | Houël., 2015 |
| Curzerene | Sesquiterpene | 37.14 | 0.56 | 0.17 | 1499 | 1497 | 2 | Houël., 2015 |
| α-Selinene | Sesquiterpene | 37.43 | 4.36 | 1.91 | 1508 | 1499 | 9 | Houël., 2015 |
| α -Muurolene | Sesquiterpene | 37.54 | 1.19 | 0.11 | 1512 | 1517 | -5 | Jalali-Heravi, Zekavat, et al., 2006 |
| Germacrene A - | Sesquiterpene | 37.59 | 0.45 | 0.00 | 1513 | 1510 | 3 | Houël., 2015 |
| β -Bisabolene | Sesquiterpene | 37.64 | 2.06 | 0.79 | 1515 | 1514 | 1 | Andriamaharavo, 2014 |
| γ-Cadinene | Sesquiterpene | 37.78 | 0.32 | 0.03 | 1520 | 1515 | 5 | Houël., 2015 |
| δ-Cadinene | Sesquiterpene | 38.06 | 0.67 | 0.09 | 1529 | 1519 | 10 | Houël., 2015 |
| Cadinene <delta-> | Sesquiterpene | 38.15 | 3.62 | 0.19 | 1532 | 1534 | -2 | Houël., 2015 |
| Calamenene <trans-> | Sesquiterpene | 38.27 | 1.19 | 0.00 | 1536 | 1524 | 12 | Houël., 2015 |
| o-Cadinene - | Sesquiterpene | 38.38 | 1.06 | 0.30 | 1540 | 1538 | 2 | Houël., 2015 |
| Elemol | Sesquiterpene | 38.73 | 0.62 | 0.27 | 1551 | 1549 | 2 | Houël., 2015 |
| Germacrene B | Sesquiterpene | 38.86 | 2.60 | 0.00 | 1555 | 1557 | -2 | Oliveira, Leitao, et al., 2006 |
| α -Calacorene | Sesquiterpene | 38.91 | 0.26 | 0.00 | 1557 | 1547 | 10 | Andriamaharavo, 2014 |
| Selina-3,7(11)-diene | Sesquiterpene | 39.02 | 2.39 | 0.00 | 1561 | 1562 | -1 | Facey, Porter, et al., 2005 |
| Palustrol | Sesquiterpene | 39.94 | 0.81 | 0.00 | 1591 | 1581 | 10 | Courtois, Paine, et al., 2009 |
| Spathulenol | Sesquiterpene | 40.06 | 3.27 | 0.12 | 1595 | 1594 | 1 | Sabulal, Dan, et al., 2007 |
| Ledol (Globulol) | Sesquiterpene | 40.19 | 0.17 | 2.12 | 1600 | 1608 | -9 | Shivashankar, Roy, et al., 2012 |
| Caryophyllene oxide | Sesquiterpene | 40.36 | 0.24 | 0.31 | 1605 | 1612 | -7 | Eyres, Marriott, et al., 2007 |
| Epiglobulol | Sesquiterpene | 40.44 | 1.37 | 0.88 | 1608 | 1608 | 0 | Skaltsa, Mavrommati, et al., 2001 |
| Elemenone<trans-beta-> | Sesquiterpene | 40.64 | 5.22 | 6.28 | 1615 | 1607 | 8 | Andriamaharavo, 2014 |
| Viridiflorol | Sesquiterpene | 40.71 | 1.62 | 0.09 | 1618 | 1609 | 9 | Andriamaharavo, 2014 |
| Isospathulenol | Sesquiterpene | 41.03 | 1.88 | 0.26 | 1612 | 1608 | 4 | Dehghan, Solaimanian, et al., 2007 |
| Humulene epoxide II | Sesquiterpene | 41.18 | 0.31 | 0.12 | 1634 | 1635 | -1 | Cardeal, da Silva, et al., 2006 |
| Germacrone | Sesquiterpene | 41.38 | 0.15 | 0.00 | 1649 | 1658 | -9 | Marongiu, Piras, et al., 2005 |
| Di-epi-1,10-cubenol | Sesquiterpene | 41.54 | 1.16 | 0.46 | 1647 | 1640 | 7 | Bertoli, Lepnardi, et al., 2011 |
| β -Acorenol | Sesquiterpene | 41.74 | 0.11 | 0.00 | 1643 | 1639 | 6 | Rout, Naik, et al., 2006 |
| Pogostol | Sesquiterpene | 41.77 | 0.32 | 0.00 | 1654 | 1651 | 3 | Adams, 2017 |
| Bulnesol | Sesquiterpene | 41.96 | 0.04 | 0.00 | 1661 | 1670 | -9 | Adams, 2017 |
| tau-Muurolol | Sesquiterpene | 41.99 | 2.31 | 0.08 | 1652 | 1641 | 11 | Radulovic, Blagojevic, et al., 2010 |

**TABLE SI -** Tentatively identified compounds in Essential Oils from barks and leaves of *Commiphora Leptophloeos* by GC/qMS

| Compound name | Chemical Classes | R.T. | Area % | | LTPRI | | | Reference (NIST WEB BOOK) |
|---|---|---|---|---|---|---|---|---|
| | | | Barks | Leaves | Exp | Lit. | Diff | |
| α -Muurolol | Sesquiterpene | 42.01 | 0.24 | 0.00 | 1663 | 1654 | 9 | Radulovic, Blagojevic, et al., 2010 |
| Intermedeol | Sesquiterpene | 42.08 | 0.00 | 0.10 | 1665 | 1667 | -2 | Andriamaharavo, 2014 |
| Aristol-1(10)-en-9-ol | Sesquiterpene | 42.29 | 0.24 | 0.00 | 1672 | 1680 | -8 | Andriamaharavo, 2014 |
| α -Cadinol | Sesquiterpene | 42.34 | 1.15 | 0.17 | 1674 | 1668 | 6 | Kim, Lee, et al., 2003 |
| 7-epi-α-Eudesmol | Sesquiterpene | 42.43 | 0.45 | 0.36 | 1668 | 1659 | 9 | Simoniatto, Bonani, et al., 2007 |
| tau-Cadinol | Sesquiterpene | 42.53 | 0.26 | 0.27 | 1681 | 1679 | 2 | Phutdhawong, Kawaree, et al., 2007 |
| Bisabolol <alpha-> | Sesquiterpene | 42.60 | 0.40 | 0.00 | 1683 | 1682 | 1 | Benkaci-Ali, Baaliouamer, et al., 2007 |
| α -Bisabolol | Sesquiterpene | 42.89 | 1.12 | 0.15 | 1694 | 1697 | -4 | Sabulal, Dan, et al., 2007 |
| Longifolol | Sesquiterpene | 43.28 | 0.00 | 0.20 | 1707 | 1713 | -6 | Adams, 2017 |
| (1R,7S)-Germacra-4(15),5,10(14)-trien-1β-ol | Sesquiterpene | 43.36 | 0.00 | 0.09 | 1701 | 1695 | 6 | Andriamaharavo, 2014 |
| Nootkatol | Sesquiterpene | 43.52 | 0.17 | 0.00 | 1717 | 1715 | 2 | Adams, Habte, et al., 2004 |
| Germacrone | Sesquiterpene | 43.62 | 0.00 | 0.20 | 1716 | 1708 | 8 | Andriamaharavo, 2014 |
| Juniper camphor | Sesquiterpene | 43.65 | 1.35 | 0.00 | 1719 | 1709 | 10 | Andriamaharavo, 2014 |
| Bisabolone | Sesquiterpene | 44.58 | 0.33 | 0.00 | 1755 | 1755 | 0 | Tuberoso, Kowalczyk, et al., 2005 |
| Isovalencenol | Sesquiterpene | 45.43 | 0.40 | 0.13 | 1787 | 1793 | -6 | Adams, 2017 |
| Neophytadiene | Sesquiterpene | 46.71 | 0.05 | 0.55 | 1836 | 1841 | -6 | Andriamaharavo, 2014 |
| Curcumenone | Sesquiterpene | 47.11 | 0.00 | 0.17 | 1851 | 1844 | 7 | Andriamaharavo, 2014 |
| **sesquiterpenes** | | | **79.35** | **20.80** | | | | |
| Ergost-5-en-3-ol, (3β.)- | Sterols | 77.93 | 0.00 | 1.19 | 3275 | - | | n.i. |
| gamma-Sitosterol | Sterols | 81.04 | 0.00 | 7.25 | 3359 | 3351 | 8 | Andriamaharavo, 2014 |
| 5α-Stigmasta-7,16-dien-3β-ol | Sterols | 82.94 | 0.00 | 10.62 | 3412 | 3401 | 11 | Radulovic and Dordevic, 2011 |
| **sterols** | | | **0.00** | **19.06** | | | | |
| gamma-Tocopherol | Tocopherols | 72.42 | 0.00 | 0.89 | 3072 | 3074 | -2 | Andriamaharavo, 2014 |
| DL - α -Tocopherol | Tocopherols | 74.40 | 0.00 | 1.23 | 3152 | 3150 | 3 | Andriamaharavo, 2014 |
| **tocopherols** | | | **0.00** | **2.12** | | | | |

Received for publication on 23rd July 2021
Accepted for publication on 18th December 2021