ABSTRACT – The objective of this work was to analyze the chemical composition of the essential oil of Centratherum punctatum Cass. leaves, cultivated in the Research Campus of the Museu Paraense Emílio Goeldi. The oil extraction was accomplished through the hydrodistillation method with the use of modified Clevenger. The extraction process occurred for 180 minutes. Compound identification and concentration quantification was performed by gas chromatography coupled to mass spectrometry. The study identified 31 compounds. Trans-Caryophyllene was the predominant constituent, followed by Germacrene D, α-Humulene and β-Cys-Farnesene. It is concluded that the research was successful, being possible to observe the presence of volatile compounds reported in the literature.

1. INTRODUCTION

Centratherum punctatum Cass. is a perennial plant, belonging to the family Asteraceae, with 45-60 cm of height, branched stem, perfumed foliage and purple flowers (LEITÃO FILHO, 1972; PRUSKI, 1997; BARROS, 2002). It is distributed in Central and South America, and can be found throughout Brazil (NAKAIMA, 2000). Phytochemical screening identified the presence of flavones, glycosides and phenolic compounds. Bioactive compounds of the essential oil obtained from the leaves of Centratherum punctatum point to anthelmintic, antifilarial and antihyperglycemic activities (BEVELLE et al., 1981; NISHA et al., 2007; ANI and NAIDU, 2008). However, the medicinal properties of this plant have not yet been properly explored (PHILLIPSON, 2001, GBOLADE et al., 2009, NARAYANASWAMY et al., 2011).

The essential oils can be applied in technological processes, for the synthesis of perfumes, cosmetics and drugs. The high volatility due to the increase in temperature makes it possible to use the technique of hydrodistillation extraction, commonly applied in the extraction of flowers and leaves (PINHEIRO, 2003, BIASI and DESCHAMPS, 2009). Separation, identification and quantification are generally done by gas chromatography (GC) with flame ionization detector and confirmation is done by mass spectrometry (CHOUHURY et al., 1996; SHARMA et al., 1997). The objective of this work is to analyze the essential oil of leaves of Centratherum punctatum Cass. from the Research Campus of the Emílio Goeldi Museum, in order to verify the chemical composition of its essential oil.
2. MATERIALS AND METHODS

2.1. Obtainment and preparation of the raw material

Samples of *Centratherum punctatum* were obtained at the Research Campus of the Museu Paraense Emílio Goeldi, located in Belém, Pará, Brazil. The collected samples were dehydrated in an air conditioned room at temperature of 17.9 °C and relative humidity of 41.6% for 45 hours. After drying, the leaves were manually separated from the branches, and trimmed. After the trimming process, the leaves were homogenized and weighed for the subsequent process of extracting the essential oil. The humidity of the dehydrated raw material was determined in humidity determiner-scale infrared.

2.2. Hydrodistillation and Gas Chromatography

The extraction of the essential oil was performed by mixing 20g of raw material (processed leaves) with 500 ml of distilled water, a modified Clevenger apparatus and a thermostated bath with circulation of chilled water. The process lasted 180 minutes. The product obtained (hydrolyzate plus essential oil) was centrifuged in a centrifuge (Q-22T18, Quimis Aparelhos Científicos LTDA, Brazil) with a rotation of 3000 rpm for 5 minutes. After this time, a small amount of anhydrous Na$_2$SO$_4$ (99% purity, Alphatec, Brazil) was added to the product and the centrifugation was performed for further 5 minutes. The essential oil was mixed with 1 ml of hexane, stored in a vial and identified for further chromatographic analysis. The oil yield was determined by equation 1.

$$R_o (\%) = \left( \frac{m_o}{m_a \left(1 - \frac{U_a}{100}\right)} \right) \times 100$$

Where: $R_o$ is the oil yield in dry basis, $m_o$ is the oil mass, $m_a$ is the sample mass and $U_a$ is the sample humidity.

The chemical composition of the essential oil was analyzed by gas chromatography coupled to mass spectrometry (Shimadzu QP - 2010 Plus). The identification and quantification of the compounds were performed from the analysis of retention times and retention indices compared with standard samples and literature data from libraries contained in the GCMS Postrun Analysis software (ADAMS, 2006; FFNSC and NIST11).

3. RESULTS AND DISCUSSION

The humidity of the dehydrated leaves of *Centratherum punctatum* was 10.17%. The oil yield was low (only traces). As the amount of oil was less than 0.1 ml, it is recommended to collect a larger quantity of fresh raw material for use in processes. The compounds identified in the essential oil with the respective retention times, retention indices and concentration are shown in Table 1. Trans-Caryophyllene was the predominant constituent, followed by Germacrene D, α-Humulene and β-Cys-Farnesene. Together, these constituents correspond to 59.84% of the essential oil. The results show that concentrations of Germacrene D, α-Humulene, bicyclogermacrene and viridiflorol were higher than those found by
Ogunwande et al. (2005), whose concentrations were 6.4%, 4.1%, 3.2% and 1.4%, respectively.

Table 1 – Chemical composition of the essential oil of Centratherum punctatum leaves.

| Compound                  | RT   | RI   | C%   |
|---------------------------|------|------|------|
| δ-Elemene                 | 21.641 | 1329 | 1.56 |
| Cyclosativene             | 23.283 | 1366 | 2.10 |
| α-Copaene                 | 23.568 | 1373 | 3.80 |
| β-Bourbonene              | 23.917 | 1381 | 0.19 |
| β-Elemene                 | 24.183 | 1387 | 0.74 |
| Sibirene                  | 24.933 | 1404 | 0.15 |
| Trans-Caryophyllene       | 25.492 | 1417 | 32.11|
| β-Copaene                 | 25.925 | 1427 | 0.76 |
| α-Trans-Bergamotene       | 26.083 | 1430 | 3.79 |
| β-Cis-Farnesene           | 26.425 | 1438 | 7.45 |
|                          | 26.567 | 1442 |      |
| α-Humulene                | 27.025 | 1452 | 8.83 |
| α-Farnesene               | 27.217 | 1457 | 0.43 |
| Germacrene D              | 28.125 | 1478 | 11.45|
| γ-Curcumene               | 28.258 | 1481 | 2.90 |
| Valencene                 | 28.467 | 1486 | 1.23 |
| Bicyclgermacrene          | 28.733 | 1492 | 4.96 |
| Isocarylphene             | 28.875 | 1496 | 1.02 |
| β-Curcumene               | 29.358 | 1507 | 0.21 |
| δ-Cardine                 | 29.683 | 1515 | 3.61 |
| Cis-Serquisabinene Hydrate | 30.775 | 1542 | 0.50 |
| Hedicariol                | 30.942 | 1546 | 0.44 |
| Spathulenol               | 32.083 | 1574 | 0.69 |
| Trans-Serquisabinene Hydrate | 32.292 | 1579 | 2.91 |
| Artedouglesia oxide B     | 32.467 | 1583 | 0.33 |
| Viridiflorol              | 32.800 | 1591 | 4.34 |
|                          | 32.917 | 1594 |      |
| Ledol                     | 33.200 | 1601 | 0.40 |
| α- Caryophyllene          | 34.500 | 1634 | 0.47 |
| Cubenol                   | 34.717 | 1640 | 1.03 |
| α-Cadinol                 | 35.225 | 1653 | 0.70 |
| β-Epi-Bisabolol           | 35.875 | 1669 | 0.66 |
| α-Bisabolol               | 36.417 | 1683 | 0.24 |
| **Total**                 | 100  |      |      |

*RT: Retention time; RI: Retention Indices; C: Concentration.
4. CONCLUSION

In this study it was observed the presence of volatile compounds in the essential oil obtained from the leaves of *Centratherum punctatum*, as reported in the literature. 31 compounds were identified, with Trans-Caryophyllene being the predominant constituent, followed by Germacrene D, α-Humulene and β-Cis-Farnesene.

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