Chemical Composition of the Essential Oil of *Psidium caudatum* McVaugh

Xiomara Yáñez*, Martha Lucía Pinzón, Fredy Solano and Luis Roberto Sánchez

Department of Biology and Chemistry, University of Pamplona, Pamplona, Norte de Santander, Colombia. Fax: (+57) 097 5682750.

* Author to whom correspondence should be addressed; e-mail: xioya@hotmail.com

Received: 2 September 2001; in revised form: 17 September 2002 / Accepted: 19 September 2002 / Published: 30 September 2002

---

Abstract: The chemical composition of the essential oil of *Psidium caudatum* McVaugh was investigated and thirty-two compounds were identified by HRGC-MS. The main constituents were terpinen-4-ol (47.72%), γ-terpinene (11.58%) and α-terpinene (6.70%).

Keywords: Chemical composition, essential oil, terpinen-4-ol, *Psidium caudatum* McVaugh.

---

Introduction

The Myrtaceae family consists of some 75 genera and nearly 3000 species of mainly tropical evergreen trees and shrubs. The main areas of distribution are the American and Asian tropics and Australia. The genus Psidium contains about 100 species mainly native to regions ranging from Mexico to Uruguay. In Colombia, *Psidium caudatum* McVaugh, syn. *Calycolpus moritzianus* (O.Berg) Burret and *Psidiopsis moritziana* (O. Berg), commonly known in the region as "arrayán", is a small tree of 5-7 m whose leaves are green, very narrow and opposite [1-3].
Similarly to *Melaleuca alternifolia* oil (tea tree oil) of Australia, the main constituent of the essential oil obtained by hydrodistillation of the leaves of *P. caudatum* McVaugh is terpinen-4-ol, amounting to between 25-45% [1]. The essential oil of *M. alternifolia* consists largely of cyclic monoterpenes of which about 50% are oxygenated and about 50% are hydrocarbons. It exhibits a broad-spectrum of antimicrobial activity that can be principally attributed to the terpinen-4-ol content [4,5].

**Results and Discussion**

The average yield of essential oil obtained after hydrodistillation of the leaves of *P. caudatum* McVaugh was about 1%. Table 1 reports the chemical composition of the essential oil under study. The various compounds were identified by comparison of their Kováts retention indexes, determined utilizing a non-logarithmic scale on both polar (INNOWAX) and non-polar (HP-5) columns, and by comparison of the mass spectra of each GC component with those of standards and with reported data [6,7].

High resolution gas chromatography-mass spectrometric (MRGC-MS) analysis and Kováts Index values showed that its principal components are the monoterpenes terpinen-4-ol (47.72%), γ-terpinene (11.58%), α-terpinene (6.70%), limonene (5.20%), α-pinene (4.49%), 1,8-cineole (eucaliptol) (3.95%), α-terpineol (3.05%), β-terpinene (2.89%), β-pinene (2.66%), p-cymene (2.22%) and α-terpinolene (2.22%).

**Conclusions**

The high content of the oxygenated monoterpene terpinen-4-ol (47.72%) present in the essential oil from the leaves of *P. caudatum* shows that this plant has a commercial potential similar to that of the Australian species *M. alternifolia*.

**Acknowledgments**

To Doctora Elena Stashenko of National School of Chromatography, at the Industrial of Santander University, Bucaramanga (Colombia).

**Experimental**

**Plant Material**

Fresh leaves of *P. caudatum* McVaugh were collected around El Naranjo, Pamplona, Norte de Santander (Colombia). The plant material was classified by Mr. Roberto Sánchez and a specimen has been deposited with the University Herbarium.
Isolation of the Essential Oil

The essential oil was obtained by the hydrodistillation method, using a Clevenger apparatus. The temperature and pressure of hydrodistillation were 120°C and 560 mmHg respectively. The distillation time was three hours. The resulting pale yellow oil was then dried over anhydrous sodium sulphate and 30 µL were solubilized in 1 mL of dichloromethane before the GC injection. 1 µL of this solution was directly used for analysis.

Essential Oil Analysis

The oil was investigated by capillary HRGC and HRGC-MS. HRGC analysis of the sample was performed on a Hewlett-Packard (HP) 5890A Series II gas chromatograph equipped with a split/splitless injector (250 °C, split ratio 1:30) and a FID operated at 250 °C. Chromatographic data were processed with an HP ChemStation 3365-II. Two columns of different polarities were used: a HP-5 fused silica capillary column (50 m x 0.25 mm i.d., film thickness 0.25 µm) and an INNOWAX fused silica capillary column (50 m x 0.25 mm i.d., film thickness 0.25 µm). The oven temperature was maintained at 50 °C for 5 min after injection, then programmed at 2.5 °C/min to 250 °C for the HP-5 column or to 180 °C for the INNOWAX column. Helium was used as carrier gas, the inlet pressure was 152 kPa and the linear velocity was 19 cm/s for both columns. Air and hydrogen flow rates were 300 and 30 mL/min. Nitrogen was used as a make-up gas at a flow rate of 30 mL/min. 1.0 µL of the solution of essential oil in dichloromethane was injected. The identity of the components was assigned by comparison of their retention indices, relative to C8-C24 n-alkanes, and mass spectra with corresponding data of components of reference oils [6,7].

A Hewlett-Packard (HP) 5890A Series II gas chromatograph interfaced to an HP 5972 mass selective detector (MSD) with an HP MS ChemStation data system was used for mass spectrometric identification of the GC components and quantitative composition. The percentage composition of the oils was computed, by the normalization method, from the HRGC peak areas without using correction factors. 1.0 µL of the essential oil solubilized in dichloromethane was injected using the split flow technique. The column used was a 60 m x 0.25 mm i.d. fused silica capillary column coated with 0.25µm film of 5% phenylmethylsiloxane. The oven temperature was maintained at 50 °C for 5 min after injection and then programmed at 3°C min⁻¹ to 250 °C (25 min). Helium was used as carrier gas, the inlet pressure was 200 kPa, the linear velocity 1 mL/min (70 °C), split flow 10mL/min. The injector temperature was kept at 250 °C. The temperatures of the ionization chamber and transfer line were 180 and 285 °C, respectively. The electron energy was 70 eV. Mass spectra were obtained by automatic scanning of the mass range m/z 30-300 a.m.u. at 2.4 scan/s. Chromatographic peaks were checked for homogeneity with the aid of the mass chromatograms of the characteristic fragment ions reported in the NBS 75K and WILLEY 138 databases.
Table 1. Chemical Composition of Colombian *Psidium caudatum* McVaugh oil extracted from the fresh leaves.

| Peak Number | Compound             | Experimentally determined Kováts Indexes | HRGC-MS Peak area [%] |
|-------------|----------------------|------------------------------------------|-----------------------|
|             |                      | HP-5 | INNOWAX |                        |                       |
| 1           | α-Tricyclene         | 924  | -       | 1.22                  |                       |
| 2           | α-Pinene             | 930  | 1092    | 4.49                  |                       |
| 3           | β-Terpinene          | 973  | -       | 2.89                  |                       |
| 4           | β-Pinene             | 975  | 1136    | 2.66                  |                       |
| 5           | β-Myrcene            | 992  | 1166    | 0.77                  |                       |
| 6           | α-Phellandrene       | 1002 | -       | 0.88                  |                       |
| 7           | Δ³-Carene            | 1008 | -       | 0.11                  |                       |
| 8           | α-Terpinene          | 1117 | -       | 6.70                  |                       |
| 9           | p-Cymene             | 1026 | -       | 2.22                  |                       |
| 10          | Limonene             | 1031 | 1217    | 5.20                  |                       |
| 11          | 1,8-Cineole (eucalyptol) | 1034 | 1230    | 3.95                  |                       |
| 12          | cis-β-Ocimene        | 1043 | -       | 0.13                  |                       |
| 13          | trans-β-Ocimene      | 1053 | 1250    | 0.37                  |                       |
| 14          | γ-Terpinene          | 1063 | -       | 11.58                 |                       |
| 15          | α-Terpinolene        | 1088 | -       | 2.22                  |                       |
| 16          | Linalool             | 1103 | 1517    | 0.43                  |                       |
| 17          | cis-Menth-2-en-1-ol  | 1124 | -       | 0.92                  |                       |
| 18          | trans-Menth-2-en-1-ol| 1145 | -       | 0.60                  |                       |
| 19          | Terpinen-4-ol        | 1185 | -       | 47.72                 |                       |
| 20          | α-Terpineol          | 1195 | 1661    | 3.05                  |                       |
| 21          | Methyl geranate      | 1328 | -       | 0.22                  |                       |
| 22          | β-Caryophyllene      | 1422 | 1575    | 0.47                  |                       |
| 23          | α-Humulene           | 1457 | 1641    | 0.19                  |                       |
| 24          | Germacrene D         | 1485 | 1687    | 0.20                  |                       |
| 25          | γ-Cadinene           | 1511 | 1759    | T                     |                       |
| 26          | α-Cadinene           | 1568 | -       | T                     |                       |
| 27          | δ-Cadinol            | 1639 | 2122    | T                     |                       |
| 28          | Muurolol T           | 1645 | 2187    | T                     |                       |
| 29          | (E,E)-Farnesol       | 1664 | 2340    | 0.51                  |                       |
| 30          | Cedryl acetate       | 1762 | -       | T                     |                       |
| 31          | γ-Eudesmol acetate   | 1778 | -       | T                     |                       |
| 32          | (E,E)-Farnesyl acetate | 1812 | 2234    | 0.05                  |                       |

T= Trace
References

1. Weiss, E.A. Essential Oil Crops. Cab International: New York, USA, 1997; pp 235-333.
2. Takhtajan, A. Diversity and Classification of Flowering Plants. Columbia University Press: New York, 1997; p 289.
3. Gergensen, P.M.; León Yáñez, S., Eds. Catalogue of the Vascular Plants of Ecuador, 1999.
4. Sowthwell, I.A.; Hayes, A.J.; Markham, J.L; Leach, D.N. The search for optimally bioactive Australian tea tree oil. Acta Hort. 1993, 334, 265-275.
5. Cox, S.D.; Mann, C.M.; Markham, J.L.; Gustafson, J.E.; Warmington, J.R.; Wyllie, S.G. Determining the antimicrobial Actions of Tea Tree Oil, Molecules. 2001, 6, 87-91.
6. Adams, R.P. Identification of essential Oil Components by Gas Chromatography/Mass Spectroscopy. Allured Publishing Corporation: Carol Stream Illinois, USA, 1995; 469p.
7. Jennings, W.; Shibamoto, T. Qualitative Analysis of Flavor and Fragrance Volatiles by Glass Capillary Gas Chromatography. Academic Press: New York, USA, 1980.

Sample Availability: Samples are available from the authors.

© 2002 by MDPI (http://www.mdpi.org) Reproduction is permitted for noncommercial purposes.