

Bicuiba: study of the chemical diversity of a plant with ethnobotanical uses among the Pataxós.

Maria Elisa A. P. Teixeira (IC),¹ Massuo Jorge Kato (PQ)¹
maria.elisa.teixeira@usp.br

¹ Instituto de Química, USP

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Highlights

Characterization of the molecular diversity in different parts of *Virola officinalis* through spectroscopic and spectrometric analyses of the extracts, fractions and purified compounds.

Abstract

The Myristicaceae family comprises approximately 500 species across 20 genera, mainly distributed in tropical regions [1]. Among this family is *Virola officinalis* Warb., known as bicuiba, an endemic plant of the Atlantic Forest that has ethnopharmacological importance. As an example of its medicinal applications, the fat obtained from the seeds is used to treat various diseases, particularly fungal skin infections [2]. Despite the extensively ethnobotanical applications and numeral phytochemical studies of *Virola* fruits [2], no specific research has been conducted on this species. Thus, the objective of the project is to characterize the molecular diversity in various parts of its fruits (pericarp, aril and seeds), stems, adult leaves, roots, and seedlings through spectroscopic and spectrometric analyses of the extracts, fractions and purified compounds. *V. officinalis* collected in Arraial d'Ajuda (BA) underwent extractions of their different parts (roots, leaves, stem, pericarp, aril and seed). For that, the plant material was dried, crushed and macerated in dichloromethane:methanol (2:1). The resulting extracts were filtered and concentrated under vacuum in a rotary evaporator. The ¹H NMR analyses of the aril and seed extracts indicated that the initial isolation steps would be performed on the seed extracts. For defatting the seed extract, a 20 g aliquot of the extract was dissolved in hot ethanol and allowed to crystallise at room temperature. This process facilitates the separation of the fat as a colourless solid, while the mother liquor was extracted with hexane. Therefore, the hexane fraction, ethanol-water fraction, and a semi-solid material were subjected to ¹H NMR analysis. An additional purification step was performed by submitting 20 g of the crude seed extract to a vacuum liquid chromatographic column (VLC, 13 x 12 cm – L x h) using 36-70 µm flash silica and hexane:ethyl acetate gradient, resulting in 23 fractions. Some of these fractions were analysed by ¹H NMR. TLC and NMR comparisons of the aril and seed extracts from *Virola* fruits suggested a similar chemical profile. The purification step was initially carried out using the seed extracts. The ¹H NMR analysis of seed revealed signals of triglycerides and furofuran lignans. In addition, the ¹H NMR displayed signals around δ 18 ppm, with suggested the presence of enones [2]. In subsequent steps, liquid chromatography coupled with mass spectrometry and gas chromatography analyses will also be performed on all extracts to enable a preliminary characterization of major compounds, which will then be purified and subjected to full characterization using spectroscopic methods.

[1] Rodrigues, W. A. (2010). Flora of Bahia: Myristicaceae. SITIENTIBUS série Ciências Biológicas, 10(1), <https://doi.org/10.13102/scb7959> 138–146.

[2] Kato, M. J., Yoshida, M., Gottlieb, O. R., 1990. Lignoids and arylalkanones from fruits of *Virola elongata*. Phytochemistry 29, 1799-1810.

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