CHEMICAL DIFFERENTIATION BETWEEN BACCHARIS TRIMERA (LESS.) DC AND BACCHARIS MICROCEPHALA (LESS.) DC USING UNTARGETED METABOLOMIC ANALYSIS

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ABSTRACT

Baccharis trimera (Less.) DC, widely used for gastrointestinal diseases2, is the most relevant species of the genus Baccharis because it is listed in the 6th edition of the Brazilian Pharmacopoeia1. Accurate identification of this species is essential to ensure quality control. However, it becomes a challenging practice due to the morphological similarity with other species of the genus, such as Baccharis microcephala3. This study aimed to chemically discriminate them using untargeted metabolomics and mass spectrometry. Five samples of each species were collected in different regions of Brazil and in different years, always during flowering. After grinding, ten mg of winged stems and 2 mL of 70% hydroethanolic solution (EB) were used to obtain the extracts, which were subjected to an ultrasound bath for 20 min. After centrifugation and filtering, 2 µL of each extract was analyzed by Ultra-High Performance Liquid Chromatography coupled to High-Resolution Mass Spectrometer (UHPLC-HRMS). The data obtained were processed and analyzed using MZmine and Weka software. Data processing generated a data matrix containing 854 variables, which after multivariate analysis using J48 Classify allowed determining the variable 63POS (m/z 597.4505 at RT 9.68 minutes) as an important discriminant between B. trimera and B. microcephala. This variable was dereplicated with molecular formula (C38H60O5), suggesting it is a triterpene (CAS-771531-45-4). Thus, it is assumed that this variable can serve as a chemical marker for such studied species and that it has never been described for Asteraceae family. Therefore, this study allowed the

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differentiation of two Baccharis species based on the monitoring of a single triterpene, offering a practical and effective approach to aid in the quality control of B. trimera.

Keywords: Chemotaxonomy, Chemical annotation, LC-MS, Metabolomics, Dereplication.

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