

ANNOTATION OF COMPOUNDS PRESENT IN *BACCHARIS TRIMERA* AND *BACCHARIS CRISPA* USING THE GNPS PLATFORM

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ABSTRACT

Baccharis trimera, known as carqueja, is listed in the 6th Edition of the Brazilian Pharmacopeia¹. However, because of its similarity to other species of the same genus, it is easily adulterated. This highlights the need of new methodologies to improve the quality control of this plant material. The present study aimed to differentiate between *B. trimera* and *B. crispa* by their chemical profiles using metabolomics and mass spectrometry. For this, ten samples of aerial parts from each species were collected from different regions of Brazil over different years, always during the flowering season. After collection, the species were identified, dried and pulverized. A 70% hydroethanolic extract was prepared using 10 mg of each sample, then filtered and analyzed by Ultra-High Performance Liquid Chromatography coupled to High-Resolution Mass Spectrometer (UHPLC-HRMS). The resulting data were preprocessed using the MZmine software, then uploaded to the Global Natural Products Social Molecular Networking (GNPS)² platform, where molecular networks were formed based on the fragmentation patterns of the compounds. Annotated compounds were compared with the literature review data for the species *B. trimera* and *B. crispa*³. The GNPS analysis facilitated the formation of molecular networks, with three large networks belonged to the flavonoid class, subdivided into networks of aglycosylated flavonoids, C-glycosylated flavonoids and flavonoids with glycosylation in the B ring — compounds uncommon within the *Baccharis* genus. Dereplication revealed literature known compounds such as rutin, kaempferol 3-O-rutinoside and apigenin³. Overall, 134 compounds were annotated for *Baccharis trimera* and *Baccharis crispa*, of which 48

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compounds were known, while 86 remain uncharacterized. Unannotated m/z values within the same network suggested their classification are part of the same class to which they are inserted. Therefore, further studies are necessary to make it possible to dereplicate more compounds, improving the quality control of the therapeutic species *B. trimera*.

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

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