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Use of metabolomics for the chemotaxonomy of *Baccharis* (Asteraceae)

Rosana Casoti¹, Gustavo Heiden², Fernando Batista Da Costa¹

¹AsterBioChem Research Team, Laboratory of Pharmacognosy, School of Pharmaceutical Sciences of Ribeirão Preto, University of São Paulo, Ribeirão Preto, SP, Brazil.

²Embrapa Clima Temperado, Pelotas, RS, Brazil.

Baccharis comprises 433 plant species classified into 7 subgenera (*Baccharis*, *Coridifolia*, *Heterothalamulopsis*, *Heterothalamus*, *Molina*, *Oblongifolia* and *Tarchonanthoides*) according to a phylogenetic-based infrageneric classification [1]. This work aimed to use a LC-MS untargeted metabolomics approach to study the metabolic fingerprint of *Baccharis*. For this study, 306 samples representative of all the seven subgenera were sampled. The leaves were grinded with a mortar and pestle in the presence of liquid nitrogen. Extraction was carried out with EtOH:H₂O (7:3 v/v) in ultrasonic bath (20 min, 25 °C). The analysis of the extracts was carried out by UHPLC-ESI-HRMS (C18 column, 150 x 3 mm, 3 µm) using a MeCN-H₂O gradient (2 - 100% MeCN, 0.4 mL/min flow rate, 24 min each run). The data matrix (positive-negative modes) was transformed to logarithmic scale and analyzed by hierarchical cluster analysis (HCA) in software R. As a result, we observed that the *Baccharis* species were clustered in 10 subgroups according to their chemical similarity. The clustering corresponded to the phylogenetic infrageneric classification based on molecular markers. The majority of the biological replicates of *Baccharis* collected in different places and years were clustered together in the HCA, which suggests that most of the species share a very similar metabolic fingerprint independent on the environment they come from. Besides, the morphologically heterogeneous subgenus *Baccharis* section *Aphyllae* presented similar fingerprint among its species, thus highlighting the importance of metabolomics in the chemotaxonomy of complex groups. From our LC-MS analysis, we conclude that the main classes of chemical markers responsible for the HCA clusters are represented by diterpenes; the flavonoids comprise the second most important class in the chemotaxonomic study of this genus. Therefore, we conclude that chemotaxonomic studies based on LC-MS-based untargeted metabolomics can be used as an important auxiliary tool in the taxonomic study of *Baccharis* and give support to a more robust classification of this genus. **References:** [1] HEIDEN, G. Systematics of *Baccharis* (Asteraceae: Astereae). Ph.D. Thesis. University of São Paulo, 2014. **Acknowledgements:** FAPESP (grants #2012/14397-7 and #2014/26866-7).

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