Chemotaxonomic study of Baccharis subgen. Tarchonanthoides (Asteraceae) based on metabolomics approach and multivariate analysis

R Casoti [1], G Heiden [2], FB Da Costa [1]

- [1]University of São Paulo, School of Pharmaceutical Sciences, Ribeirão Preto 14040 – 903, Brazil.
- [2]Embrapa Clima Temperado, Pelotas, RS 96010 – 971, Brazil

- Congress Abstract

The genus *Baccharis* comprises ca. 400 species and has a very complex and unclear taxonomy. Species of the *Baccharis* subgenus *Tarchonanthoides* are classified into four sections based on their morphological characteristics: *Canescentes* (CA), *Coridifoliae* (CO), *Curitybensis* (CU) and *Tarchonanthoides* (TA) [1]. We report herein a chemotaxonomic study of 21 species of this subgenus based on chromatographic fingerprints using LC-MS and multivariate analysis. The EtOH:H_2O extract (7:3 v/v) was prepared by sonication for 20 min at 25 °C. The extracts were analyzed by UHPLC-ESI-HRFTMS using ACE column (150×3 mm, 3 µm) and gradient MeCN-H2O (2 to 100% MeCN) in 30 min. Negative mode mass data were deconvoluted and aligned with the MZmine 2.10 software. Hierarchical clustering analysis (HCA) and principal component analysis (PCA) were calculated with the SIMCA-P 13.0.2.0 and R3.1.0 software [2]. The results obtained by PCA and HCA were similar to the taxonomical classification. Nevertheless, the PCA indicated that the 21 species are clustered into three and not four groups. Interestingly, the same result was obtained by HCA; however, two of the three groups are very close to each other. Moreover, one species from both the CA and CU groups showed the same chemical profile as those from the TA group, thereby contradicting their position based on the morphological classification. Among several compounds that are important for the chemotaxonomic classification, we observed that a diterpenoid was important for the CO group and a flavone for the groups TA and CU, which clustered together. A kaurenone, which was pointed out as an important variable for discriminating the CO and TA groups from the CA group, is absent in the latter. Thus, our chemotaxonomic study based on metabolomics approach and multivariate analysis can be used as an auxiliary tool in the taxonomic study of *Baccharis*, and can also help in identifying which compounds are important for discriminating between each group.

Keywords: Baccharis, chemotaxonomy, LC-MS, multivariate analysis

References:

[1] Heiden G, Pirani JR. Phytotaxa 2012; 60: 41 – 49.

[2] Ward JH. J. Am. Statist. Assoc. 1963; 58: 236 – 244.