



Rapid method for the classification of *Baccharis* species by Fourier Transform Infrared (FT-IR) spectroscopy and chemometrics analysis

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Abstract: Authentication of herbal drugs is an essential step in quality control to avoid problems such as adulteration and incorrect identification of botanical materials. Accurate information ensure the patient's safety, and promotes the effectiveness of treatment [1-2]. Spectroscopic technics associated with chemometrics analysis are used to discriminate herbal drugs [3]. Fourier Transform Infrared Spectroscopy (FT-IR) is among technics that offer significant advantages in authentication process, with low cost, ease of sample preparation, and rapid analysis [2-4]. In this context, the aim of this study was the use Fourier Transform Infrared Spectroscopy with chemometric analysis (FTIR-PCA) as a tool for samples classification of *Baccharis* species from the Atlantic Forest. To meet this requirement, 28 specimens were collected in Curitiba and Piraquara, Paraná, Brazil. The areal parts were dried at room temperature, powdered (N₂ liquid) and sieved (42 mesh). The samples were analyzed on a Bruker® Vertex 70 FT-IR spectrometer, using reflectance drift module. Spectra were acquired in mid-infrared region (MIR) at 400-4000 cm⁻¹, 64 scans, and resolution of 4 cm⁻¹. The FT-IR data spectra were assessed using principal components analysis (PCA) with pre-processing by normalization to constant sum, log transformation and auto scaling. The classification of samples in five groups was possible due to the comparison with authentic samples of *B. trimera*, *B. articulata*, *B. organensis*, *B. uncinella* and *B. aracetubaensis*. The procedure was considered rapid, reproducible and with minimal sample preparation.

References:

- [1] Rohman, A., Nugroho, A., Lukitaningsih, E., and Sudjadi. 2014. Application of Vibrational Spectroscopy in Combination with Techniques for Authentication of Herbal Medicine. *Applied Spectroscopy Reviews*. 49:603–613.
- [2] Wei, Y., Fan, W., Zhao, X., Wu, W., and Lu, H. 2015. Rapid Authentication of *Dendrobium officinale* by Near-Infrared Reflectance Spectroscopy and Chemometrics. *Analytical Letters*. 48:817–829.
- [3] Gad, H. A., El-Ahmady, S. H., Abou-Shoer, M. I., and Al-Azizi, M. M. 2012. Application of Chemometrics in Authentication of Herbal Medicines: A Review. *Phytochemical Analysis*. 24:1-24.
- [4] Meilan, A. C., Goodman, A. M., Baron, M. G., and Rodriguez, J. G. 2014. A Specific Case in the Classification of Woods by FTIR and Chemometric: Discrimination of *Fagales* from *Malpighiales*. *Cellulose*: 21:261-273