Chemometric analysis applied in intact lichens samples using (HR-MAS) ^{1}H NMR and IR data for chemotaxonomic discrimination.

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Lichens present a difficult morphologic differentiation and usually the chemical analysis are very employed for its taxonomic classification, mainly due to the secondary metabolites to be relatively constants for this organisms[1]. The chemotaxonomic lichens classification usually is realised by colour reactions, chromatography, fluorescence and mass spectrometry analysis[2]. However, this majority analysis involve pre-treatment samples process with a high time and reagents consumption. Therefore, fast analysis methods that dispense the samples manipulation are very required, being able to present great importance for lichens chemotaxonomy.

In this work we focus the application of HR-MAS ^{1}H NMR (High Resolution Magic Angle Spinning) and IR, both techniques using intact samples associated with chemometric analysis. For this purpose, eleven species of lichens sample from six genera and two different families were powdered in a cryogenic mill. ^{1}H HR-MAS NMR spectra were obtained on a Bruker 9.4 Tesla DRX 400 Bruker spectrometer, equipped with a 4 mm HR-MAS probehead and zirconia rotor. IR spectra were registered in a Bomem Hartmann & Braun MB-Series model 102 spectrometer. All spectra were used as input variable on the *Pirouette*® software to perform chemometric analysis by PCA and HCA methods.

Chemometrics analysis of HR-MAS ^{1}H NMR and IR spectra, has permitted to correlate the families, genera and species. In figure 1, we can observe the discrimination between Phisciaceae and Parmeliaceae families in the HR-MAS ^{1}H NMR data with only one sample present an unusual behaviour. In figure 2, the PCA scores plot show families discrimination using IR data (Parmeliaceae family is presented in hatched square).

In comparison with others traditional techniques, HR-MAS ^{1}H NMR and IR allied with chemometric have provided a fast and economic method for lichens chemotaxonomy. Both methods was useful for lichens analysis and has permitted the satisfactory discrimination between families, genera and species.

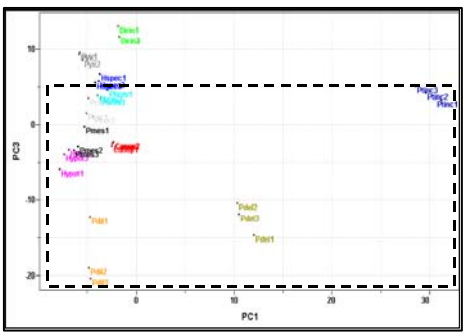

Figure 1: HCA plot of all lichens in HR-MAS NMR analysis (similarity 0,217).

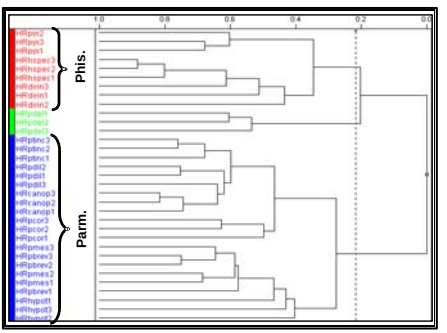

Figure 2: PCA scores plot of all lichens in IR analysis. (PC1xPC3, 21.9 and 14.6%).

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References

[1] Quilhot W.; Leighton G.; Flores E.; Fernandes E.; Pena W.; Guzman G. *Acta Farm. Boranense*, **1987**, *6*(1): 15-22.

[2] Honda N.K.; Vilegas W. *Quím. Nova*, **1998**, 21(6): 110-125.