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Taxonomic Discrimination of Higher Plants by ^{1}H NMR

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Objectives

This study describes an efficient taxonomic classification of higher plants by 1H NMR spectroscopy using multivariate analysis.

Materials and Methods

1. Materials: Leaf samples of five species and one variety and two cultivars of higher plants (*Rosa multiflora* Thunb., *R. multiflora* var.*platyphylla* Thory, *R. rugosa* Thunb., *S. karmtschaticum* Fisch., *Catharanthus roseus* (L.) G. Don cv. Cooler Grape, C. *roseus* (L.) G. Don cv. Cooler Peppermint, and *Lilium longiflorum* Thunb. cv. Casablanca) were subjected to 1H nuclear magnetic resonance spectroscopy (NMR) for spectral fingerprinting.
2. Methods: Freeze-dried plant material (15 mg) was weighted into an sterile 1.5 ml Eppendorf tube. D2O:CD3OD (1 ml, 80:20) containing 0.005% w/v TSP-*d*4 (sodium salt of trimethylsilylpropionic acid) was added to each sample. The contents of the tube were mixed thoroughly and then heated at 50C in a water bath for 10 min. After cooling, the samples were centrifuged at 13,000 rpm for 5 min. All NMR spectra were collected on a Varian UNIT 500 NMR spectrometer at a temperature of 298 K and presaturation pulse was used for water suppression. Each spectrum consisted of 60 scans of 32 k data points and 1H NMR chemical shifts in the spectra were referenced to TSP-*d*4 at 0.00 ppm. The NMR spectra were collected on three different runs.

Results and Discussion

NMR data of these plants for total metabolites, aliphatics, carbohydrates, aromatics, or aliphatics plus aromatics were analyzed by principal component analysis (PCA) in five different manners. Hierarchical dendrograms based on PCA of total metabolites or carbohydrates did not agree with the known taxonomy of the plants. However, dendrograms based on PCA of aliphatics plus aromatics were in agreement with the known taxonomy. A few different carbohydrate compounds seem to occupy a major portion of the total metabolites, which would hide a great chemical diversity of aliphatics and aromatics in plants in PCA. These results suggest that aliphatics and aromatics in plants detected by NMR enable taxonomic discrimination.

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