



METABOLOMICS AND THE BIOASSAY-GUIDED PURIFICATION OF BIOACTIVE METABOLITES

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One of the most popular strategies for isolating bioactive natural products (BNPs) from plant crude extracts is the bioassay-guided fractionation; this process can be described as “find and follow” the pharmacological activity along the fractionation process using biological assays, with the final aim to purify and identify the BNPs responsible for the activity. Although this strategy has proven to be successful, it can at times be repetitive, time-consuming, labor-intensive and, consequently, expensive, since it can require the application of a wide variety of chromatographic techniques and numerous biological evaluations.

In order to speed up the isolation of BNPs from plant crude extracts, while reducing the amounts of chemical and biological waste, new strategies have been developed; these include correlating the variation of the chemical composition (i.e. chromatographic profile) of the crude extract and/or the purified fractions with their biological activity using chemometric analysis methods, which allow the detection of BNP's without isolating them. Chemometric studies have been previously used to detect the BNP's responsible for the antioxidant, cytotoxic, tyrosinase inhibition, and lymphocyte proliferative capacity activities of phytochemically-known plants.

In this presentation we'll discuss the use of *Colubrina greggii* S. Watson var. *yucatanensis* MC Johnst. (Rhamnaceae) as a model to investigate the use of chemometric analysis combined with data from a leishmanicidal bioassay, using Principal Component Analysis (PCA) and Orthogonal Projections to Latent Structures (O-PLS), to detect BNP's in crude extracts from plants having little or no phytochemical information. Additionally, the use of ¹H-NMR metabolomic profiling for both the detection of anthelmithic BNPs in the extract of *Lysiloma latisiliquum* (L.) Benth (Leguminosae) and the chemotaxonomic characterization of ecotypes of *Cocos nucifera* (L.) will be mentioned.