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BOOK OF ABSTRACTS

**EVALUATION OF SEASONAL VARIATION IN UPLC FINGERPRINTS OF
CHRYSOBALANUS ICACO L. (CHRYSOBALANACEAE) BY
CHEMOMETRICS
ASSOCIATED TO SOIL CHEMICAL ANALYSIS**

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Chrysobalanus icaco leaves are traditionally used in Brazil as a hypoglycemic. This pharmacological activity has already been experimentally proved [1]. However, the biosynthesis of secondary metabolites are frequently affected by environmental conditions and variations in the total content and/or of the relative proportions of these compounds can take place [2] and alter the desired therapeutic effect. In this context, this work aims to study the effect of seasonality in UPLC fingerprints of *C. icaco* by chemometrics and to assess the soil fertility results. Twenty-two batches of wild *C. icaco* leaf and their soil samples were collected in the wet and dry season from 14 different cities in the northeast of the state of Pará (Brazil). The fingerprint analysis was performed on a Waters Acquity UPLC with photodiode array (PDA) detection acquiring at 273 nm. The hydroalcoholic extracts (70% v/v) (triplicate) were separated on an Agilent Zorbax Eclipse XDB-C18 (2.1 mm × 50 mm, 1.8 µm) column with a gradient mobile phase consisting of solvents A (1% aqueous formic acid, v/v) and B (acetonitrile). The flow rate was 0.3 mL/min and injection was 1 µL. Data files were converted to ARW files using Empower software (Waters), transferred to Excel[®] and input into Matlab[®] for peak alignment and chemometric analysis, by Principal Component Analysis (PCA). Correlated Optimized Warping (COW) [3] was used to accurate alignment of chromatograms. Then, the chromatograms were normalized and mean centered. Principal Component Analysis (PCA) was applied to evaluate the effect of seasonality in UPLC fingerprints of *C. icaco* samples. The first three PCs represent 80.01% of the total variance (PC1 = 42.56%, PC2 = 26.85% and PC3 = 10.60%). Examining the space defined by scores of first and second PCs, most samples of the same origin tends to cluster itself near. Indeed, some of *C. icaco* samples were located on the positive and negative side of PC2 axis separated like wet or dry season sample. Regarding soil chemical analysis, the macro elements (N, P, K, Ca and Mg) were analyzed quantitatively and it was observed that the higher potassium concentration determine the location of the *C. icaco* sample more negative in PC2 axis. The variables accounting for these separations were identified from the PC2 loadings plot. The results evidence that *C. icaco* samples from different geographical origin and harvested in the wet and dry season have varied the UPLC fingerprints. This approach should be refined to enable real and thorough understanding of plant interaction with the environment.

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