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ABSTRACT BOOK

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Faculty of Sciences of the University of Lisbon

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P-195 UPLC FINGERPRINTING ASSOCIATED WITH CHEMOMETRIC ANALYSIS TO EVALUATE THE POLYMORPHISM OF *CHRYSOBALANUS ICACO* L. (CHRYSOBALANACEAE)

Nádia Elígia Nunes Pinto Paracampo[a,b],*, Ronei Jesus Poppi[b] and José Alberto Fracassi da Silva[b]

[a] Embrapa Eastern Amazon, 66095-100 Pará, Brazil

[b] Chemistry Institute, State University of Campinas, 13083-970 São Paulo, Brazil

[*] nadia.paracampo@embrapa.br

Chrysobalanus icaco L. is a single polymorphic species that varies mainly in leaf shape and size, and in fruit color and size. These different forms frequently grow side by side without any ecological separation and it is not possible to subdivide this species using information based on herbarium material alone [1]. However, *C. icaco* leaves are widely used in Brazilian´s folk medicine for treatment of diabetes [2] and it is known that any change in extract constituents can completely alter the desired therapeutic effect. This study attempts to discriminate *C. icaco* morphotypes using ultra-performance liquid chromatography (UPLC) fingerprinting combined with chemometrics. Twenty-five batches of wild *C. icaco* leaf collected from 15 different cities in the state of Pará (Brazil) were investigated. Three morphotypes have been distinguished by the mature fruit color: white (pale-yellow), rose and black (dark-purple). 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 (50 mm × 2.1 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 Pro software (Waters), transferred to Excel® and input into MALTAB® for peak alignment and chemometric analysis. Correlated Optimized Warping (COW) [3] was used to accurate alignment of retention time. Then, the chromatograms were normalized and mean centered. Principal Component Analysis (PCA) was applied to classify and distinguish between *C. icaco* samples. It can be seen from the 3D-

projection plot of PCA of three principal components (Figure 1) the relationships between the 25 batches based on the chemical constituents and could be readily divided into two relative groups: I (Batch Nº 1-12, white and black morphotypes) and II (Batch Nº 13-25, rose morphotype). The peaks accounting for these separations were identified from the PCA loadings plot. Additionally, mass spectrometry coupled to UPLC will be used for further characterization of these peaks. This approach allowed for the clear classification of batches into two groups representing samples originating from the three morphotypes.

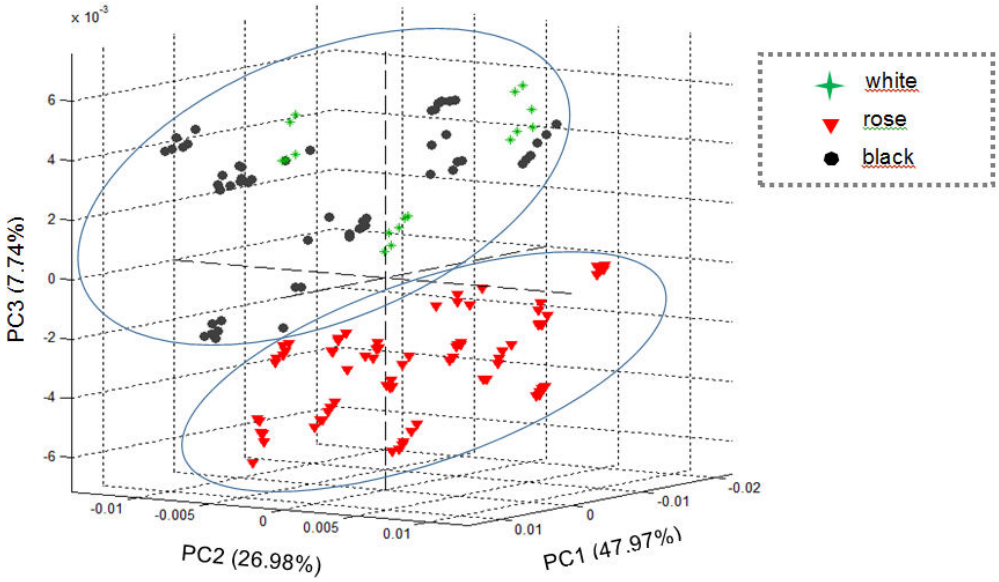

Figure 1. 3D-projection plots of PCA of three principal components for the 25 *C. icaco* L. batches.

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