Evaluation of the polyphenol profile of jabuticaba peel flours by FTIR analysis

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Jabuticaba (Plinia sp.) is a Brazilian fruit, and its dark peel is a source of bioactive compounds, especially polyphenols. However, little is known about how much the content of these compounds may vary between jabuticaba samples, given that native crops tend to have a more dissimilar composition, influenced by environmental conditions. Robust analysis methods such as high performance liquid chromatography (HPLC) are expensive and time consuming, and Fourier-transform infrared spectroscopy (FTIR) spectroscopy together with chemometric models may be a simpler and reliable strategy for routine analysis. The objectives of this work were to evaluate the composition of polyphenols in jabuticaba peel flour (JPF) from different provenances and employ FTIR together with chemometrics to predict the polyphenol profile. Twenty eight flour samples (JPF) were produced by drying, milling and sifting jabuticaba peels. The main phenolic compounds were quantified by HPLC. The samples were also analyzed in a FTIR-ATR Spectrophotometer. The main compounds identified in the JPF were cyanidin-3-glucoside (C3G) (ranging from 352 to 1009 mg/100 g), ellagic acid (EA) (164 to 335 mg/100 g) and delphinidin-3-glucoside (D3G) (95 to 203 mg/100 g). PCA analysis indicated that samples were separated into two groups according to phenolics (PC1) and anthocyanin /EA (PC2) contents. EA presented a moderate correlation ($r = 0.69$; $p = 0.00$) with the content of total extractable phenolics, as opposed to C3G ($r = 0.45$; $p = 0.02$) and D3G ($r = 0.48$; $p = 0.01$), confirming that the Folin-Ciocalteu method is not selective for anthocyanins. In the FTIR spectra, two bands commonly found in phenolics were identified: 1390-1330 cm-1 and 1260-1180 cm-1, associated to interaction between O–H angular deformation and C–O stretching. Three PLS models were constructed. The best model was the one for C3G ($R^2 = 0.92$), followed by D3G ($R^2 = 0.87$) and EA ($R^2 = 0.83$). All models showed low calibration, cross validation and prediction errors, confirming the potential of FTIR and PLS for quantification of phenolic compounds.