Comparison between FT-NIR and Micro-NIR in the evaluation of Acerola fruit quality, using PLS and SVM regression algorithms

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Acerola (Malphighia emarginata) is a typical Brazilian super-fruit characterized by a huge amount (from 1.0 to 4.5 mg/100 g) of ascorbic acid, an excellent antioxidant of the free radicals in water phase. Fresh acerola fruit is mainly transformed with a very high postharvest waste, up to 40%, due to the high perishability of acerolas. Nowadays the most important part of the production is used for vitamin C natural powder production; other common ways of commercialization are acerola fresh fruit, frozen flesh and bottled juice. Due to these considerations, the aim of this work is to estimate in a non-destructive manner, in acerola fruit, titratable acidity and ascorbic acid content.

The 117 samples analysed were characterized by different ripeness stages and the data were obtained in fourteen sampling days. For the non-destructive acquisitions, two different NIR device were used: a Perkin Elmer Frontier FT-Spectrometer, working in the range of 12000 – 4000 cm-1, equipped with a Reflectance Accessory (NIRA); a MicroNIR 1700 (950 – 1650 nm), an ultra-compact and low-cost device created by JSDU. Regarding calibration parameters, the titratable acidity was obtained by a titration of 1g of acerola's juice, diluted in 50mL of distilled water, with a solution of NaOH 0,1N and the results were expressed in malic acid percentage. The quantification of ascorbic acid was carried out by the titration of 1g of acerola's juice, diluted in 100mL of oxalic acid (0.5%), with a solution of DFI (2,6-dichlorophenol indophenol, 0.02 %). The results were expressed in mg of ascorbic acid /100 g of acerola juice.

The elaboration of spectral data obtained with the NIR devices, requires a multivariate statistical approach for extracting useful information from the acquired signals. The spectral data were modelled using two different regression algorithms, PLS (partial least square) and SVM (support vector machine). The first one algorithm is used because of its simplicity, good performance and easy accessibility while SVM is intended to model non-linear relations with high dimensional input vector. The data were divided in two sets: the first one used for the calibration (77 fruit) and the second one as external test set (40 fruits).

The mean results of the traditional quality parameters are as follows: the acid ascorbic content is equal to 2750 ± 517 mg/100g and titratable acidity is 2.20 ± 0.24 g/100g, expressed as malic acid. The variability of chemical parameters is low and appears to follow a non-strictly linear profile. Regression models obtained with Micro-NIR spectra give better results using SVM algorithm, for both ascorbic acid and titratable acidity estimation. Regarding vitamin C, R2 in calibration is 0.71 with RMSEC equal to 221mg/100g, while for titratable

acidity a R2 of 0.78 with RMSEC of 0.11g/100g was obtained. For the external prediction R2 is equal to 0.65 and 0.72 for ascorbic acid and titratable acidity, respectively. NIR data give comparable results both using SVM and PLS algorithms with lower errors for SVM regression.

Prediction ability of Micro-NIR appears to be suitable for on field monitoring; non-linear regression modelling is required.