Laboratory Scientific Report

Proof of Concept on Hardness Prediction of Yam Tubers using NIRS

High-Throughput Phenotyping Protocols (HTPP), WP3

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Ethics: The activities, which led to the production of this document, were assessed and approved by the CIRAD Ethics Committee (H2020 ethics self-assessment procedure). When relevant, samples were prepared according to good hygiene and manufacturing practices. When external participants were involved in an activity, they were priorly informed about the objective of the activity and explained that their participation was entirely voluntary, that they could stop the interview at any point and that their responses would be anonymous and securely stored by the research team for research purposes. Written consent (signature) was systematically sought from sensory panelists and from consumers participating in activities.

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ABSTRACT

Flour from numerous varieties of yams, representing the hardness diversity, were analyzed using Near Infrared Spectroscopy (NIRS). A total of 78 data were analyzed using the Chemflow software. The data pretreatment was standard normal variate and Savitzky Golay algorithm. Calibrations were developed using NIPALS Partial Least Square regression (PLSR), using the standard Wold's algorithm with 4 blocs cross validation. Principal component analysis (PCA) was performed before PLS regression. The coefficient of determination in cross validation (R^2CV), the standard error in calibration (SEC) and in cross validation (SECV), the standard error in prediction (SEP) and the coefficient of correlation (R) were calculated.

The objective was to evaluate yam flour samples for hardness parameter prediction, using NIRS.

Key Words: Near Infrared Spectroscopy, yam, flour, Chemflow, hardness

1 MATERIALS

A total of 78 data were analyzed and evaluated for hardness parameter prediction using NIRS. These samples include flour from numerous varieties of yams, representing the hardness diversity, send by CIRAD collaborators (D. Cornet and G. Arnau).

2 DATA ANALYSIS

Using the Chemflow software (Rossard et al., 2016), models were developed in order to examine the structure of the data as well as outliers detection. The data pretreatment used was standard normal variate and Savitzky Golay algorithm with first order derivative with a 13 size of the window and a 2 degree of polynom. Calibrations were developed using NIPALS Partial Least Square regression (PLSR), using the standard Wold's algorithm with 4 blocs cross validation and 20 latent variables. Principal component analysis (PCA) was performed before PLS regression. The Q and T^2 multivariate distances were used as criteria for selecting those samples in the population that were more variable on the basis of the spectra features, and thus outliers were detected. Of the overall set of 73 remaining samples, 75% were used for cross-validation as the calibration set, while the remaining 25% were used as the validation set for testing calibration model, according to random algorithm. The coefficient of determination in cross validation (R^2CV), the standard error in calibration (SEC) and in cross validation (SECV), the standard error in prediction (SEP) and the coefficient of correlation (R) were calculated.

3 RESULTS AND DISCUSSION

With reference method, yam samples hardness ranged from 1.197 to 11.59 Newton (N) with a mean of 5.74, a median of 5.70, a standard deviation (SD) of 2.82 and coefficient of variation of 49.21%. This high variability was acceptable to perform calibration and validation curve generation.

The PCA score plot of PC1 and PC2 of the samples analyzed showed no major clusters or groups. The first PC explains 77.67% of the variation in the spectra, while the second explains 11.47%. Five outliers were detected with Q values over 0.005. Statistics for the PLSR calibration developed showed that SEC, R^2CV and SECV for hardness parameter were respectively 1.66 ; 0.73 ; and 2.2 N at 8 latent variables. The RPD value (SD/SEP ratio), was 1.7. The SEP obtained was 1.68 (N), which is good as it is close to the SEC.

Correlation plot of the NIR prediction of the validation set revealed a positive relationship (Figure 1.), with a r=0.76 correlation, which indicated the model can predict hardness but with variation between the reference values and NIR prediction.

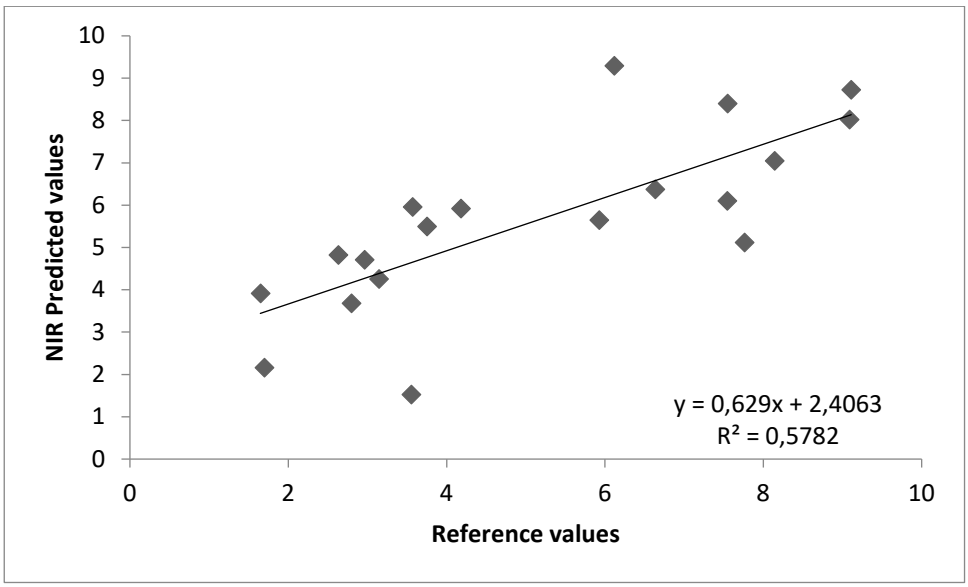

Figure 1. Correlation plot of validation set for Hardness NIR prediction model in yam flour

4 REFERENCE FOR CHEMFLOW SOFTWARE

Rossard, V., Boulet, J. C., Gogé, F., Latrille, E., Roger, J.-M. (2016). ChemFlow, chemometrics using Galaxy. Presented at Galaxy Community Conference - GCC2016, Bloomington, USA (2016-06-24-2016-07-29).

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