Laboratory Scientific Report

Proof of Concept on Physico-Chemical and Textural Prediction of Yam Tuber 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

This study focusses on the ability of Near Infrared spectroscopy to predict chemical and Textural properties of Yam Tubers. To investigate it, numerous varieties of yams coming from a core collection (CIRAD-INRAe, Guadeloupe) and representing of the chemical and textural diversity were analyzed.

A total of 174 samples were analyzed for their: DM, Starch, Protein and sugar contents in wet chemistry and for their texture properties (Hardness, Cohesiveness, Adhesiveness, Springiness and Extensibility) using a texturometer. The same samples were analyzed for their reflectance spectra in Near Infrared. Two replications of yam flour (dried) sample were scanned on a FOSS-NIR-Systems model 6500 scanning monochromator (FOSS-NIRSystems, Silver Spring, MD) with the autocup sampler.

The whole sample set was divided in 3 data sets: learning set (N93), test set (N= 31) and external validation set (n= 41). Learning set was used in combination with the test set to set up the best fitting model in terms of error of prediction (SEP) and R^2. The external validation set was used to evaluate the performances of this model.

The MPLS regression algorithm implemented in Winisi Software (Infrasoft International, Port Mathilda, USA) was used to develop the models. The performances of the different models ranged in terms of R^2 between 0.66 (extensibility) and 0.94 (sugar) and in terms of prediction error (estimated on external validation samples) SEP between 0.11 (for Cohesiveness) and 2.22 (Adhesiveness). The SEP were for DM = 1.58%, for sugar = 0.56%, for protein = 0.29% and for starch = 1.46%.

This study demonstrated that it is possible to develop efficient predictive models based on NIRS spectra of Yam flour samples. These models are efficient for quantification of chemical parameters (starch, sugar, protein, DM). Models are less efficient, but promising, regarding textural parameters.

Key Words: NIRS, Yam tubers, textural properties, MPLS, chemical composition

1 MATERIALS

A total of 174 data were analyzed and evaluated for DM, Starch, Protein and sugar parameters prediction using NIRS in period 2. These samples include flour from numerous varieties of yams, representing the physico-chemicals and textural diversity, send by Cirad collaborators (D. Cornet, G. Arnau, E. Ehounou).

2 SPECTRA COLLECTION AND SAMPLE SELECTION

NIRS analysis were made in the Food processing Laboratory of INRA in Guadeloupe. Two replications of yam flour sample were scanned on a FOSS-NIR-Systems model 6500 scanning monochromator (FOSS-NIRSystems, Silver Spring, MD) with autocup. Each flour was place in a small ring cup of 36 mm diameter, and reflectance spectra (log 1/R) from 400 to 2500 nm were recorded at 2 nm intervals. Each spectrum represented the average of 32 scans, and recorded as log (1/R). Each sample were scanned twice with two independent cup in order to minimize the effect of particle size. The average spectrum of each sample was calculated for further chemometrics analysis. The spectroscopic procedures and data recording were conducted with Isiscan software, (FOSS, NIRS, Denmark).

Calibration equations were developped using the WinIsi IV .10.0 software, in the spectral information range of 1100-2498 nm

Before the development of calibration model, two cycles of outliers elimination were set up on the 174 samples using the center algorithm which calculate the Global H distance (GH) with a cutoff of GH=3. Following this procedure, 9 outliers samples were removed. The scatter of spectra was first corrected by a standard normal variate and derivative with 1,4,4,1 mathematical treatment. Then, samples were divided into calibration set (3/4) and external validation set (1/4) using WinIsi software.

To select appropriate and representative samples of the calibration set, the SELECT algorithm and pre-processing methods were applied upon 165 spectra. Thus, 124 spectra were used as calibration development (93 for the calibration and 31 for cross-validation) and 41 spectra for external validation set or prediction set.

Calibration and external validation

Standard error of calibration (SEC), coefficient of determination (RSQ) for calibration, coefficient of determination (1-VR) and standard error of cross-validation (SECV) for cross-validation were calculated. For each component, the prediction ability of its equation model was tested based on the coefficient of determination (R^2), standard error of performance (SEP) and the ratio SD/SEP.

3 RESULTS

3.1 Description spectra

The NIR spectra of all the yam samples revealed the obvious differences in the absorption intensities that existed among them, though all spectra closely ressembled each other. The raw NIR Spectra of the yam flour samples are shown in Fig 1. IR spectra of 165 dried yam flour of 27 genotypes, x-axis, wavelength, y-axis, absorbance. 400-900 nm is the visible range (variability due to the color of samples), and 900 – 2500 nm is the NIR range. The water peaks are not present at 1490 and 1940 nm because of dried samples.

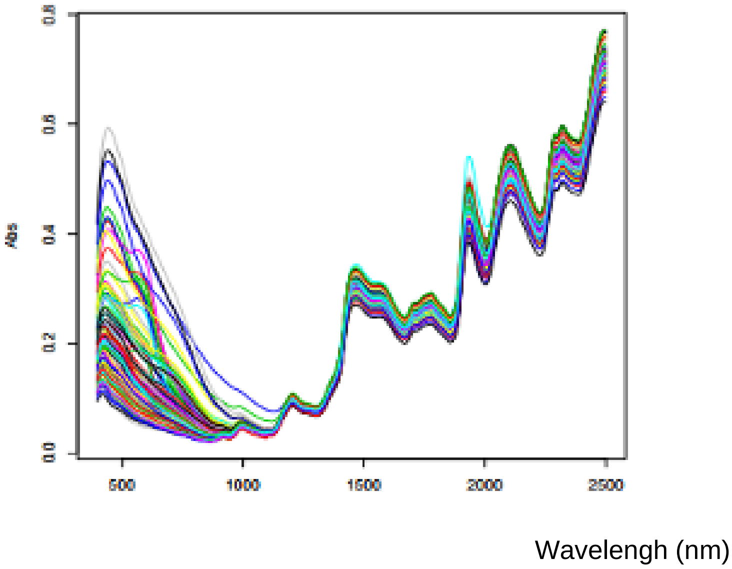

Figure 1. NIR Spectra of 174 yam samples

3.2 Description of data set for VIS/NIRS calibration

Table 1 present the results of physico-chemical and texture attributes for the calibration, validation and prediction datasets. For all variables, the range and the mean of all attributes were closely similar between the three datasets.

Table 1. Sample number (N), range, mean, and standard deviation (SD) of physico-chemical and texture attributes for the calibration, validation and prediction datasets.

	Calibration data set				**Validation data set**				**External validation or Prediction data set**			
Attribute	N	Range	Mean	SD	N	Range	Mean	SD	N	Range	Mean	SD
Dry matter (%)	93	20.30 – 38.64	29.58	3.88	31	20.63 – 36.29	29.43	3.29	41	19.80-35.18	29.33	3.99
Protein% DM	93	3.30 – 7.62	5.02	0.89	31	3.87 – 8.21	5.27	0.94	41	3.61 – 7.68	5.12	0.85
Starch_% DM	93	66.65-84.93	79.05	3.40	31	72.24 – 83.84	79.88	2.89	41	66.78 – 84.86	79.02	4.21
Sugar_% DM	93	0.436 – 12.24	3.57	2.25	31	0.50 – 9.64	2.83	1.71	41	0.61 – 11.55	3.49	2.11
Hardness N	38	1.197 - 16,72	5.40	2.75	18	1.40 – 16.72	7.21	3.88	22	1.54 – 10.02	5.09	2.64
Cohesiveness	38	0.106 – 0.812	0.31	0.16	18	0.10 – 0.54	0,.7	0.09	22	0.11 – 0.62	0.30	0.16
Adhesiveness	38	(-11.76) - (-0.18)	-3.88	2.90	18	(-8.60) - (-0.35)	-4.41	2.45	22	(-10.34) - (-0.16)	-3.64	2.78
Springiness	38	0.081 – 0.91	0.42	0.25	18	0.09 – 0.84	0.38	0.16	22	0.09 – 0.94	0.43	0.27
Extensibility	38	0.072 – 0.96	0.48	0.29	18	0.10 – 0.91	0.47	0.23	22	0.07 – 0.97	0.47	0.31

3.3 Calibration and validation of MPLS models

The results in **Table 2** showed for the calibration performances for physico-chemical and textural attributes. Physico-chemical attributes models showed good performances (RSQ>0.8). The ratio performance to deviation (SD/SECV) show that calibration model of protein and sugar content, with values higher than three, could be considered good for screening purposes (Williams, 2001). However, the calibration performance for hardness (RSQ = 0.83, 1-VR= 0.63, SD/SECV ratio = 1.67), cohesiveness (RSQ = 0.55, 1-VR= 0.23, SD/SECV ratio = 1.16), and springiness (RSQ = 0.64, 1-VR= 0.22, SD/SECV ratio = 1.28) were not good.

Table 2: Description of pretreatments, mathematical trasnformation and calibration model performances for physico-chemical and texture attributes.

Constituent	SEL	N	Mean	SD	SEC	R^2	SECV	R^2 cross val	SD/SECV
DM %		85	29,70	3,60	1,436	0,84	1,63	0,79	2.22
Protein % DM	2	82	5,01	0,86	0,179	0,96	0,24	0,92	3.55
Sugar % DM	3	82	3,16	1,64	0,322	0,96	0,42	0,93	3.91
Starch % DM	3	88	79,39	2,98	0,914	0,91	1,21	0,83	2.45
Hardness N		33	5,36	2,40	0,982	0,83	1,44	0,63	1.47
Cohesiveness		31	0,27	0,12	0,081	0,55	0,10	0,23	1.16
Adhesiveness		36	-3.47	2,36	1,074	0,79	1,90	0,34	1.25
Springiness		32	0,37	0,21	0,134	0,57	0,16	0,41	1.32
Extensibility		38	0,48	0,29	0,172	0,64	0,23	0,37	1.38

SEC: The standard error of calibration; RSQ: Coefficient of determination in calibration; SECV: Standard error of cross-validation; 1-VR: 1 minus the ratio of unexplained variance to total variance; SD/SECV: Calibration performance.

Table 3 present performances metrics of the different model applied to the validation dataset. Results confirms observations made on calibration dataset. For starch, sugars and proteins, the coefficient of determination in external validation and the predictive performance SD/SEP ratio were respectively 0.89, 2.67, 0.93, 3.49 and 0.88, 2.77. These high values permit a good estimation accuracy on the validation samples and indicate a good predictive performance. For dry matter, the SD/SEP (2.13) was moderate indicating an acceptable estimation accuracy. For the textural parameters, hardness, cohesiveness and springiness models statistical parameters R^2 and SD/SEP revealed poor performances, respectively of 0.52, 0.91; 0.55, 1.35 and 0.66, 1.34. These low values could not permit satisfactory quantitative prediction accuracy.

Table 3. Model performances on external validation dataset.

Attribute	**N**	**SEP(C)**	**SEP**	**SD**	**Bias**	**R^2**	**Slope**	**SD/SEP**
DM_%	41	1.59	1.58	3.37	-0.18	0.85	1.09	2.13
Protein	41	0.29	0.29	0.81	-0.04	0.88	0.98	2.77
Sugar	41	0.56	0.56	1.94	0.08	0.94	1.05	3.49
Starch	41	1.41	1.46	3.89	0.42	0.89	1.02	2.67
Hardness	22	1.84	1.84	1.67	-0.41	0.52	1.14	0.91
Cohesiveness	22	0.11	0.11	0.15	-0.01	0.55	0.80	1.35
Adhesiveness	22	2.08	2.22	1.72	-0.91	0.45	1.08	0.77
Springiness	22	0.19	0.19	0.24	-0.03	0.52	0.84	1.24
Extensibility	22	0.19	0.8	0.24	-0.01	0.66	1.05	1.34

N: number of samples; SEP(C): the standard error of prediction on calibration dataset; SEP: the standard error of prediction on validation dataset; R^2: coefficient of determination in external validation; SD: standard deviation; 1-VR: 1 minus the ratio of unexplained variance to total variance; RPD = SD/SEP: ratio performance to deviation.

We can see the correlation plot of validation set for dry matter, protein, starch, Sugar, and hardness prediction model in yam flour in figure 2, 3, 4 5 and 6 respectively.

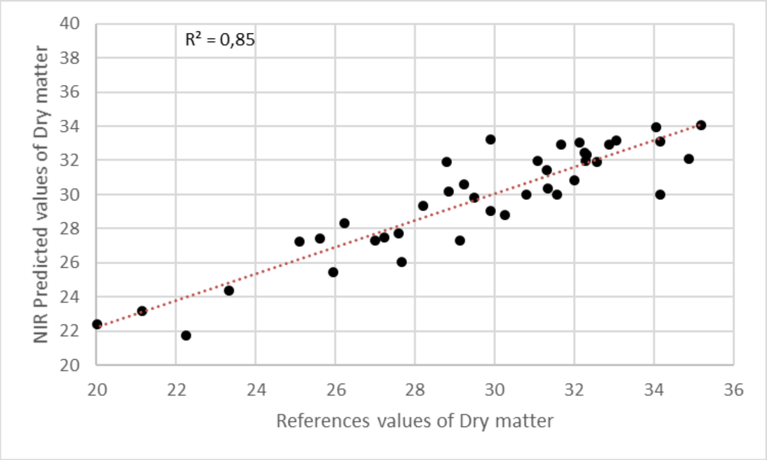

Figure 2. Correlation plot of validation set for Dry Matter NIR prediction model in yam flour

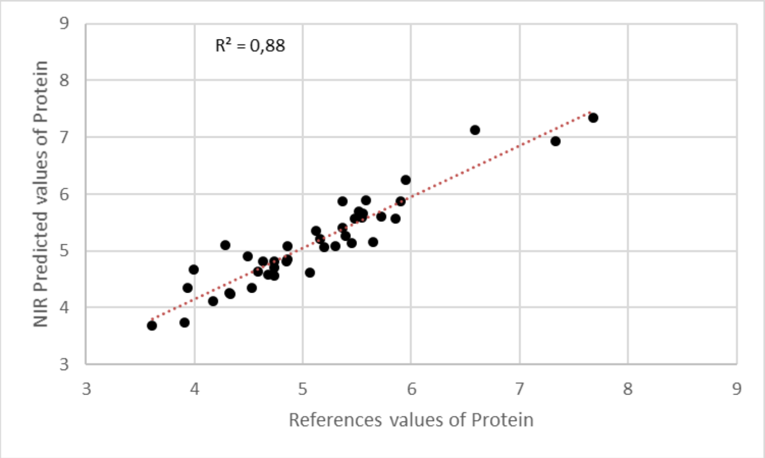

Figure 3. Correlation plot of validation set for Protein NIR prediction model in yam flour

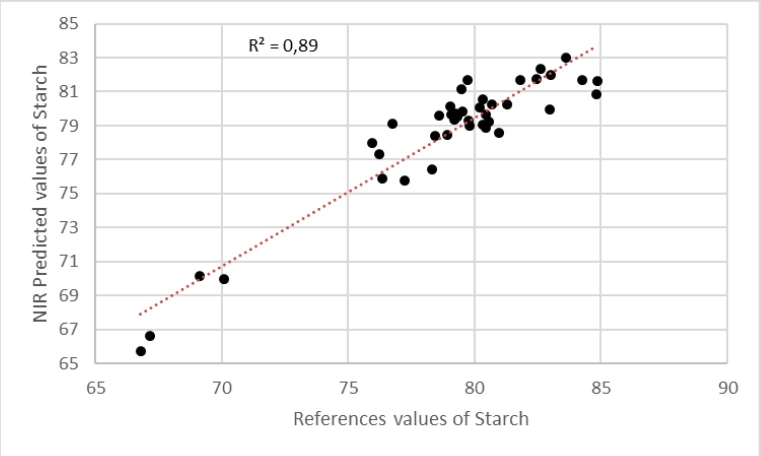

Figure 4. Correlation plot of validation set for Starch NIR prediction model in yam flour

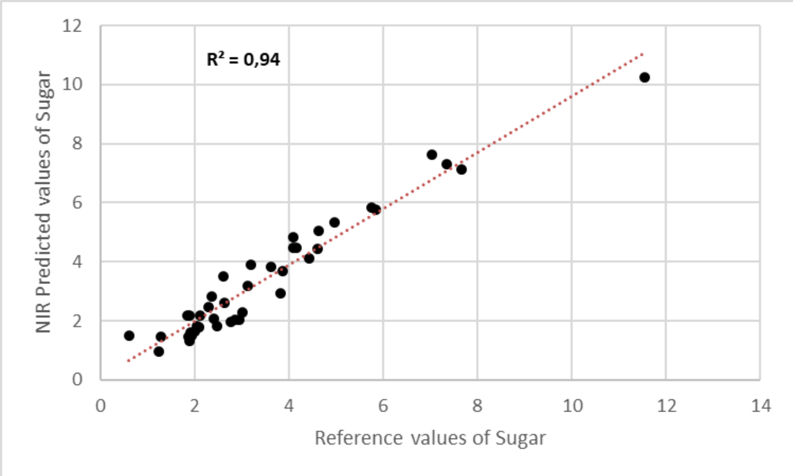

Figure 5. Correlation plot of validation set for Sugar NIR prediction model in yam flour

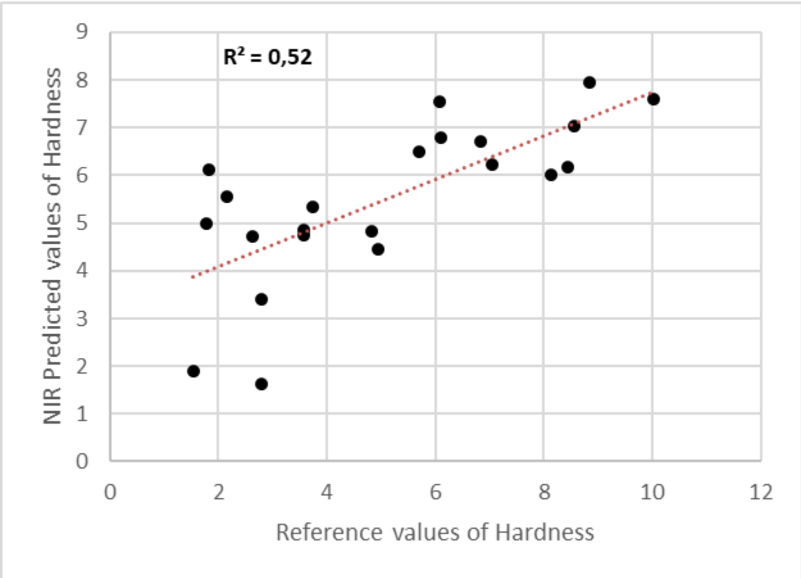

Figure 6. Correlation plot of validation set for Hardness NIR prediction model in yam flour

4 CONCLUSIONS

NIRS can be used to produce a rapid screening of dry matter, protein, sugar and starch with single calibration applied to yam *D. alata* varieties. However, textural parameters could not be satisfactorly quantitatively predicted with WinIsi software, with this dataset.

5 REFERENCES

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