Work Package 3
High-Throughput Phenotyping Protocols (HTPP)
Report Template: Existing Nirs Calibrations

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Work Package 3

High-throughput phenotyping protocols (HTPP)

REPORT TEMPLATE: EXISTING NIRS CALIBRATIONS

General identification

Constituent	Dry matter
Institute/Partner	CIAT
Country	Colombia
Project(s)[1]	RTB Harvest Plus Challenge Program
Product	Cassava
Presentation of product	Fresh Roots

Calibration description

Product	Fresh cassava
Product presentation	Ground fresh roots (puree)
Constituent	Dry Matter (DM)
unit	%
Number of developing year	10 years (2009 -2018)
Number of values	8091
Range of values	12,3% - 52,4%
Spectrometer Brand/model	FOSS/6500
Spectral range	400 nm – 2500 nm
Software used for calibration	Winisi IV (FOSS)
Regression model	LOCAL Regression / Partial Least squares
Numeric formats available for equation and b coefficients	Winisi IV, Excel, ASCII
Standard Error of Prediction	1,285%
Calibration published in scientific papers (DOI + Reference)	Belalcazar, John, et al. "High-throughput phenotyping and improvements in breeding cassava for increased carotenoids in the roots." Crop Science 56.6 (2016): 2916-2925. F. Davrieux, D. Dufour, P. Dardenne, J. Belalcazar, M. Pizarro, J. Luna, L. Londoño, A. Jaramillo, T. Sanchez, N. Morante, F. Calle, L.A. Becerra Lopez-Lavalle, and H. Ceballos, "LOCAL Regression Algorithm Improves near Infrared Spectroscopy Predictions When the Target Constituent Evolves in Breeding Populations," J. Near Infrared Spectrosc. 24, 109-117 (2016)
Observation	

Calibration summary

Between 2009 and 2018, 8091 values of Dry Matter values were collected for fresh cassava roots:

Year	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	Total

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[1] Names of projects in which the calibrations were established

Number of DM	650	645	693	1369	1758	506	612	884	334	640	8091

Descriptive Statistics for Dry Matter

Constituent	N	Minimum	Maximum	Mean	Standard Deviation
Dry Matter (%)	8091	12,29	52,44	34,34	5,65

The distribution of Dry Matter contents follows a normal curve with no extreme values (fig.1).
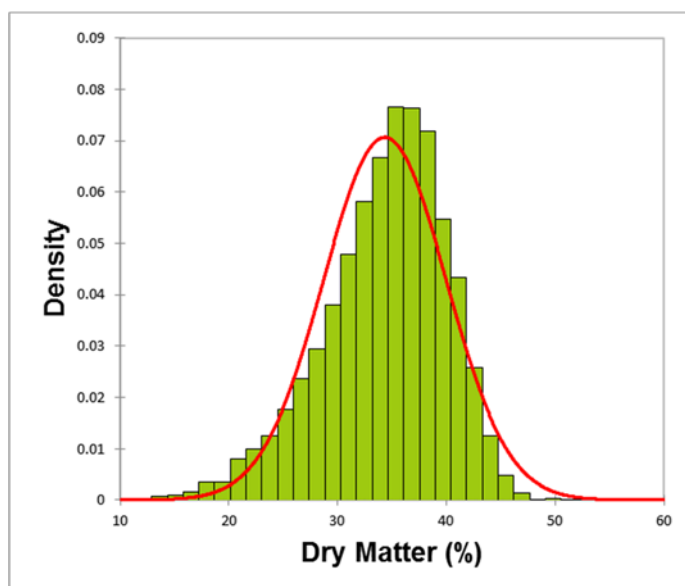

Figure 1: Histogram of Dry Matter contents

Calibration protocol

Data and statistical analyses were performed using Win-ISI 4.6 software (Infrasoft International and FOSS, Hillerod, Denmark). Spectra were corrected for light scattering using the standard normal variate and de-trend (SNVD) correction. The calibration was set up using the second derivative of SNVD corrected spectra, calculated on five data points and smoothed using Savitzky–Golay polynomial smoothing on five data points. The full spectra range was used. The WinISI 4.6 LOCAL regressions algorithm was used for calibration. Cross-validation with 4 groups (random) was used during calibration development. The Student (t) test was used to identify t-outlier samples during calibration development. Outlier detection was based on the standardized residuals with a cutoff of 2.5. Two passes of outlier elimination were used.

Calibration parameters

The LOCAL regression was optimized for the minimum and maximum numbers of similar samples to be used: the minimum number of samples was 50 and the maximum, 250. The maximum number of Partial least Squares (PLS) terms was 13.

Calibration statistics parameters

Constituent	N	SEP	Bias	Slope	R²	Wavelengths	Spectra treatments

						SNVD
DM (%)	7807	1,285	-2,153	0,945	0,947	400– 2500 nm	Second derivative (5 points) Polynomial Smooth (2nd order, five points)

N: number of samples, SEP: Standard Error of Prediction, R²: Coefficient of determination.
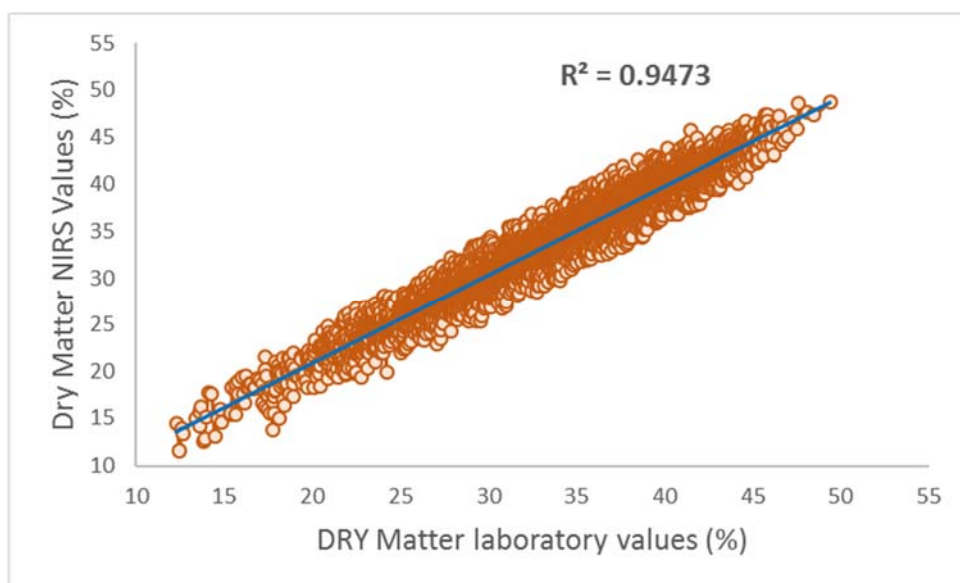

Figure 2: Scatter plot of DM Nirs predicted values versus DM laboratory values

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