

Use of NIR and PLS to predict chemical composition of Brachiaria.

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Track

8. Agriculture and food

The determination of the chemical composition of different fractions of forage is of fundamental importance for the animal performance prediction, to improve the quality of the cultivars in breeding programs and the development of different production stems.

The reflectance in the near infrared is a fast spectroscopic method, which emerged as an alternative to traditional analytical methods to be rapid, non-destructive and of low cost. This study explored the potential of partial least squares (PLS) and near infrared spectroscopy (NIRS) to predict crude protein (CP), neutral detergent fiber (NDF), acid detergent fiber (ADF), lignin (LIG) and in vitro dry matter digestibility (IVDMD) parameters of a several species of brachiarias. In total, 324 samples used in this study were selected from various cultivars of Brachiaria (*Brachiaria brizantha* cvs. Marandú, Xaraés and Piata; *Brachiaria Ruziziensis* and *Brachiaria decumbens*). The samples were collected in 2012 in trials located in 4 different regions of Brazil. Thus, we selected by Kennard-Stone algorithm 147 samples of brachiaria seeking greater representativeness of the samples. The reference method used for determining the protein was Dumas, NDF, ADF and lignin was ANKOM method, and IVDMD was the method with ruminal fluid digestion.

The Brachiaria samples of different growth stages and fractions of plant were collected at 20 cm from the ground and dried at 65 ° C to constant weight. Then, they were ground in a Wiley knife mill type, using a 1 mm sieve. The spectra were recorded on the Buchi NIRFlex N500 FT-NIR spectrometer using as sample carries a borosilicate glass Petri dish from 10000 to 4000 cm⁻¹. Data were handled with Unscrambler 10.2 software. Samples were analyzed in triplicate and all spectra were averaged 32 scans at a resolution of 4 cm⁻¹. For

this work, we measured the composition of a 147 homogenized samples and each component measurement by 4 laboratories (interlaboratory comparison). The Brachiaria samples were randomly classified into 2 subsets with representation of all grasses species; two-thirds of the samples were used to develop regression models using partial least squares (PLS), and the remaining one third of the data was used to conduct an external validation of the models.

Different math pretreatments were used (Savitzky-Golay smoothing, first derivative and mean center). The best determination coefficient (R^2) and root mean square error of prediction (RMSEP) using PLS algorithm to correlate spectral information to chemical data were CP ($R^2 = 0.97$, RMSEP = 0.60), NDF ($R^2 = 0.95$, RMSEP = 1.74) and ADF ($R^2 = 0.93$, RMSEP = 1.46), LIG ($R^2 = 0.94$, RMSEP = 0.57), DMIVD ($R^2 = 0.94$, RMSEP = 2.60). The other statistical parameters used to evaluate the predictive performance of the validation data set were RPD (ratio performance deviation) and RSEP (relative standard error of prediction) that estimated for CP (RPD = 5.9, RSEP = 7.3) NDF (RPD = 5.1, RSEP = 2.3) and ADF (RPD = 3.6, RSEP = 3.5), LIG (RPD = 4.0, RSEP = 10.1), DMIVD (RPD = 3.9, RSEP = 5.2) attesting the good prediction ability of the models. Near-infrared spectroscopy successfully quantified forage quality parameters in commercial Brachiaria, being appropriate for replacing the reference methods routinely.

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