

Use of NIRS, PLS and OPS Variable Selection to Predict Five Quality Parameters of Sweet Sorghum Juice used to Produce Bioethanol

Marcelo Sena
Cristiane Guimarães
Camila Assis
Maria Lúcia Simeone

Track

8. Agriculture and food

First generation biofuels represents a well established sustainable energy source, reducing pollutants emission in the atmosphere. A culture highly feasible to be used for the bioethanol generation in Brazil is the sweet sorghum, which is particularly promising as complementary for the diversification of sugarcane croplands due to its shorter harvest period. Sorghum breed programs have sought to develop new cultivars of higher bioethanol yield, generating a large number of juice samples that must be analysed and characterized before the fermentation. Thus, rapid and non-destructive analytical methods are required. In this work, multivariate calibration models were developed for determining five quality parameters of sorghum juice (Brix, saccharimeter reading/SR, reducing sugars/RS, Pol, apparent purity/Q) based on PLS and NIRS. All of these models were optimized by variable selection with Ordered Predictors Selection (OPS). OPS selects the most predictive variables by a systematic investigation of the PLS informative vectors (correlation coefficients, VIPscores, NAS, etc.) in a cross-validation process, leading to a great reduction in the number of variables.

500 juice samples were obtained from 275 recombinant inbred lines of sweet sorghum derived from two contrasting lines in relation to the quality and quantity of sugars. The five quality parameters were determined by appropriate reference methods. Juice samples were previously filtered in cotton and their spectra were recorded on a Büchi NIRFlex N-500 FT-NIR spectrometer, equipped with a transfectance accessory, from 10000 to 4000 cm^{-1} , with 4 cm^{-1} steps. Data were handled with Matlab, PLS_Toolbox and a homemade routine for OPS.

The analytical ranges for the parameters were 5.5-18.1°B (brix), 1.1-53.2°Z (SR), 1.2-5.2%

w/v (RS), 0.3-13.0% w/v (pol) and 9.8-83.0% w/v (Q). Samples were split in 333 for calibration and 167 for validation using the Kennard-Stone algorithm. The best models were obtained with the preprocessings first derivative, Savitzky-Golay smoothing and mean center. All the PLS models were built with 6 latent variables. Subsequently, the models were optimized by variable selection with OPS, reducing the number of wavenumbers used from 1501 (full spectra) to 50-130, depending on each parameter. All the RMSEC and RMSEP values for the OPS-PLS models were decreased. RMSEP were decreased from 0.4 to 0.3°B (brix), 3.2 to 2.1°Z (SR), 0.4 to 0.3% w/v (RS), 0.8 to 0.6% w/v (pol) and 5.8 to 5.3% w/v (Q). Correlation coefficients (r) for the reference versus predicted values were between 0.896 and 0.992. The randomness of the residuals was checked by appropriate statistical tests, assuring the linearity of the methods. The developed methods were validated by estimating figures of merit, such as trueness, precision, analytical sensitivity and bias. RPD (residual prediction deviation) was estimated between 2.4 and 6.2, attesting the good prediction ability of the models. The use of OPS allowed developing simpler, more interpretable and predictive multivariate calibration models. The NIRS methods are rapid, non-destructive and of low cost, being appropriate for replacing the more laborious reference methods, what is stressed considering the large number of samples analyzed.

Acknowledgements

CAPES for a fellowship (C.A.), Reinaldo F. Teófilo (UFV, Brazil) for the OPS routine, and FAPEMIG for the financial support.

ArquivoEditarExibirHistóricoFavoritosFerramentasAjuda

Zimbra: EntradaUse of NIR and PLS to predict c...Oral Sessions | Nir 2015

mi2015.com.br/en/node/1128International Council for Near Infrared Spectroscopy

Mais visitadosPrimeiros passosÚltimas notíciasJZ E-mail corporativoBiblioteconomia

NIR 2015
Brazil

Highlighting South America

HomeConferenceProgramCommitteesSponsorsVenueContact us

Kyoto University - Primate Research Institute - Japan

15:30 OP14 Simulation method design to link the spectral properties of dense microalgal culture to cell physiology

Riyad Bendoula, Sarah Bellini, Jean-Michel Roger - France

Irslea - UMR ITAP

15:50 OP15 Prediction of soil bulk density for a set of Scottish afforested soils: a comparison of approaches

Jean Robertson, Estefania Perez-Fernandez, J. Potts, A. Lilly

The James Hutton Institute - Scotland

ORAL SESSION 4 - AGRICULTURE AND FOOD [Tuesday 20th]

Chair: Dolores Perez-Marin

8:40 Session to Honour

Károly Kaffka, Tony Blakeney, Jim Burger and Fred McClure

9:00 OP16 Use of NIRS, PLS and OPS variable selection to predict five quality parameters of sweet sorghum juice used to produce bioethanol

Marcelo M. Senga, Cristiane C. Guimarães, Camila Assis, Maria Lúcia F. Simeone

Universidade Federal de Minas Gerais - ICEx - Chemistry - Brazil

9:20 OP17 Development of NIRS method for energetic value of high fiber cane clones

Fabrice Davrieux, Camille Roussel, Mathilde Mellin, Régis Cinier, Christophe Poser

CIRAD-UMR Qualisud, 7 chemin de l'IRAT, 97410 Saint-Pierre, La Réunion - France

9:40 OP18 The impossible made possible: providing a detailed topological map of chemical classification parameters for pork carcasses with on-line slaughter line instrumentation

Klavs Sørensen, Søren Balling Engelsen

University of Copenhagen - Department of Food Science - Spectroscopy & Chemometrics - Denmark

ORAL SESSION 5 - AGRICULTURE AND FOOD [Tuesday 20th]

Chair: Maria Lucia F. Simeone

10:20 OP19 Evolution of Vis/NIR bulk optical properties of apple skin and flesh during fruit maturation

Robbe Van Beers, Ben Aernouts, Rodrigo Watté, Ann Schenk, Bart Nicolai, Wouter Saeys

KU Leuven Department of Biosystems, MeBioS, Leuven - Belgium

10:40 OP20 Identification and quantification of bovine meat adulteration by using NIR Spectroscopy

Ernestina Casiraghi, Jose Manoel Amigo, Søren Balling Engelsen, Cristina Alamprese

University of Milan-Faculty of Agricultural and Food Science-Department of Food, Environmental and Nutritional - Italy

simeoneBealçar tudoDiferenciar maiúsculas/minúsculasOcorrência 1 de 2