Application Note AN-NIR-110

Quality control of sugarcane juice

Multiparameter determination within one minute using NIRS

Sugarcane (*Saccharum* spp.) is a very important crop for the global economy. It is often used as a raw material for the production of sugar, alcohol, yeast, and more. Brix (°Brix), Pol (%), juice purity (%), reducing sugars (%), and total recoverable sugars (Kg t^{-1}) are some of the many quality control (QC) parameters that must be analyzed in sugarcane juice. Numerous methods based on several analytical techniques are available for sugarcane juice quality control. These methods can be quite time-consuming since sample treatment is a prerequisite. A quicker alternative to these other methods is near-infrared spectroscopy (NIRS). NIRS allows the simultaneous determination of several QC constituents, without chemicals or sample preparation, in less than one minute.

EXPERIMENTAL EQUIPMENT

Sugarcane juice was analyzed by NIRS, and a total of 100 spectra were collected to create a prediction model for quantification of several QC parameters. All samples were measured with a Metrohm NIRS DS2500 Liquid Analyzer (400–2500 nm) in transmission mode with a DS2500 Holder Flow Cell (Figure 1). A flow cell with 1 mm pathlength was used in this study. This flow cell was filled via peristaltic pump. The Vision Air Complete software package from Metrohm was used for all data acquisition and prediction model development.

Table 1. Hardware and software equipment overview.

Equipment	Article number
DS2500 Liquid Analyzer	2.929.0010
DS2500 Holder Flow cell	6.7493.000
NIRS quartz cuvette flow 1 mm	6.7401.310
Vision Air 2.0 Complete	6.6072.208

Figure 1. Metrohm NIRS DS2500 Liquid Analyzer and DS2500 Holder Flow Cell used for the fast determination of several QC parameters in sugarcane juice.

RESULT

The obtained Vis-NIR spectra (Figure 2) were used to create a prediction model for quantification of Brix (°Brix), Pol (%), juice purity (%), reducing sugars (%), and total recoverable sugars (Kg t^{-1}). The quality of the prediction model was evaluated using correlation diagrams which display a very high correlation between the Vis-NIR prediction and the reference values. The respective figures of merit (FOM) display the expected precision of a prediction during routine analysis (Figures 3–8).

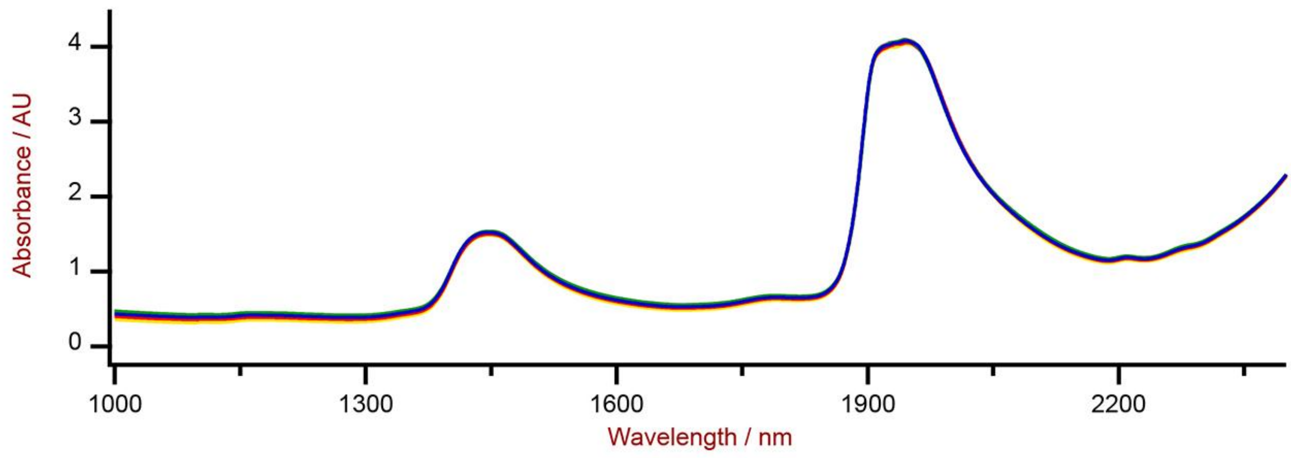

Figure 2. Selection of Vis-NIR spectra of sugarcane juice samples analyzed on a DS2500 Liquid Analyzer with a 1 mm pathlength flow cell.

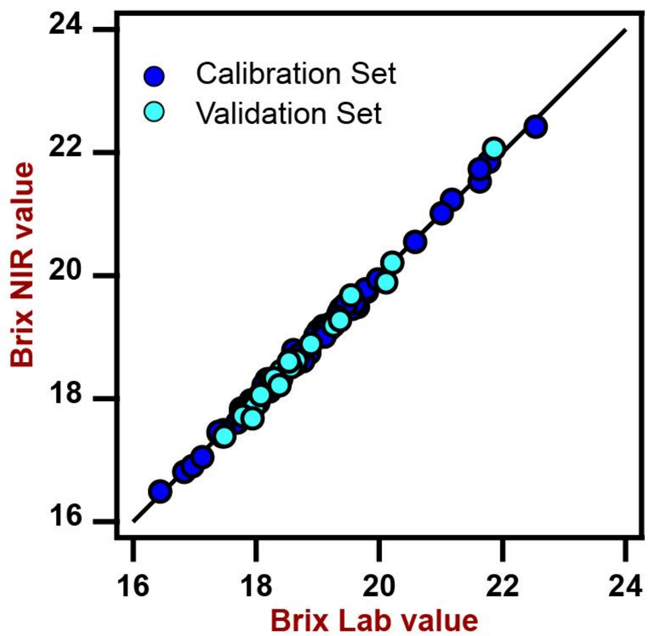

Figure 3. Correlation diagram and the respective FOMs for the prediction of Brix in sugarcane juice using a DS2500 Liquid Analyzer. Laboratory values were evaluated using a refractometer.

Figures of Merit	Value
R^2	0.9875
Standard Error of Calibration	0.1323 (°Brix)
Standard Error of Cross-Validation	0.1467 (°Brix)

Standard Error of Validation	0.138 (°Brix)

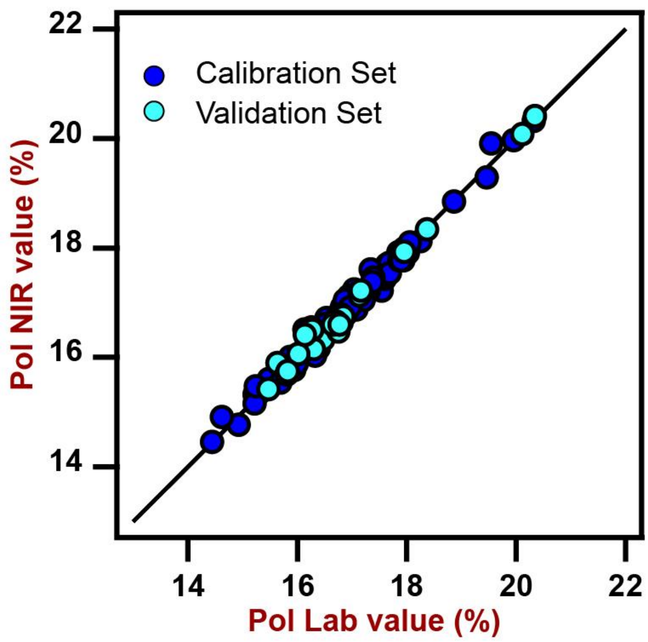

Figure 4. Correlation diagram and the respective FOMs for the prediction of Pol in sugarcane juice using a DS2500 Liquid Analyzer. Laboratory values were calculated from the sucrose reading, Brix, and a few constants.

Figures of Merit	Value
R^2	0.9833
Standard Error of Calibration	0.1506%
Standard Error of Cross-Validation	0.1851%
Standard Error of Validation	0.1388%

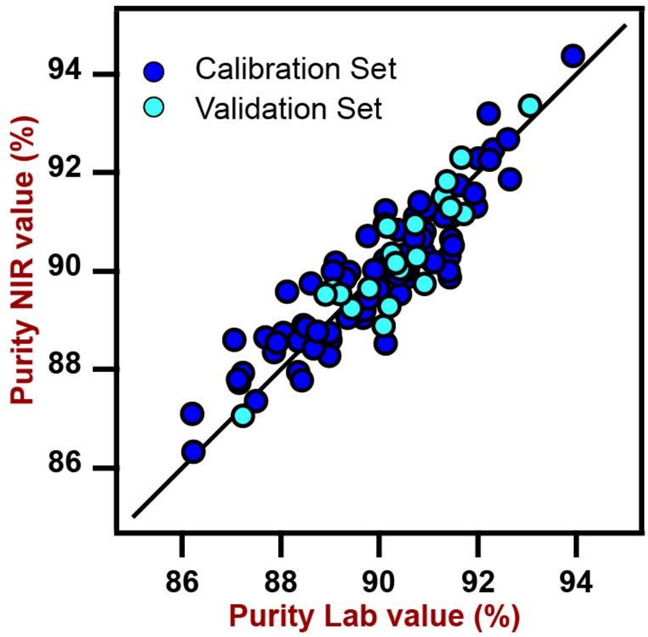

Figure 5. Correlation diagram and the respective FOMs for the prediction of sugarcane juice purity using a DS2500 Liquid Analyzer. Laboratory values were calculated using the results from Pol and Brix determinations: Purity = 100 × (Pol/Brix).

Figures of Merit	Value
R^2	0.8194
Standard Error of Calibration	0.7202%
Standard Error of Cross-Validation	0.7596%
Standard Error of Validation	0.564%

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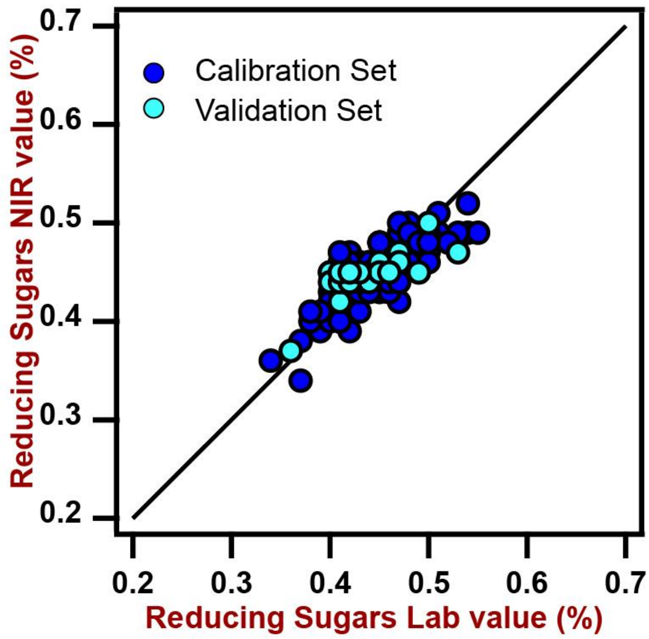

Figure 6. Correlation diagram and the respective FOMs for the prediction of reducing sugars in sugarcane juice using a DS2500 Liquid Analyzer. Laboratory values were measured with ion chromatography (IC).

Figures of Merit	Value
R^2	0.6497
Standard Error of Calibration	0.0263%
Standard Error of Cross-Validation	0.0291%
Standard Error of Validation	0.0249%

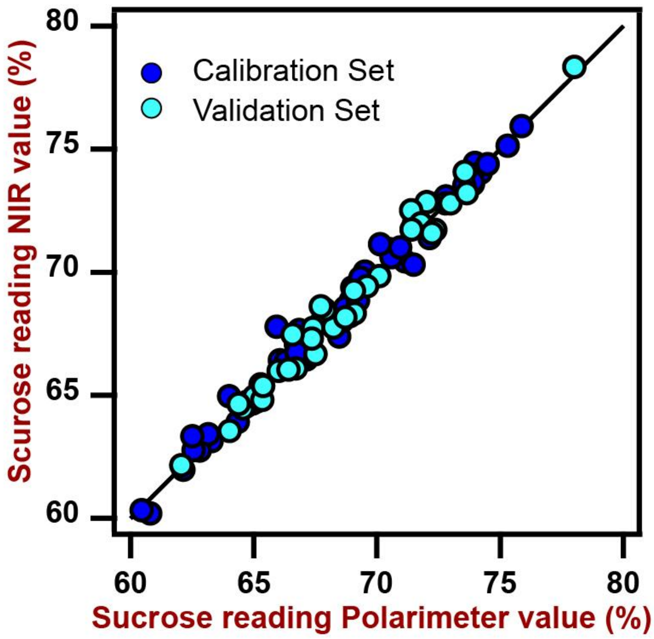

Figure 7. Correlation diagram and the respective FOMs for the prediction of sucrose reading in sugarcane juice using a DS2500 Liquid Analyzer. Laboratory values were evaluated with a polarimeter.

Figures of Merit	Value
R^2	0.9911
Standard Error of Calibration	0.5388%
Standard Error of Cross-Validation	0.6604%
Standard Error of Validation	0.497%

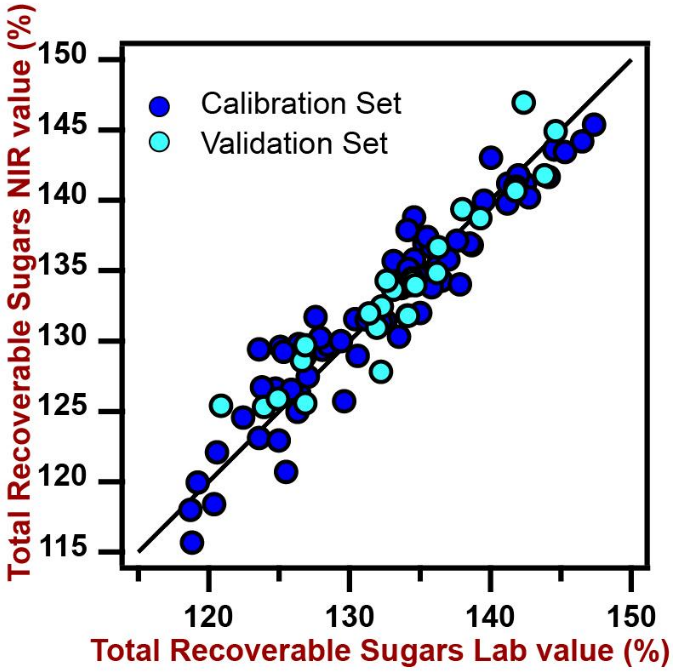

Figure 8. Correlation diagram and the respective FOMs for the prediction of total recoverable sugars in sugarcane juice using a DS2500 Liquid Analyzer. Laboratory values were evaluated using Pol and reducing sugars values: TRS = (9.5263 × Pol) – (9.05 × RS).

Figures of Merit	Value
R^2	0.9463
Standard Error of Calibration	2.2985%
Standard Error of Cross-Validation	2.5118%
Standard Error of Validation	1.9074%

CONCLUSION

This Application Note demonstrates the feasibility to determine Brix, Pol, juice purity, reducing sugars, and total recoverable sugars in sugarcane juice with NIR spectroscopy. Vis-NIR spectroscopy enables a fast and highly accurate alternative to other standard methods (Table 2). No sample preparation is required, and results are delivered in less than a minute.

Table 2. Time to result overview for the different quality control parameters typically measured in sugarcane juice.

Parameter	Method	Time to result
Brix	Refractometer	1 min
Pol	Calculated from Pol and Brix, as well as the application of a few constants	10 min sample preparation (clarification & filtration) + 1 min polarimeter + 1 min refractometer
Purity	Calculated from Pol and Brix	Purity = 100 × (Pol/Brix)
Reducing sugars (RS)	Ion Chromatography	10 min sample preparation (clarification & filtration) + 40 min IC
Sucrose reading	Polarimeter	10 min sample preparation (clarification & filtration) + 1 min polarimeter
Total recoverable sugars (TRS)	Calculated from Pol and reducing sugars	TRS = (9.5263 × Pol) – (9.05 × RS)

Internal reference: AW NIR CH-0073-042023

CONTACT

Metrohm France
13, avenue du Québec - CS 90038
91978 VILLEBON COURTABOEUF CEDEX

info@metrohm.fr

CONFIGURATION

DS2500 Liquid Analyzer

Spectroscopie proche infrarouge robuste pour le controle qualité en laboratoire et en environnement de production.

L'analyseur DS2500 Liquid Analyzer est la solution éprouvée et souple destinée aux analyses de routine d'échantillons liquides, tout au long de la chaine de fabrication. Sa conception robuste fait du DS2500 Liquid Analyzer un appareil insensible à la poussière, à l'humidité et aux vibrations, et donc particulièrement adapté aux rudes conditions d'un environnement de production.

Le DS2500 Liquid Analyzer couvre l'ensemble de la gamme spectrale de 400 à 2500 nm, chauffe les échantillons jusqu'à 80 °C et est compatible avec divers flacons à usage unique et cuves en quartz. Le 2500 Liquid Analyzer, lequel s'adapte à vos exigences individuelles en matière d'échantillons, vous permet d'obtenir des résultats précis et reproductibles en moins d'une minute. Avec sa détection du support d'échantillon intégrée et le logiciel Vision Air intuitif, un maniement simple et sur est également garanti pour l'utilisateur.

En présence de grandes quantités d'échantillons, l'utilisation d'une cellule à flux continu associée à un robot passeur d'échantillons Metrohm peut augmenter considérablement la productivité.