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).

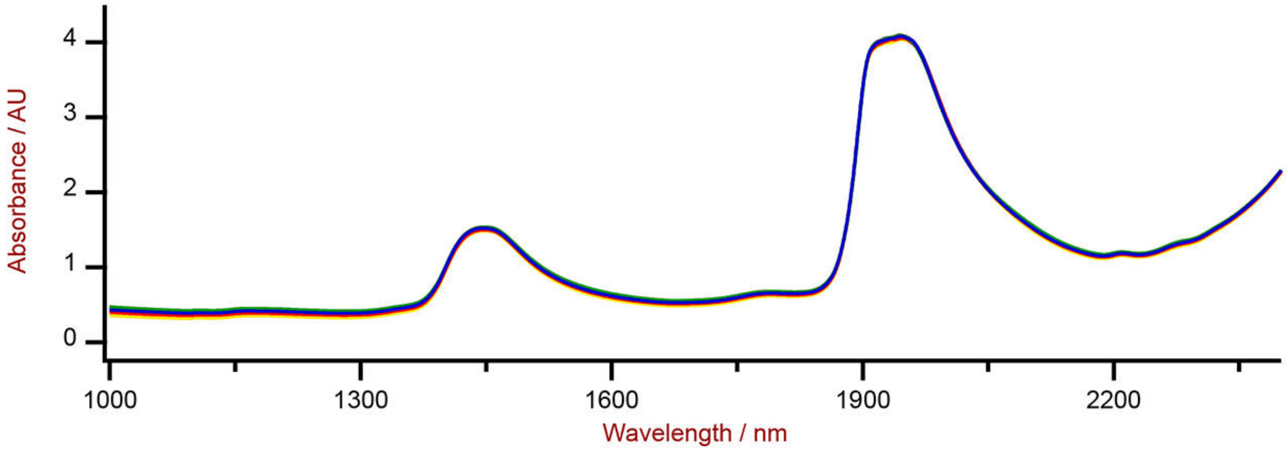

Figure 2. Selection of Vis-NIR spectra of sugarcane juice samples analyzed on a DS2500 Liquid Analyzer with a 1 mm pathlength flow cell.

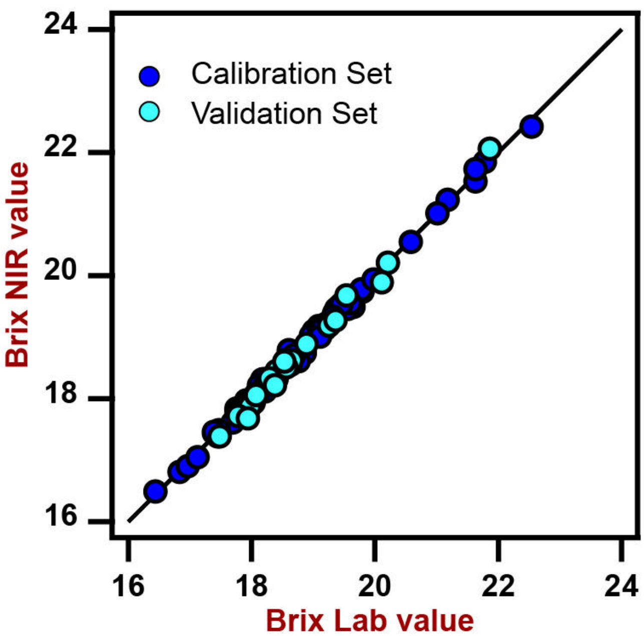

Figure 3. Correlation diagram and the respective FOMs for the prediction of Brix in sugarcane juice using a DS2500 Liquid Analyzer. Laboratory values were evaluated using a refractometer.

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)

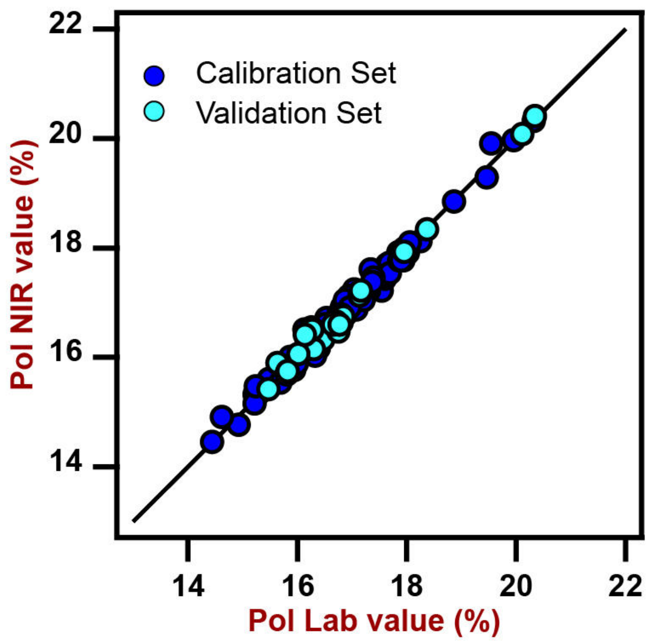

Figure 4. Correlation diagram and the respective FOMs for the prediction of Pol in sugarcane juice using a DS2500 Liquid Analyzer. Laboratory values were calculated from the sucrose reading, Brix, and a few constants.

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%

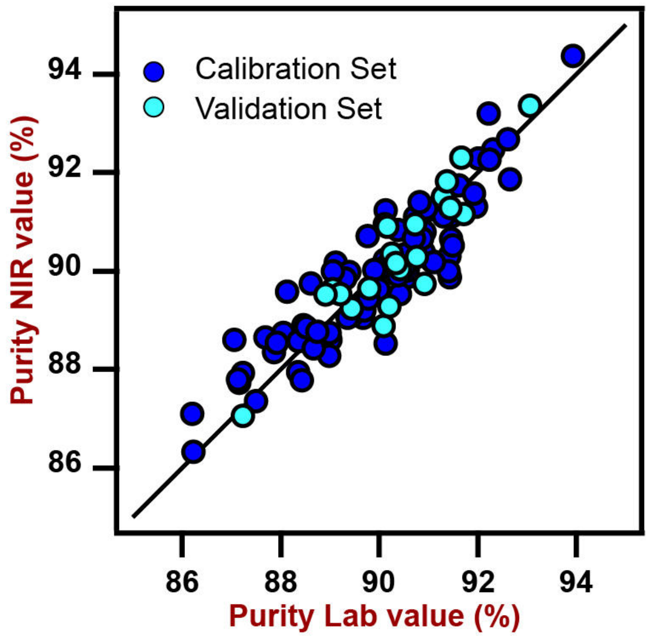

Figure 5. Correlation diagram and the respective FOMs for the prediction of sugarcane juice purity using a DS2500 Liquid Analyzer. Laboratory values were calculated using the results from Pol and Brix determinations: Purity = 100 × (Pol/Brix).

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%

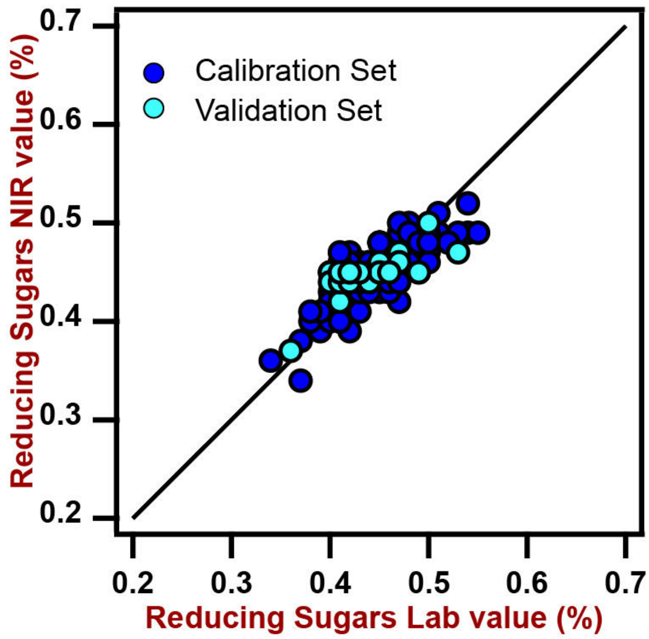

Figure 6. Correlation diagram and the respective FOMs for the prediction of reducing sugars in sugarcane juice using a DS2500 Liquid Analyzer. Laboratory values were measured with ion chromatography (IC).

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%

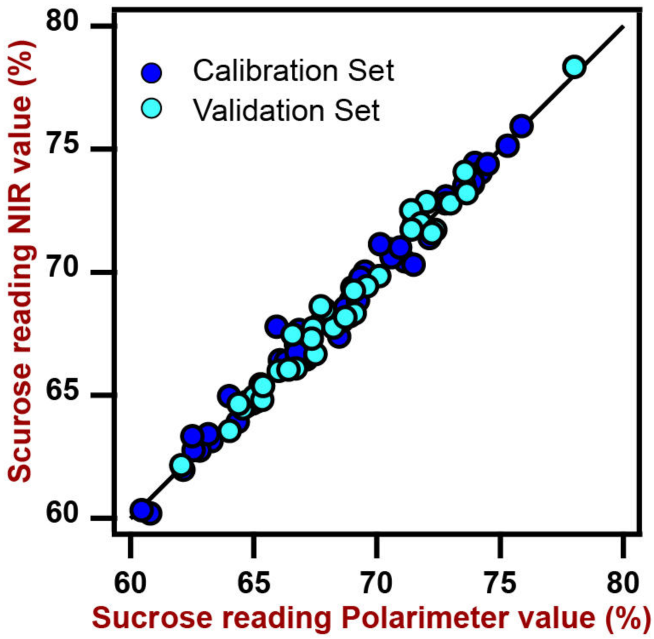

Figure 7. Correlation diagram and the respective FOMs for the prediction of sucrose reading in sugarcane juice using a DS2500 Liquid Analyzer. Laboratory values were evaluated with a polarimeter.

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%

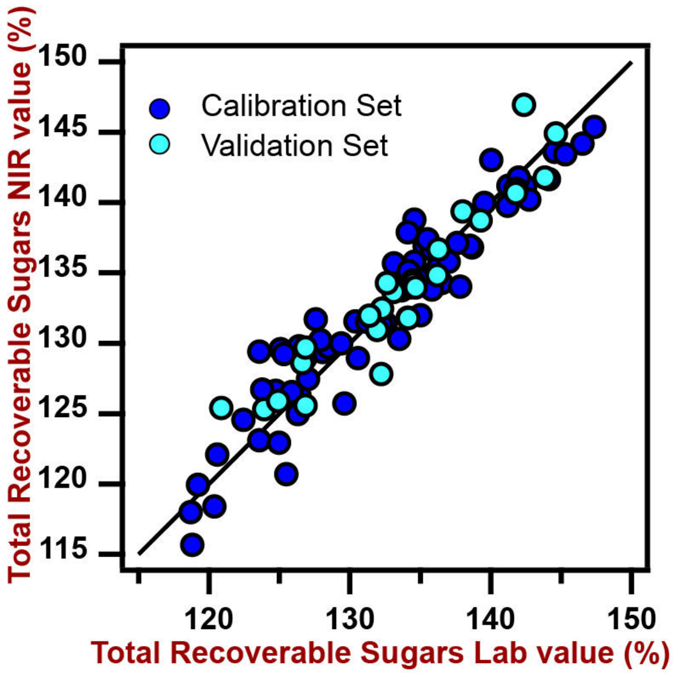

Figure 8. Correlation diagram and the respective FOMs for the prediction of total recoverable sugars in sugarcane juice using a DS2500 Liquid Analyzer. Laboratory values were evaluated using Pol and reducing sugars values: TRS = (9.5263 × Pol) – (9.05 × RS).

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

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CONFIGURATION

DS2500 Liquid Analyzer

Robust near-infrared spectroscopy for quality control, not only in laboratories but also in production environments.

The DS2500 Liquid Analyzer is the tried and tested, flexible solution for routine analysis of liquids along the entire production chain. Its robust design makes the DS2500 Liquid Analyzer resistant to dust, moisture and vibrations, which means that it is eminently suited for use in harsh production environments.

The DS2500 Liquid Analyzer covers the full spectral range from 400 to 2500 nm, heats samples up to 80°C and is compatible with various disposable vials and quartz cuvettes. The DS2500 Liquid Analyzer is thus adaptable to your individual sample requirements and helps you obtain accurate and reproducible results in less than one minute. The integrated sample holder detection and the self-explanatory Vision Air Software also ensure simple and safe operation by the user.

In the case of larger-sized sample quantities, productivity can be considerably increased by using a flow-through cell in combination with a Metrohm sample robot.