Application Note AN-NIR-109

Determination of Brix, fructose, glucose, and sucrose with NIRS

Cost-effective multiparameter analysis within one minute

Sucrose, glucose, and fructose are three common sugars that are absorbed differently in the body. Each of these sugars has slightly different effects. A major factor regarding their effects on our health is whether these sugars occur naturally in foods or have been added during a processing stage. The determination of the individual sugars and Brix (°Bx, a measure of dissolved sugar content) are key quality parameters in the food industry.

Determination of these parameters can be done using e.g., high-performance liquid chromatography (HPLC), ion chromatography (IC), and thin-layer chromatography (TLC). However, these methods can be time-consuming and incur high running costs. On the other hand, near-infrared spectroscopy (NIRS) allows the simultaneous determination of many sugars without chemicals or any sample preparation in less than a minute.

EXPERIMENTAL EQUIPMENT

A total of 50 spectra of aqueous solutions of glucose, fructose, and sucrose were prepared to create a prediction model for quantification. All samples were measured with a Metrohm NIRS DS2500 Liquid Analyzer (400–2500 nm, **Figure 1**) in transmission mode with a holder for flow cells. A flow cell with 1 mm pathlength was used for this application. Data acquisition and prediction model development were performed with the Vision Air Complete software package from Metrohm.

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 used for the quantification of glucose, fructose, sucrose, and total sugars (Brix) in aqueous samples.

RESULT

The obtained Vis-NIR spectra (Figure 2) were used to create a prediction model for quantification of glucose, fructose, sucrose, and Brix. 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 3–6).

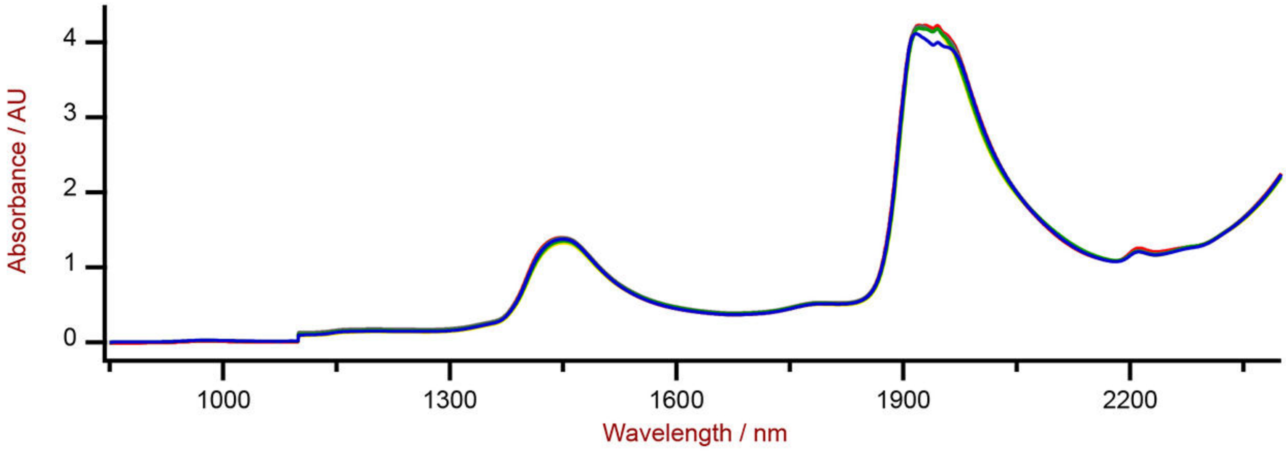

Figure 2. Selection of Vis-NIR spectra of an aqueous mixture of glucose, fructose, and sucrose analyzed on a DS2500 Liquid Analyzer.

RESULT FRUCTOSE CONTENT

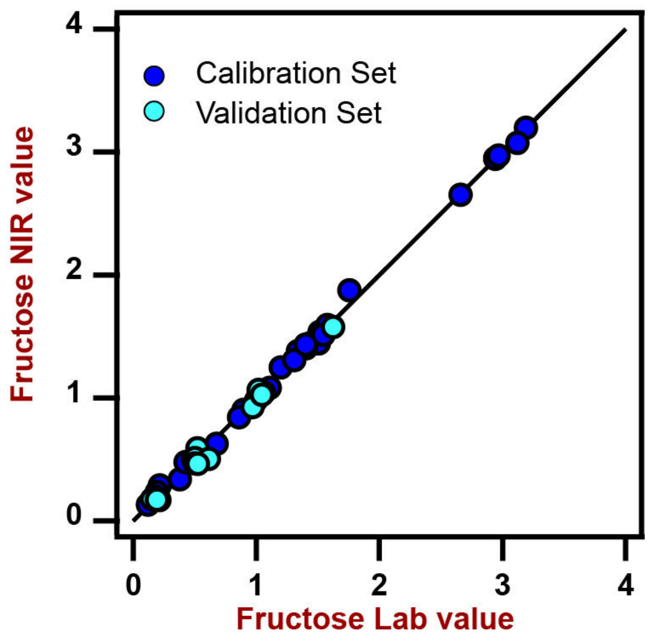

Figure 3. Correlation diagram and the respective figures of merit for the prediction of fructose content in an aqueous sugar mixture using a DS2500 Liquid Analyzer.

Figures of Merit	Value
R2	0.9882

Standard Error of Calibration	0.04%
Standard Error of Cross-Validation	0.06%
Standard Error of Validation	0.05%

RESULT GLUCOSE CONTENT

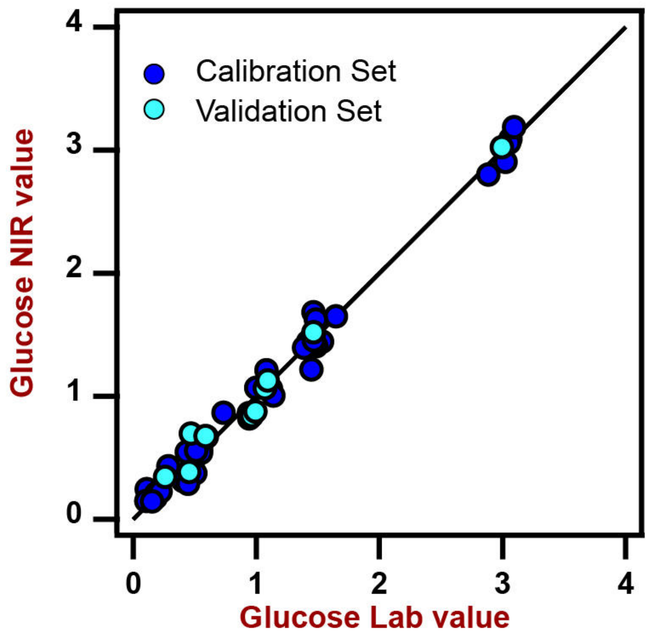

Figure 4. Correlation diagram and the respective figures of merit for the prediction of glucose content in an aqueous sugar mixture using a DS2500 Liquid Analyzer.

Figures of Merit	Value
R2	0.9877
Standard Error of Calibration	0.11%
Standard Error of Cross-Validation	0.12%
Standard Error of Validation	0.10%

RESULT SUCROSE CONTENT

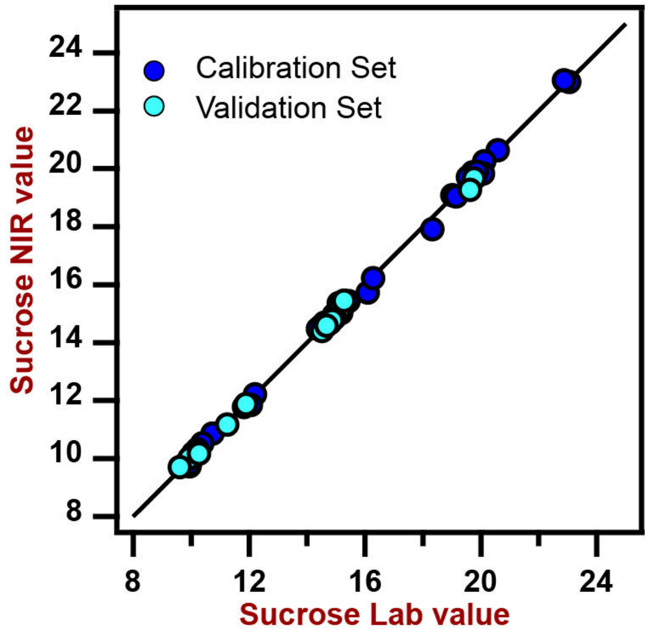

Figure 5. Correlation diagram and the respective figures of merit for the prediction of sucrose content in an aqueous sugar mixture using a DS2500 Liquid Analyzer.

Figures of Merit	Value
R2	0.9886
Standard Error of Calibration	0.16%
Standard Error of Cross-Validation	0.16%
Standard Error of Validation	0.13%

RESULT BRIX

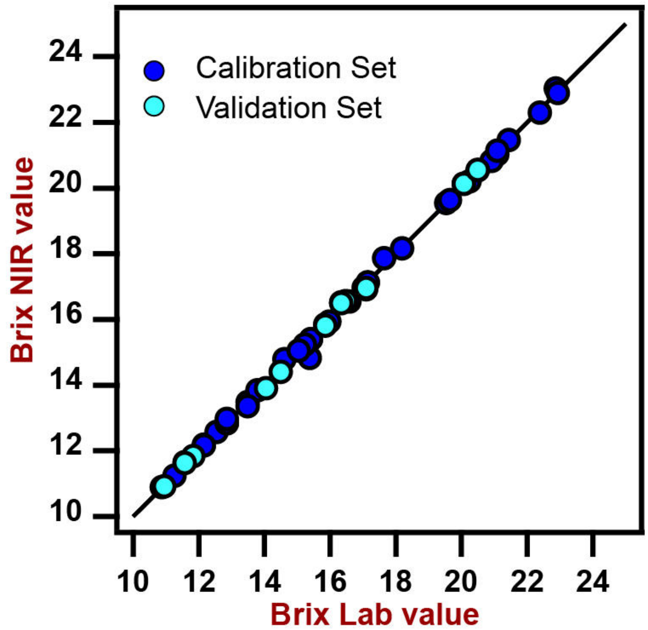

Figure 6. Correlation diagram and the respective figures of merit for the prediction of Brix (total sugars) in an aqueous mixture of sugars using a DS2500 Liquid Analyzer. The lab value was evaluated using a refractometer.

Figures of Merit	Value
R2	0.9988
Standard Error of Calibration	0.13 (°Brix)
Standard Error of Cross-Validation	0.15 (°Brix)
Standard Error of Validation	0.09 (°Brix)

CONCLUSION

This Application Note demonstrates the feasibility to determine glucose, fructose, sucrose, and Brix in aqueous samples with NIR spectroscopy. Vis-NIR spectroscopy is a faster, easier, highly accurate alternative to other standard analytical methods (Table 2).

Table 2. Time to result overview for the different parameters.

Parameter	Method	Time to result
Glucose, Fructose, Sucrose	HPLC	~5 min (preparation) + ~40 min (HPLC)
Brix	Refractometer	~1 min

Internal reference: AW NIR CH-0072-042023

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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.