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.

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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.

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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**).
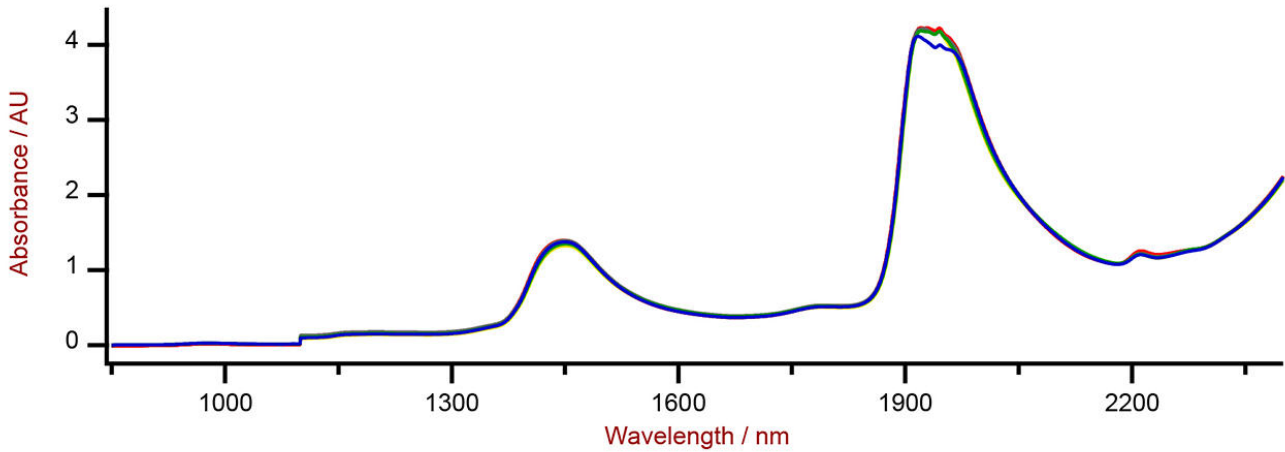

Figure 2. Selection of Vis-NIR spectra of an aqueous mixture of glucose, fructose, and sucrose analyzed on a DS2500 Liquid Analyzer.
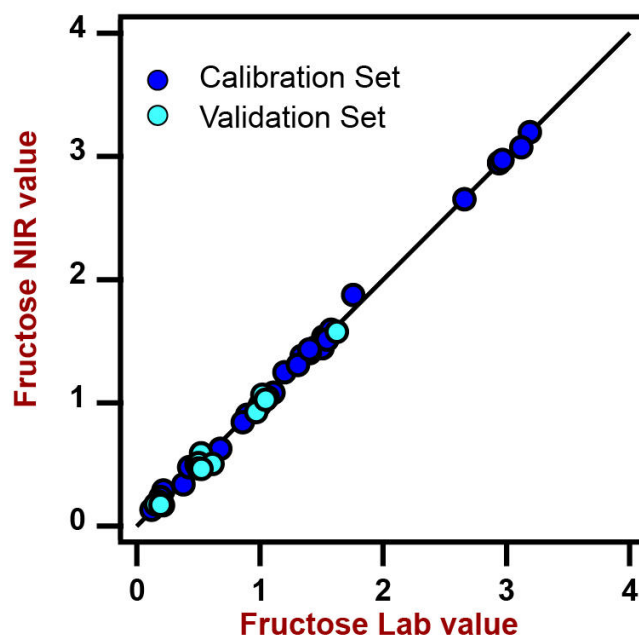
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RESULT FRUCTOSE CONTENT

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
R^2	0.9882
Standard Error of Calibration	0.04%
Standard Error of Cross-Validation	0.06%
Standard Error of Validation	0.05%

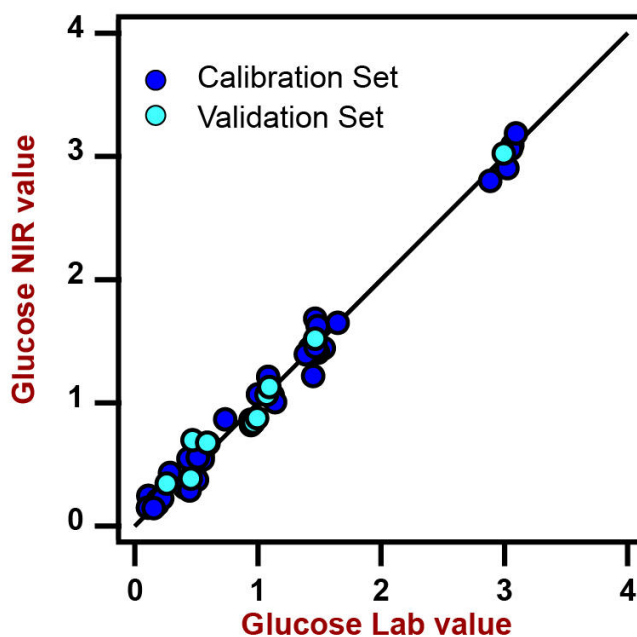Ω Metrohm

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
R^2	0.9877
Standard Error of Calibration	0.11%
Standard Error of Cross-Validation	0.12%
Standard Error of Validation	0.10%

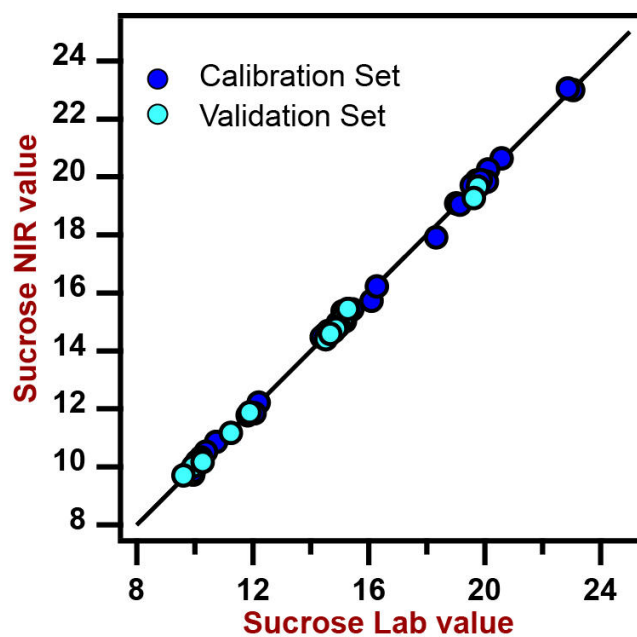Ω Metrohm

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
R^2	0.9886
Standard Error of Calibration	0.16%
Standard Error of Cross-Validation	0.16%
Standard Error of Validation	0.13%

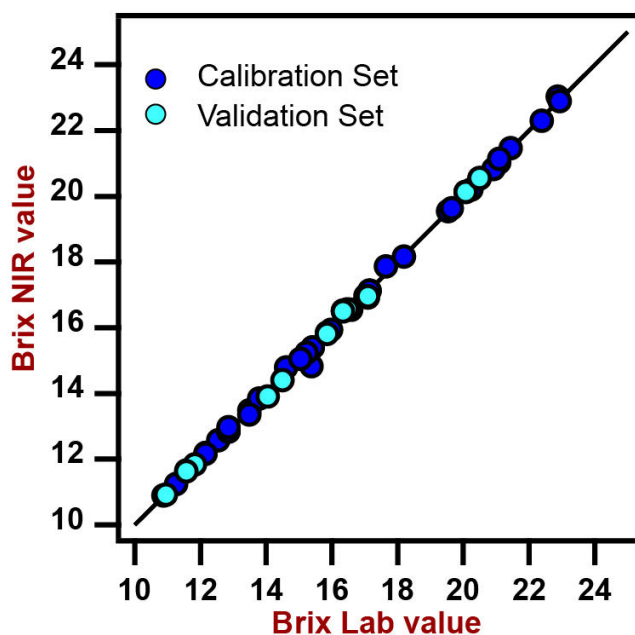Ω Metrohm

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
R^2	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).

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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

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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.

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