Application Note AN-NIR-108

Quality control of sugars in fruit juice

Fast multiparameter determination of sugars with NIRS

Fruit juices are produced and consumed for their refreshing character, nutritional benefits, and as a good source of instant energy. Since juices are sweet beverages, the determination of different sugar components is highly important in this industry. In particular, the sugars fructose, glucose, and sucrose are controlled and monitored. Traditional laboratory analysis for the determination of these sugars in fruit juices involves the use of liquid chromatography as well as polarimetric and refractive index measurements. This combination of techniques takes a significant amount of time for the complete analysis and requires different types of laboratory equipment. Near-infrared spectroscopy (NIRS) is an analytical technique that allows the simultaneous determination of glucose, fructose, and sucrose in fruit juices in less than one minute. Additionally, no chemicals are required, and sample preparation is not necessary when using NIR spectroscopy.

EXPERIMENTAL EQUIPMENT

A total of 27 samples, including aqueous solutions of glucose (0–8 g/100 mL), fructose (0–8 g/100 mL), and sucrose (0–8 g/100 mL), were prepared to create a prediction model for quantification. All samples were measured in transmission mode on a Metrohm NIRS DS2500 Liquid Analyzer (400–2500 nm, Figure 1) with a holder for 2 mm vials. For convenience, disposable vials with a pathlength of 2 mm were used, which made cleaning of the sample vessels unnecessary.

Samples of 10 different fruit juices were measured with this setup. The content of glucose, fructose, and sucrose was predicted using the prediction models mentioned above. Ion chromatography (IC) was used as the reference method to measure the concentration of different sugars in the juice samples. The Metrohm software package Vision Air Complete was used for all data acquisition and prediction model development.

Figure 1. Metrohm NIRS DS2500 Liquid Analyzer used for the determination of various sugars in fruit juices.

RESULT

The obtained Vis-NIR spectra (Figure 2) were used to create a prediction model for quantification of glucose, fructose, sucrose, and total sugars. 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). The Standard Error of Prediction (SEP) for every component measured in this study is shown in Figure 7.

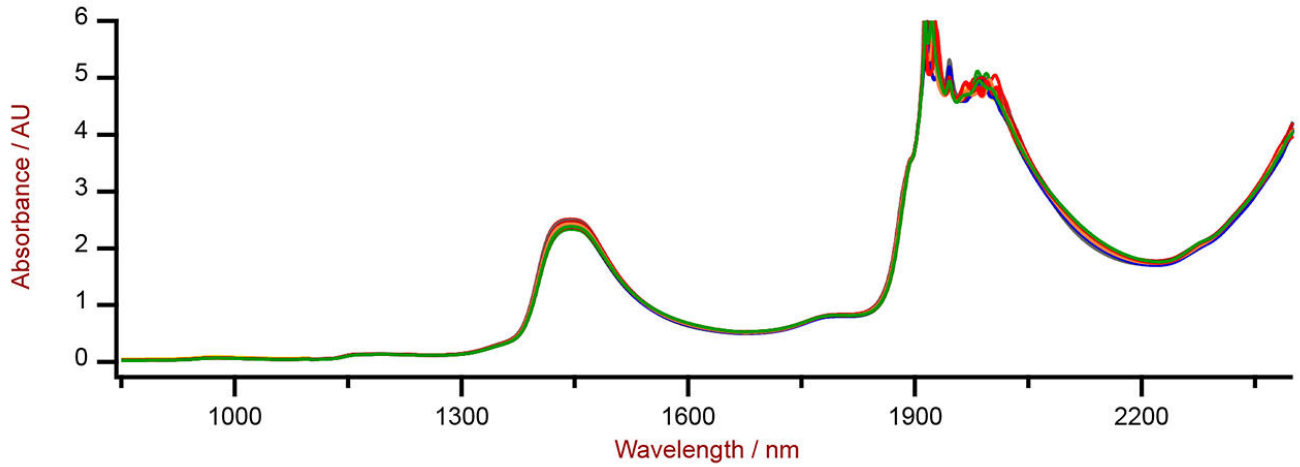

Figure 2. Selection of Vis-NIR spectra of an aqueous mixture of glucose, fructose, and sucrose analyzed on a DS2500 Liquid Analyzer.

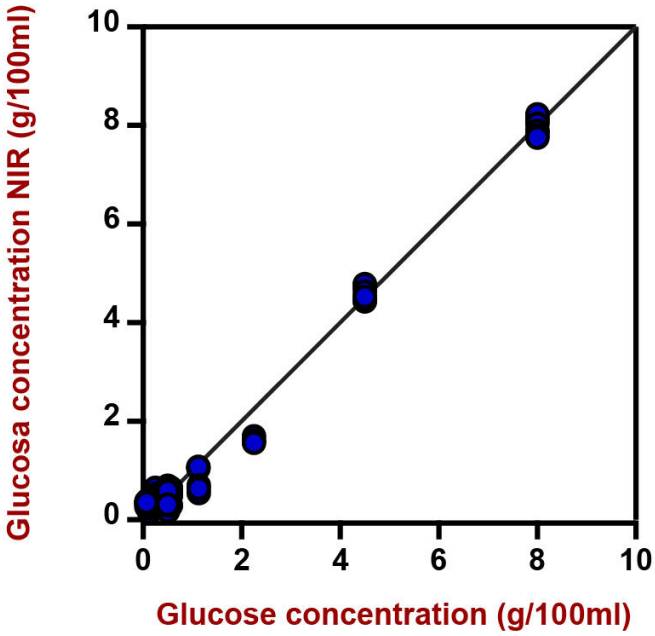

Figure 3. Correlation diagram and the respective figures of merit for the prediction of glucose in an aqueous mixture of sugars using a DS2500 Liquid Analyzer. The lab value was evaluated with IC.

Figures of Merit	Value
R2	0.9913
Standard Error of Calibration	0.2586 (g/100 mL)

Standard Error of Cross-Validation	0.2633 (g/100 mL)

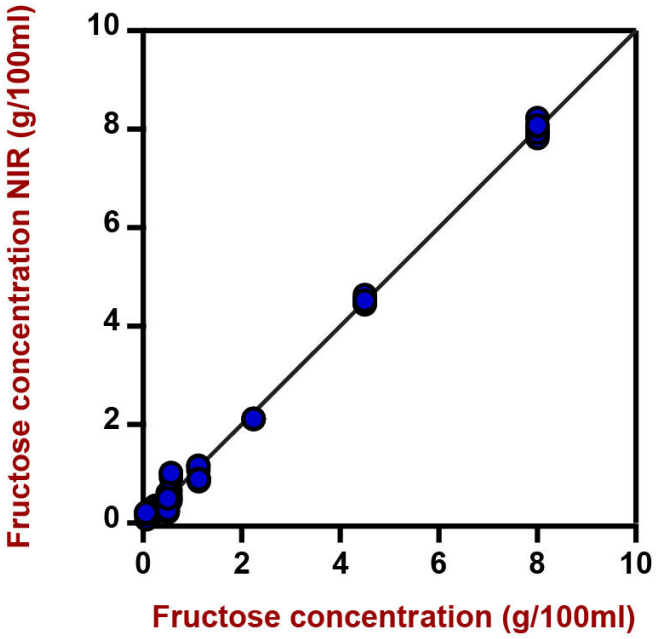

Figure 4. Correlation diagram and the respective figures of merit for the prediction of fructose content in an aqueous mixture of sugars using a DS2500 Liquid Analyzer. The lab value was evaluated with IC.

Figures of Merit	Value
R2	0.9967
Standard Error of Calibration	0.1682 (g/100 mL)
Standard Error of Cross-Validation	0.1876 (g/100 mL)

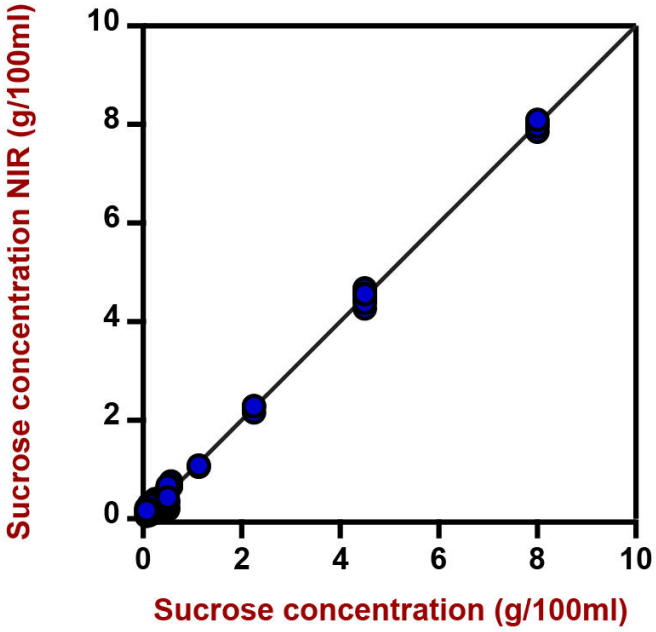

Figure 5. Correlation diagram and the respective figures of merit for the prediction of sucrose content in an aqueous mixture of sugars using a DS2500 Liquid Analyzer. The lab value was evaluated with IC.

Figures of Merit	Value
R2	0.9902
Standard Error of Calibration	0.2390 (g/100 mL)
Standard Error of Cross-Validation	0.2401 (g/100 mL)

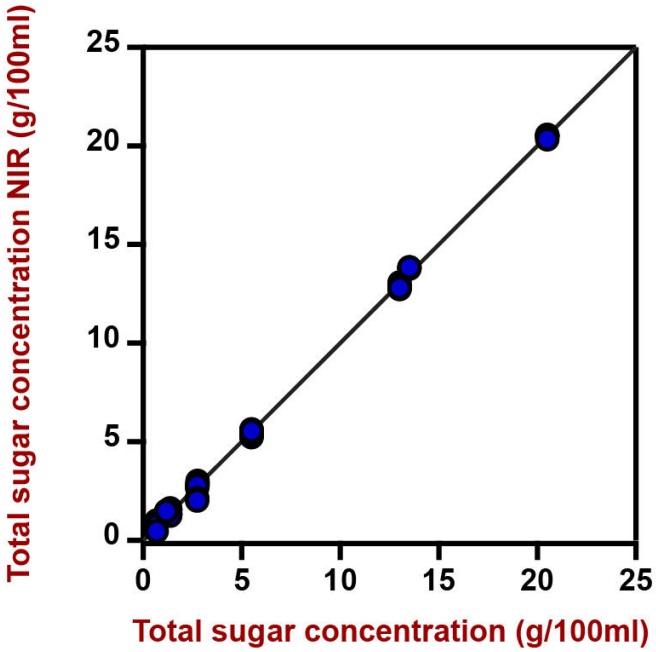

Figure 6. Correlation diagram and the respective figures of merit for the prediction of total sugars in an aqueous mixture of sugars using a DS2500 Liquid Analyzer. The lab value was evaluated with a refractometer.

Figures of Merit	Value
R2	0.9985
Standard Error of Calibration	0.2718 (g/100 mL)
Standard Error of Cross-Validation	0.2770 (g/100 mL)

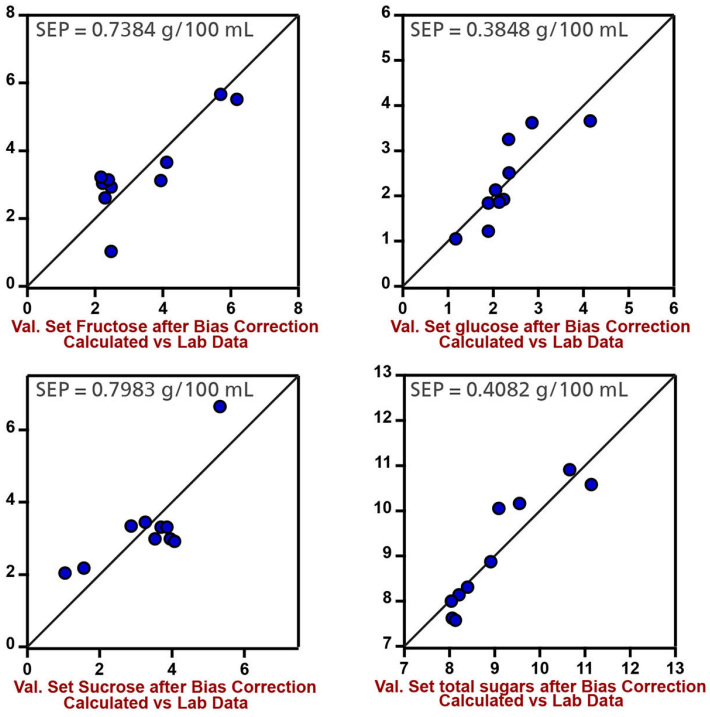

Figure 7. Validation plots of fructose, glucose, sucrose, and total sugars in fruit juices 1 to 10 with SEP (Standard Error of Prediction).

CONCLUSION

This Application Note demonstrates the feasibility to determine glucose, fructose, sucrose, and total sugars in juices with near-infrared spectroscopy. Vis-NIR spectroscopy offers users fast and highly accurate results without the need for highly trained analysts, chemicals, or sample preparation. Therefore, NIRS represents a suitable alternative to other standard methods like liquid chromatography (Table 2).

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CONTACT

Metrohm Česká republika
s.r.o.
Na Harfě 935/5c
190 00 Praha
office@metrohm.cz

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.