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.

Table 1. Hardware and software equipment overview.

Equipment	Article number
DS2500 Liquid Analyzer	2.929.0010
DS2500 Holder 2 mm vials	6.749.2000
Disposable vials, 2 mm	6.7402.070
Vision Air 2.0 Complete	6.6072.208

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.

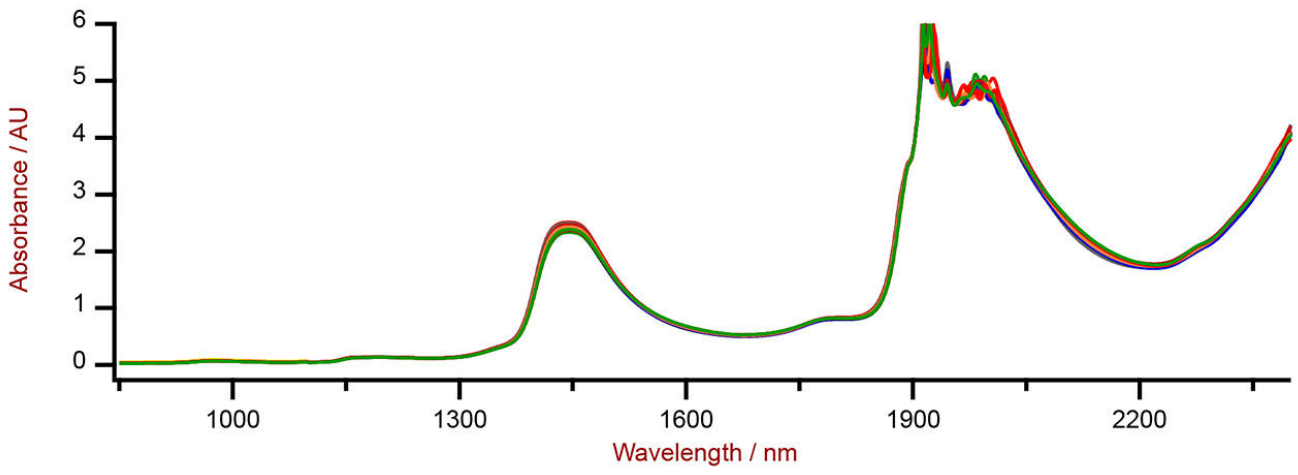

Figure 2. Selection of Vis-NIR spectra of an aqueous mixture of glucose, fructose, and sucrose analyzed on a DS2500 Liquid Analyzer.

RESULT GLUCOSE CONTENT

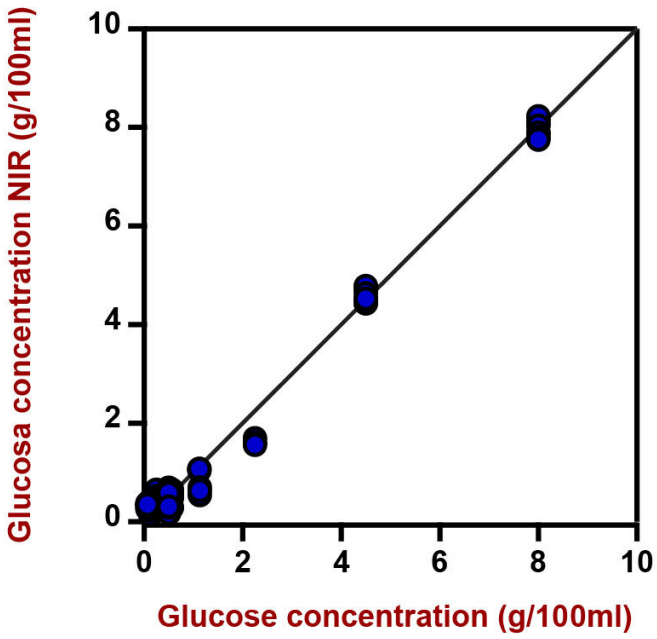

Figure 3. Correlation diagram and the respective figures of merit for the prediction of glucose in an aqueous mixture of sugars using a DS2500 Liquid Analyzer. The lab value was evaluated with IC.

Figures of Merit	Value
R^2	0.9913

Standard Error of Calibration	0.2586 (g/100 mL)
Standard Error of Cross-Validation	0.2633 (g/100 mL)

RESULT FRUCTOSE CONTENT

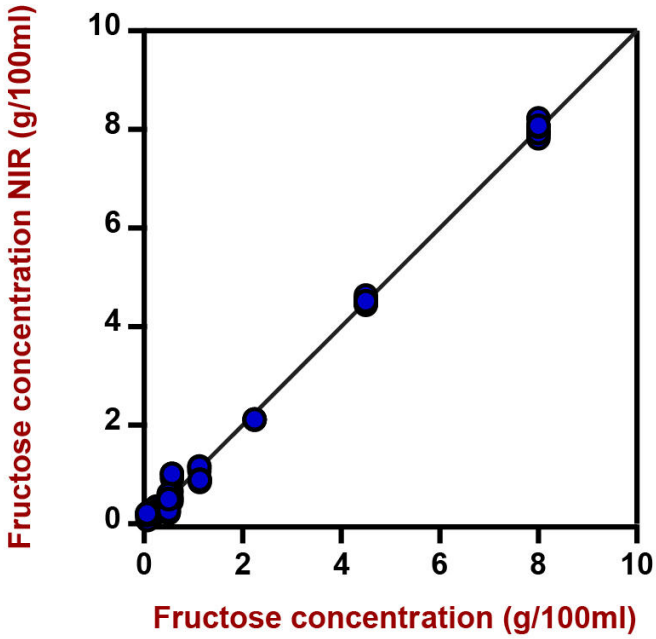

Figure 4. Correlation diagram and the respective figures of merit for the prediction of fructose content in an aqueous mixture of sugars using a DS2500 Liquid Analyzer. The lab value was evaluated with IC.

Figures of Merit	Value
R^2	0.9967
Standard Error of Calibration	0.1682 (g/100 mL)
Standard Error of Cross-Validation	0.1876 (g/100 mL)

RESULT SUCROSE CONTENT

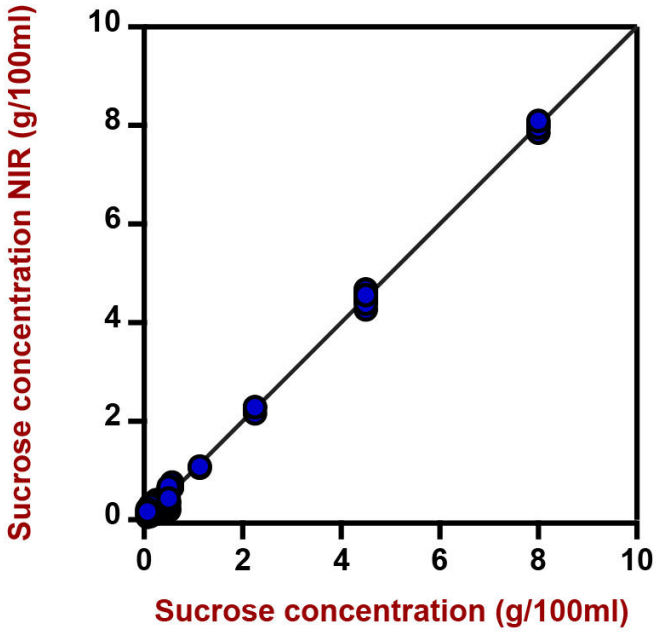

Figure 5. Correlation diagram and the respective figures of merit for the prediction of sucrose content in an aqueous mixture of sugars using a DS2500 Liquid Analyzer. The lab value was evaluated with IC.

Figures of Merit	Value
R^2	0.9902
Standard Error of Calibration	0.2390 (g/100 mL)
Standard Error of Cross-Validation	0.2401 (g/100 mL)

RESULT TOTAL SUGAR CONTENT

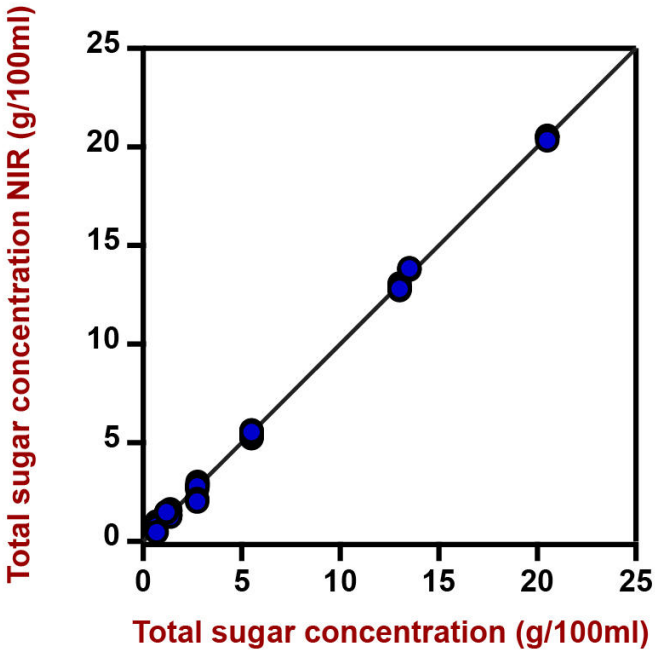

Figure 6. Correlation diagram and the respective figures of merit for the prediction of total sugars in an aqueous mixture of sugars using a DS2500 Liquid Analyzer. The lab value was evaluated with a refractometer.

Figures of Merit	Value
R^2	0.9985
Standard Error of Calibration	0.2718 (g/100 mL)
Standard Error of Cross-Validation	0.2770 (g/100 mL)

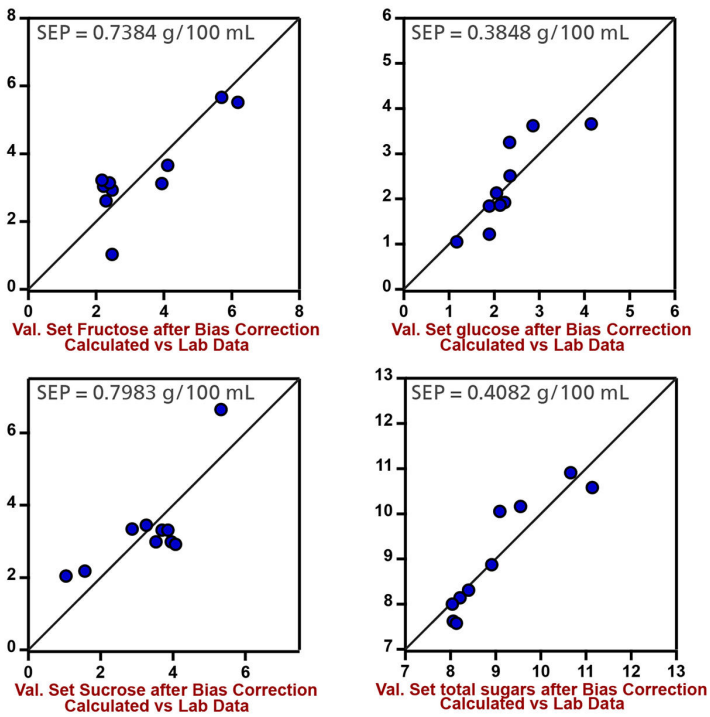

Figure 7. Validation plots of fructose, glucose, sucrose, and total sugars in fruit juices 1 to 10 with SEP (Standard Error of Prediction).

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).

Table 2. Time to result overview for the different sugars commonly analyzed in juices.

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

Internal reference: AW NIR CH-0071-042023

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CONFIGURATION

DS2500 Liquid Analyzer
固的近外光,用于生境和室中的量。

DS2500 Liquid Analyzer 是一成熟且活的解决方案,其用于在整个生中行液体常分析。其固的使 DS2500 Liquid Analyzer 不受灰、潮湿、振的影,因此非常用于在劣的生境中使用。

DS2500 Liquid Analyzer 覆盖 400 至 2500 nm 的整个光范,将品加至 80° C 高温,并与各不同的一次性小瓶和石英比色皿兼容。因此,DS2500 Liquid Analyzer 可的个性化品要求,助在一分内得精和具有可重性的果。借助集成的品架装置和自的 Vision Air 件,保了用能松和安全地行操作。

如果是大的品量,可通将流通池与一个 Metrohm 机器人自器搭配使用的方法著提高生率。