



Application Note AN-NIR-109

利用近红外光谱测定白利糖度、果糖、葡萄糖和蔗糖

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 ($^{\circ}$ 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**).

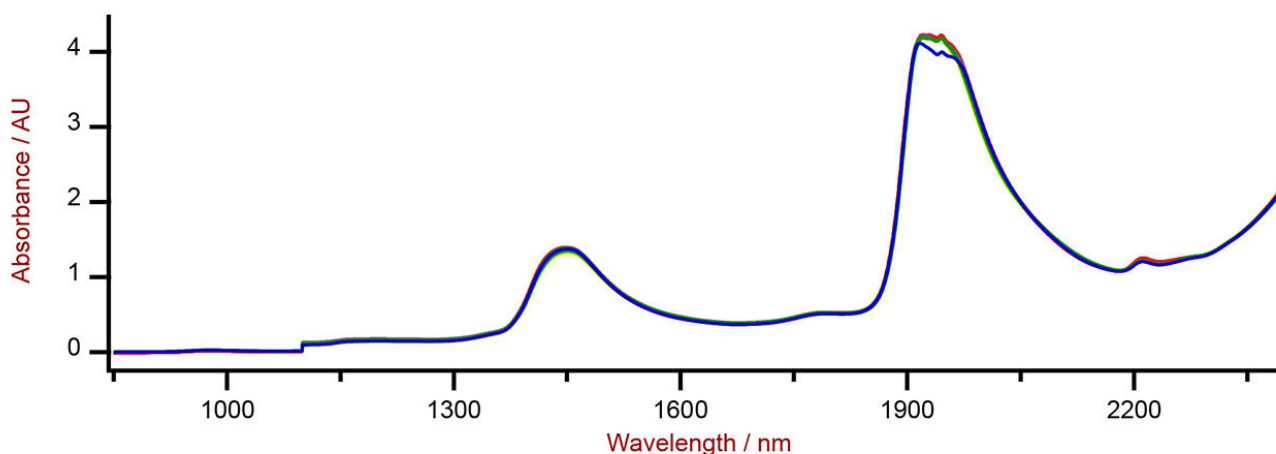


Figure 2. Selection of Vis-NIR spectra of an aqueous mixture of glucose, fructose, and sucrose analyzed on a DS2500 Liquid Analyzer.

RESULT FRUCTOSE CONTENT

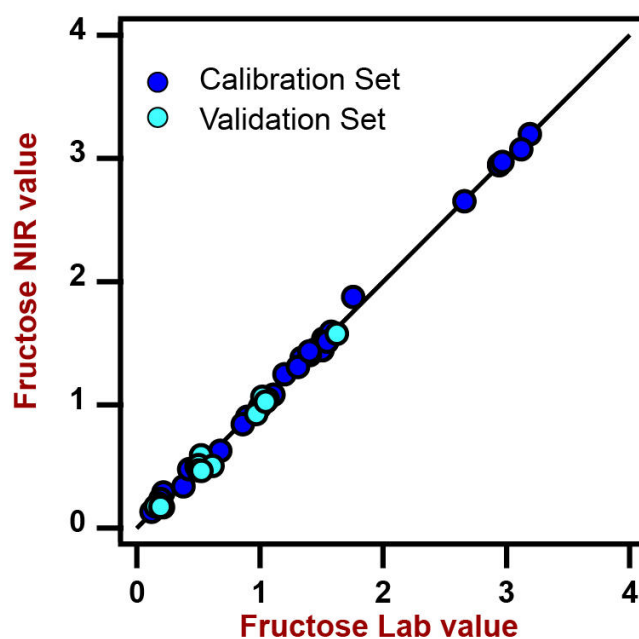


Figure 3. Correlation diagram and the respective figures of merit for the prediction of fructose content in an aqueous sugar mixture using a DS2500 Liquid Analyzer.

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

RESULT GLUCOSE CONTENT

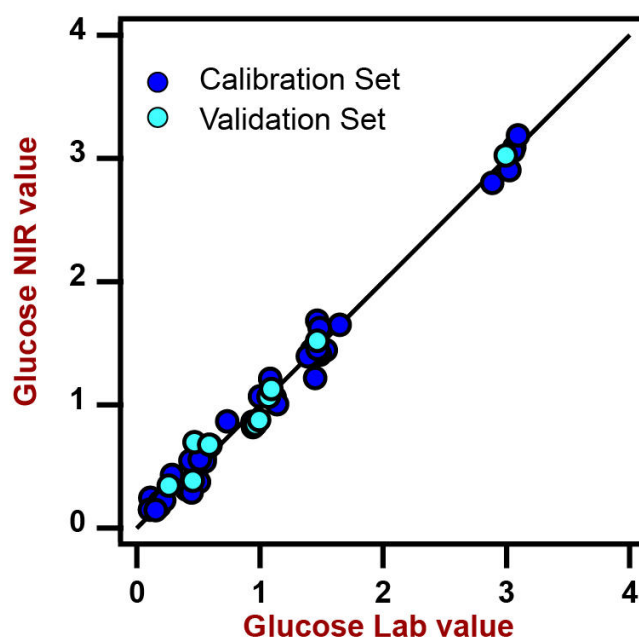


Figure 4. Correlation diagram and the respective figures of merit for the prediction of glucose content in an aqueous sugar mixture using a DS2500 Liquid Analyzer.

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

RESULT SUCROSE CONTENT

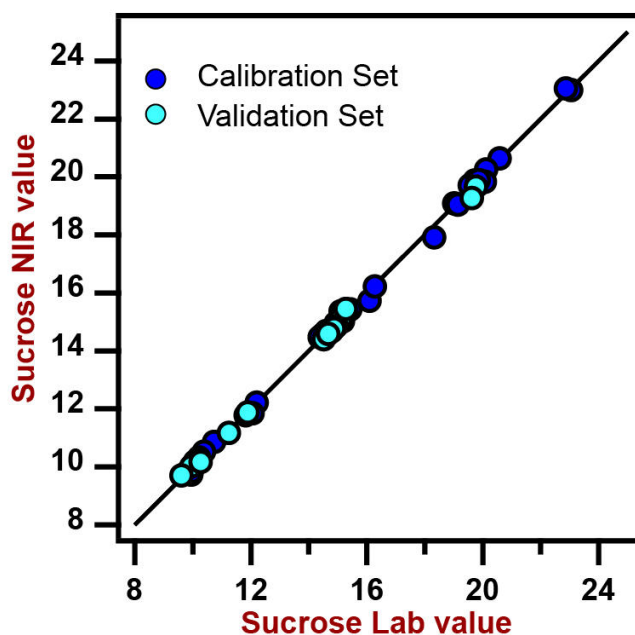


Figure 5. Correlation diagram and the respective figures of merit for the prediction of sucrose content in an aqueous sugar mixture using a DS2500 Liquid Analyzer.

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

RESULT BRIX

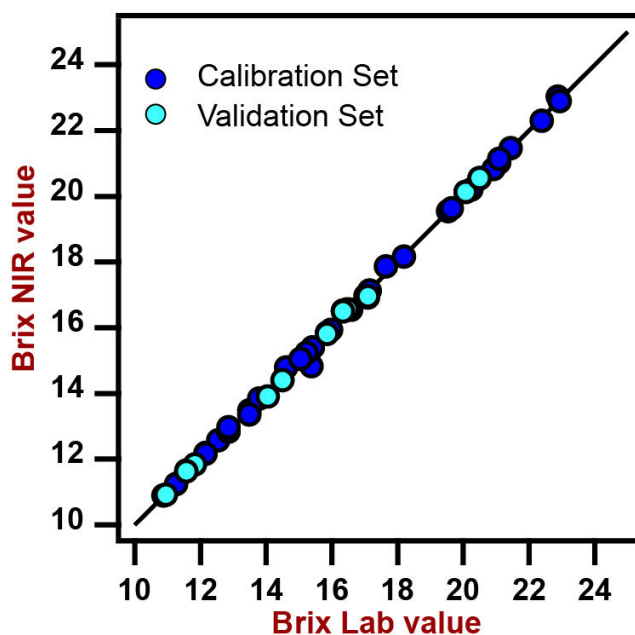


Figure 6. Correlation diagram and the respective figures of merit for the prediction of Brix (total sugars) in an aqueous mixture of sugars using a DS2500 Liquid Analyzer. The lab value was evaluated using a refractometer.

Figures of Merit	Value
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).

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

坚固结实的近红外光谱仪,用于生产环境和试验室中的质量检查。

DS2500 Liquid Analyzer 是一种成熟且灵活的解决方案,其用于在整个生产链中进行液体常规分析。其坚固结实的设计使 DS2500 Liquid Analyzer 不受灰尘、潮湿、振动的影响,因此非常适用于在恶劣的生产环境中使用。

DS2500 Liquid Analyzer 覆盖 400 至 2500 nm 的整个光谱范围,将样品加热至 80° C 高温,并与各种不同的一次性小瓶和石英比色皿兼容。因此,DS2500 Liquid Analyzer 可适应您的个性化样品要求,帮助您在几分钟内获得精确和具有可重现性的结果。借助集成的样品架识别装置和自带的 Vision Air 软件,还保证了用户能轻松和安全地进行操作。

如果是较大的样品量,则可通过将流通池与一个 Metrohm 机器人自动进样器搭配使用的方法显著提高生产率。