

Application Note AN-NIR-108

Measuring Brix and individual sugars in fruit juices with NIR spectroscopy

Fast multiparameter determination of sugars with NIRS

Fruit juices are produced and consumed for their refreshing character, nutritional benefits, and for a quick energy boost. The determination of different sugar components in these sweet beverages is highly important in this industry. In particular, fructose, glucose, and sucrose are controlled and monitored. Fruit juice sugar content analysis usually involves the use of polarimetric and refractive index measurements as well as high-performance liquid chromatography (HPLC). These measurements take a significant amount of time and require different types of laboratory equipment. Near-infrared spectroscopy (NIRS) is a chemical-free analytical technique that can simultaneously measure glucose, fructose, glucose, and Brix in juices in a few seconds. Sample preparation is not necessary when using NIRS, and automation with an OMNIS Sample Robot makes the analysis even easier.

EXPERIMENTAL EQUIPMENT

A total of 15 samples, including aqueous solutions of glucose (1–8 g/100 mL), fructose (1–8 g/100 mL), and sucrose (1–8 g/100 mL), were prepared to create prediction models for quantification. All samples were measured in transmission mode on an OMNIS NIR Analyzer Liquid (1000–2250 nm) with a 2 mm cuvette flow-cell and a holder for flow-through cells (Figure 1). For liquid transfer, the built-in peristaltic pump from the OMNIS Sample Robot S Pick&Place was used.



Figure 1. OMNIS NIR Analyzer Liquid and OMNIS Sample Robot S Pick&Place with pipetting system.

Samples of six different fruit juices (various orange juices, pineapple juice, multifruit juice, and apple juice) were measured with this setup. The sugar concentration, glucose (%), fructose (%), sucrose (%), and Brix (° Brix) were predicted using the prediction models mentioned above. Ion chromatography (IC) was used as the primary reference method to measure the concentration of different sugars in the juice samples (according to AN-P-072) and a digital refractometer was used to measure Brix. OMNIS Software was used for all data acquisition and prediction model development.

RESULT

The obtained NIR spectra (Figure 2) were used to create a prediction model for quantification of glucose, fructose, sucrose, and Brix. The quality of the prediction models was evaluated using correlation diagrams which display a very high correlation between the 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).

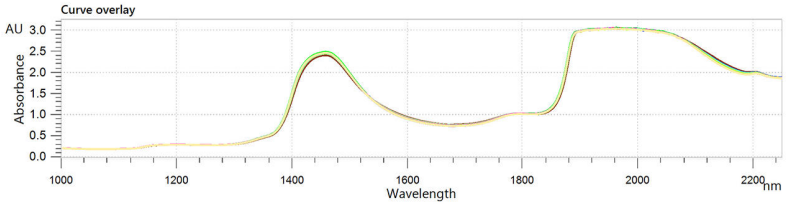


Figure 2. NIR spectra of a mixture of glucose, fructose, and sucrose in water analyzed on an OMNIS NIR Analyzer Liquid.

RESULT FRUCTOSE CONTENT

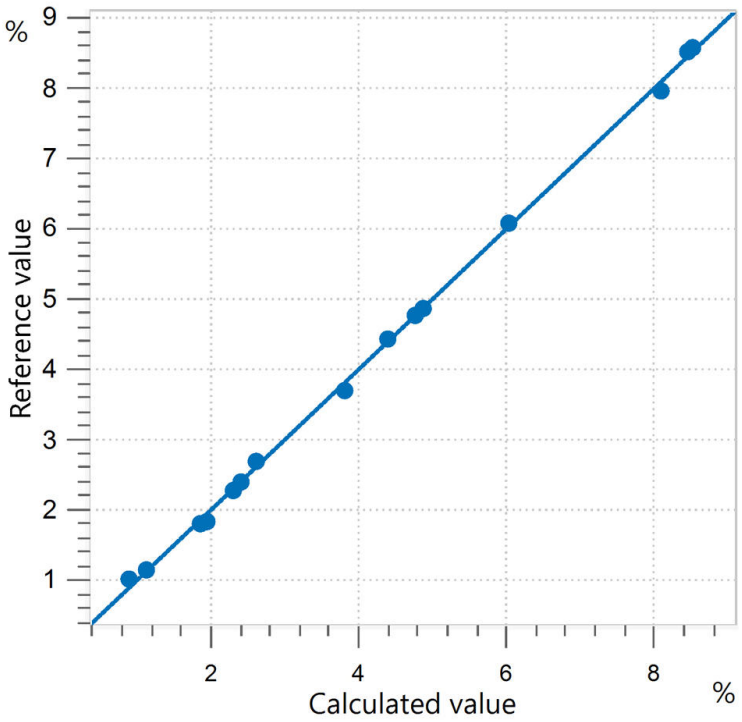


Figure 3. Correlation diagram and the respective figures of merit for the prediction of fructose content in a mixture of sugars in water using an OMNIS NIR Analyzer Liquid.

R^2	SEC (%)	SECV (%)
0.999	0.06	0.07

RESULT GLUCOSE CONTENT

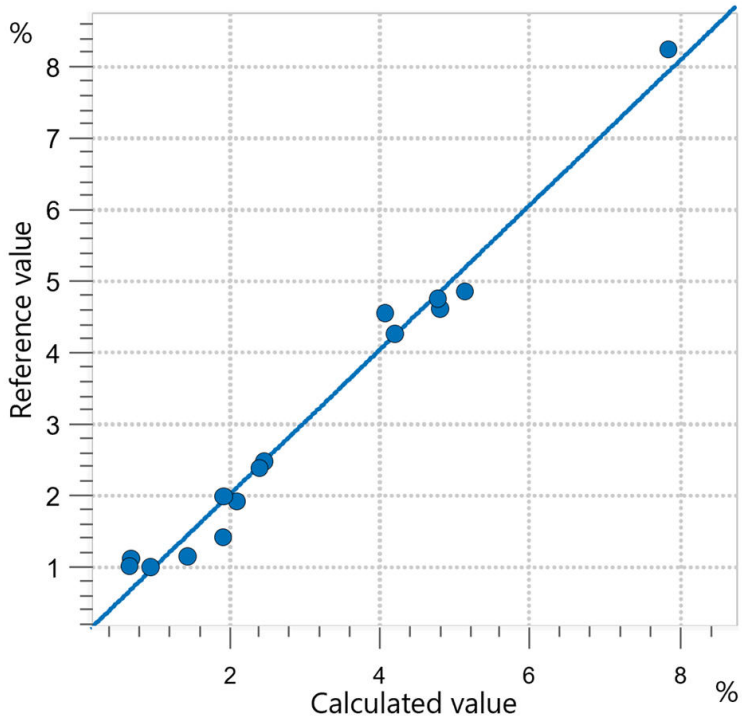


Figure 4. Correlation diagram and the respective figures of merit for the prediction of glucose content in a mixture of sugars in water using an OMNIS NIR Analyzer Liquid.

R^2	SEC (%)	SECV (%)
0.981	0.21	0.28

RESULT SUCROSE CONTENT

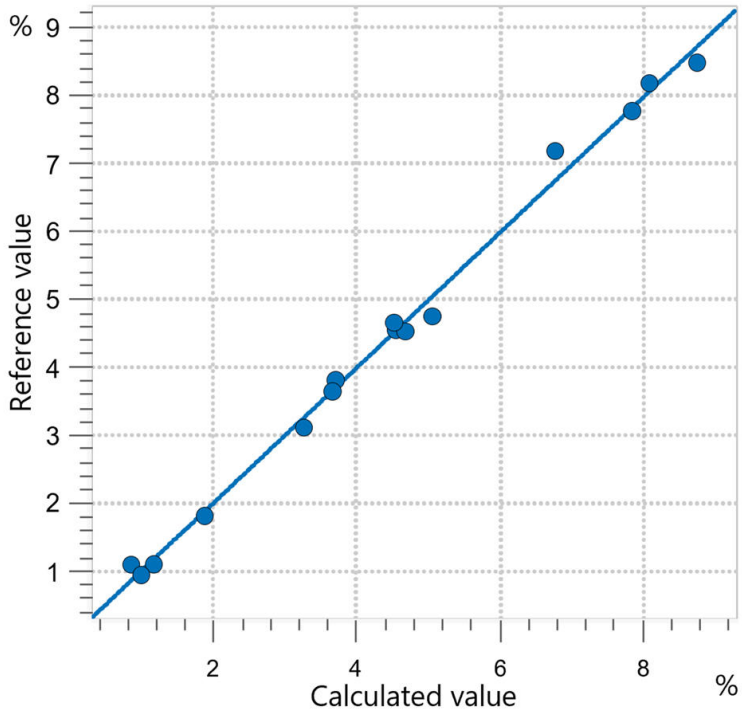


Figure 5. Correlation diagram and the respective figures of merit for the prediction of sucrose content in a mixture of sugars in water using an OMNIS NIR Analyzer Liquid.

R^2	SEC (%)	SECV (%)
0.995	0.14	0.18

RESULT BRIX

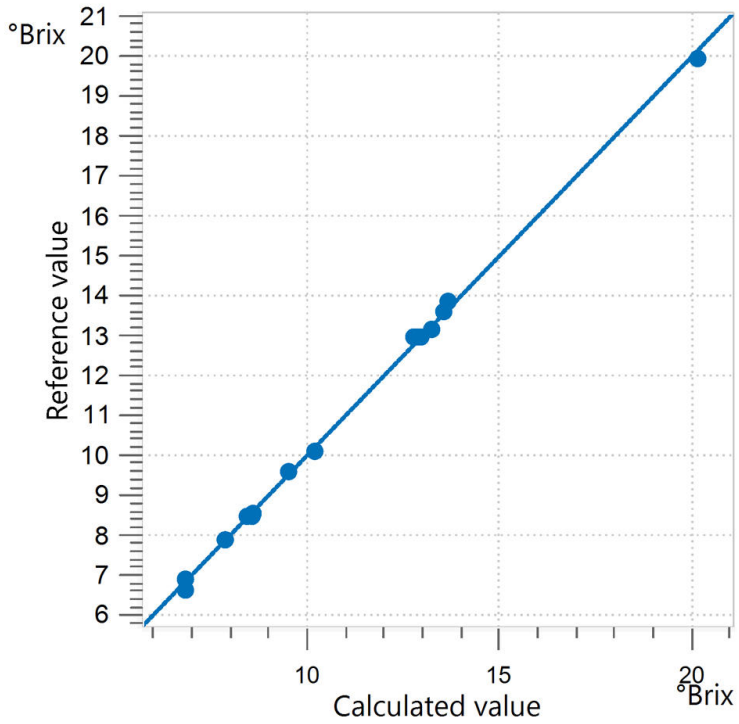


Figure 6. Correlation diagram and the respective figures of merit for the prediction of Brix in a mixture of sugars in water using an OMNIS NIR Analyzer Liquid.

R^2	SEC (%)	SECV (%)
0.999	0.08	0.12

PREDICTED VALUES OF COMMERCIAL FRUIT JUICES

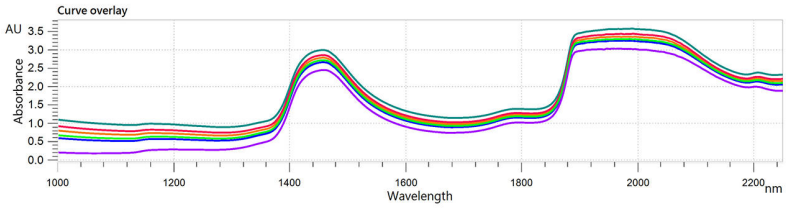


Figure 7. NIR spectra of fruit juice samples analyzed on an OMNIS NIR Analyzer Liquid.

Using the prediction models described earlier, commercial fruit juices samples were measured with NIR spectroscopy (Figure 7) using the automated setup in Figure 1. The predicted values of glucose, fructose, sucrose, and Brix in commercial fruit juices (1 to 6) are shown in Tables 2–5.

Table 2. NIR-predicted results of Brix compared with reference method (refractometer).

Fruit juice no.	Brix Refractometer (° Brix)	Brix Predicted NIR (° Brix)
1	11.32	11.11
2	11.32	10.96
3	12.59	12.68
4	11.32	10.94
5	11.63	11.79
6	11.06	11.74

Table 3. NIR-predicted results of fructose compared with reference method (IC).

Fruit juice no.	Fructose (%) (IC)	Fructose Predicted NIR (%)
1	2.47	2.27
2	2.29	2.79
3	2.47	2.73
4	2.22	2.55
5	4.08	3.09
6	5.70	5.80

Table 4. NIR-predicted results of sucrose compared with reference method (IC).

Fruit juice no.	Sucrose (%) (IC)	Sucrose Predicted NIR (%)
1	3.7	2.6
2	3.86	4.21
3	5.33	4.77
4	3.95	3.33
5	3.09	2.94
6	1.04	3.29

CONCLUSION

This Application Note demonstrates the feasibility to determine glucose, fructose, sucrose, and Brix in various fruit juices with near-infrared spectroscopy. NIR spectroscopy offers users fast and extremely accurate results without the need for highly trained analysts, chemicals, or sample preparation. Therefore, NIRS represents a suitable alternative to the traditional HPLC and Brix analysis methods (Table 6). Additionally, the possibility of automating NIR spectroscopy for fruit juice analysis saves even more time and costs. Measuring sugar content in fruit juice has never been easier.

Table 6. Time to result overview for the different sugar parameters commonly analyzed in juices.

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

CONTACT

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CONFIGURATION



OMNIS NIR Analyzer Liquid

用于液体样品的近红外光谱仪。

OMNIS NIR Analyzer 按照瑞士质量标准开发和制造,是用于整个生产链中常规分析的近红外光谱解决方案。最新技术的应用以及与现代 OMNIS Software 的集成,体现在这款 NIR 光谱仪的速度、操作性和灵活应用上。

OMNIS NIR Analyzer Liquid 的优势概览:

- 液体样品测量时间小于 10 秒
- 样品温度调节范围为 25–80 ° C
- 自动检测样品容器的放入和移除
- 可轻松集成至自动系统,或与其它分析技术(滴定)联用。
- 支持多种不同路径长度的样品容器



NIRS 12.5 mm 2 mm

流通式石英比色皿可用于持续监控例如片剂溶解过程和反应动力学。其耐高压性和专有的防气泡性能使全部测量均十分方便。

由高纯度和均质的石英玻璃制成的窗口可确保在波长为 200 nm - 2500 nm 范围内具有超过 80% 的透射性能。

有不同的层厚可供选购:

0.5 mm 层厚,容积 = 175 µL(**订货号:67401300**)

1 mm 层厚,容积 = 350 µL(**订货号:67401310**)

2 mm 层厚,容积 = 700 µL(**订货号:67401320**)

5 mm 层厚,容积 = 1750 µL(**订货号:67401330**)

10 mm 层厚,容积 = 3500 µL(**订货号:67401340**)

尺寸:高 x 长 x 宽 = 35 mm x 12.5mm x 12.5 mm

窗口高度 = 8.5 -15 mm

和 XDS Rapidliquid Analyzer 的 NIRS 间距支架和 DS2500 Liquid Analyzer 的 DS2500 支架兼容。



OMNIS NIR

适合流通池的 OMNIS NIR Analyzer 的比色皿支架 (6.7401.300; 6.7401.310; 6.7401.320; 6.7401.330; 6.7401.340)。

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A WHOLE NEW LEVEL OF PERFORMANCE

OMNIS

允许单机版 OMNIS 软件在一台 WindowsTM 计算机上运行。

特性:

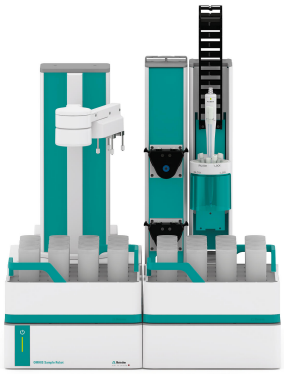
- 该许可证已含有一份 OMNIS 设备许可证。
- 须通过万通许可授权平台进行激活。

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A WHOLE NEW LEVEL OF PERFORMANCE

Quant Development

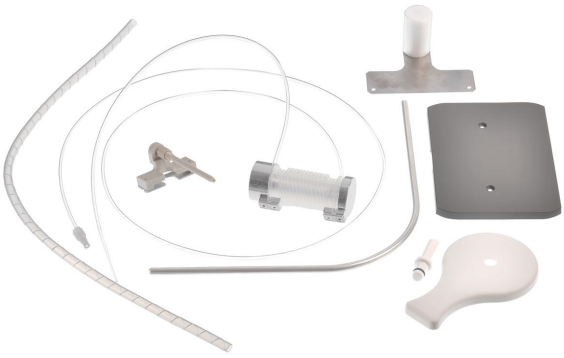
用于在独立 OMNIS Software 安装套件中编写和编辑量化模型的软件许可证。



OMNIS Sample Robot S Pick and Place

OMNIS Sample Robot S 具有一个“蠕动”泵模块(2 通道)和一个 Pick&Place 模块以及大量附件,可直接进入全自动滴定。此系统具有两个样品盘位置,可用于 32 个 120 mL 的样品盘。此模块化系统供货时已完全安装完毕,因此可在极短时间内投入运行。

该系统也可根据需要扩展配备另外两台蠕动泵以及多加一个 Pick&Place 模块,由此使通量翻倍。如果需要更多工作台,则可将此 Sample Robot 扩展为 L 规格款型的 OMNIS Sample Robot,由此可使七个样品盘的样品在多达四个 Pick&Place 模块上并行处理,将样品通量扩大四倍。



OMNIS

完整附件组,用于将 OMNIS Sample Robot Pick&Place 改装为可进行移液的仪器型号。该套件可安装在所有版本 OMNIS Sample Robot(大号、中号和小号)上。