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).

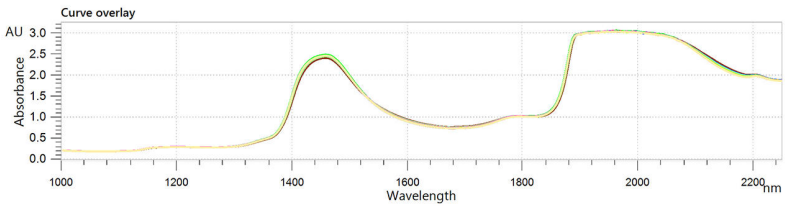

Figure 2. NIR spectra of a mixture of glucose, fructose, and sucrose in water analyzed on an OMNIS NIR Analyzer Liquid.

RESULT FRUCTOSE CONTENT

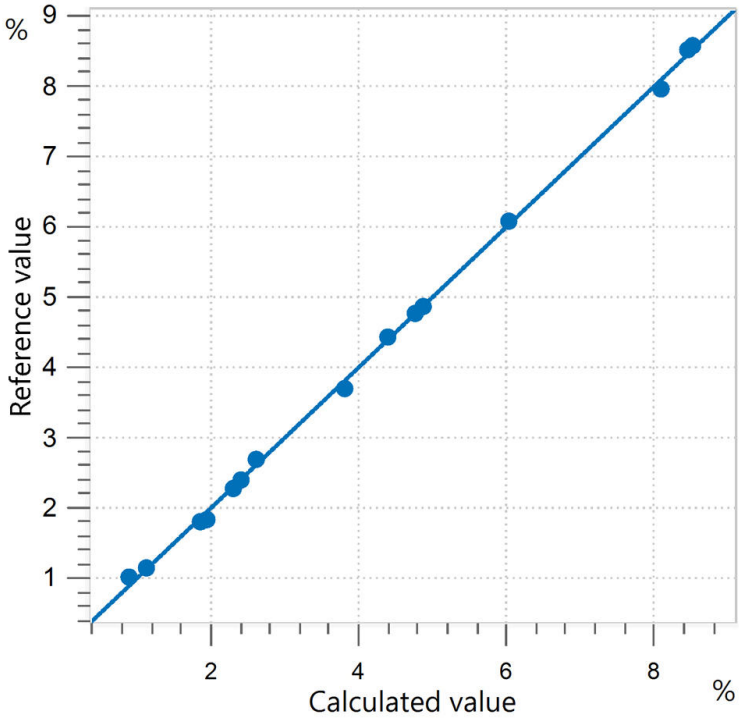

Figure 3. Correlation diagram and the respective figures of merit for the prediction of fructose content in a mixture of sugars in water using an OMNIS NIR Analyzer Liquid.

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

RESULT GLUCOSE CONTENT

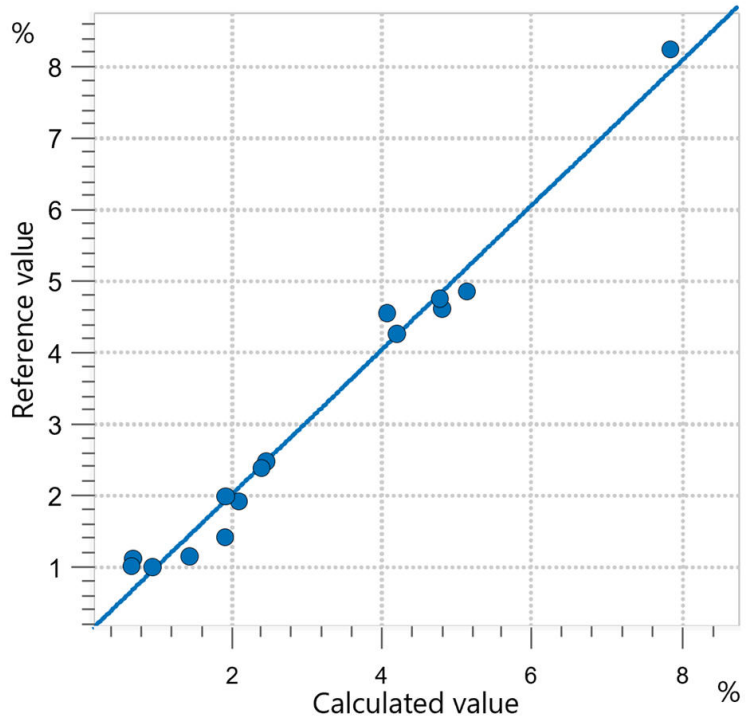

Figure 4. Correlation diagram and the respective figures of merit for the prediction of glucose content in a mixture of sugars in water using an OMNIS NIR Analyzer Liquid.

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

RESULT SUCROSE CONTENT

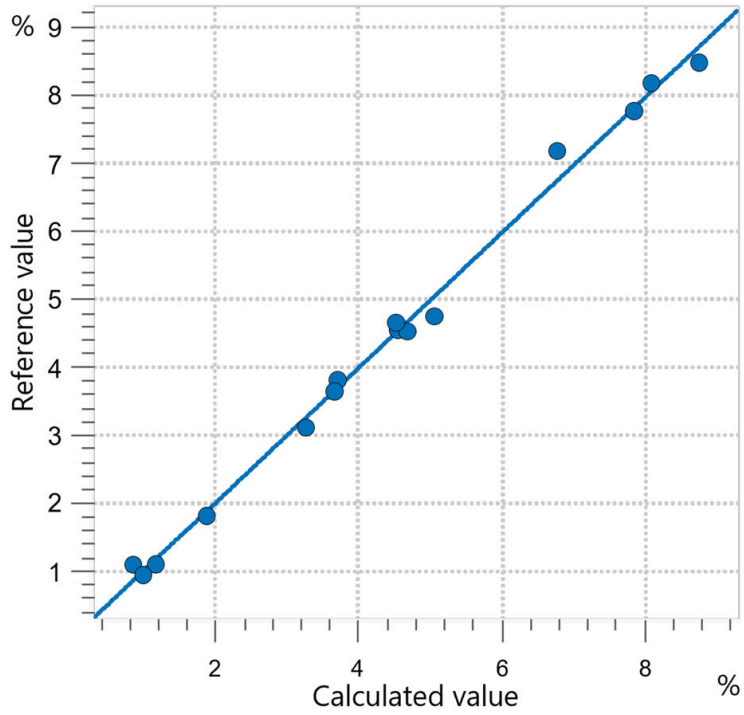

Figure 5. Correlation diagram and the respective figures of merit for the prediction of sucrose content in a mixture of sugars in water using an OMNIS NIR Analyzer Liquid.

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

RESULT BRIX

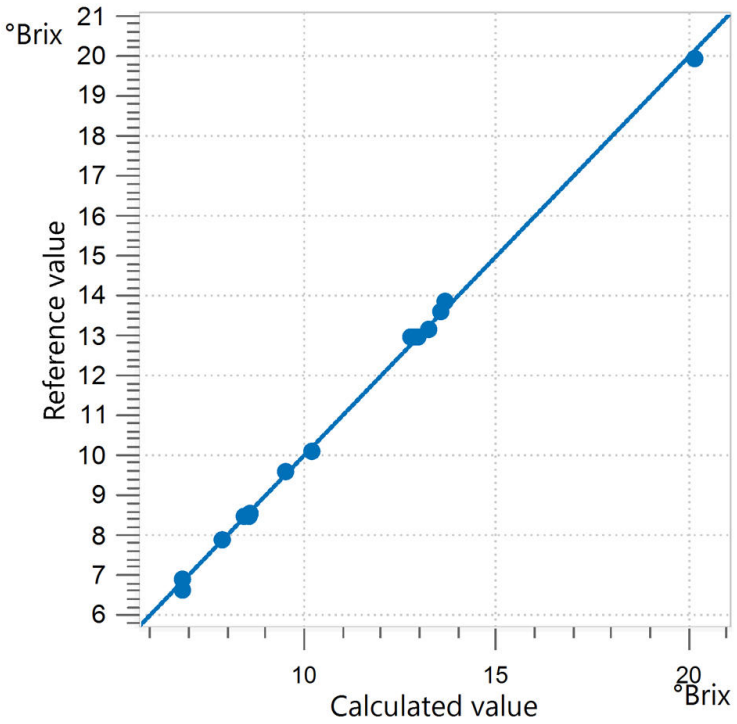

Figure 6. Correlation diagram and the respective figures of merit for the prediction of Brix in a mixture of sugars in water using an OMNIS NIR Analyzer Liquid.

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

PREDICTED VALUES OF COMMERCIAL FRUIT JUICES

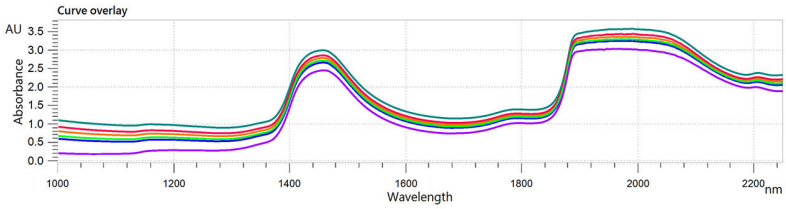

Figure 7. NIR spectra of fruit juice samples analyzed on an OMNIS NIR Analyzer Liquid.

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 1–4.

Table 1. 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 2. 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 3. 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 5). 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 5. 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

Near-infrared spectrometer for liquid samples.

Developed and produced in accordance with Swiss quality standards, the OMNIS NIR Analyzer is the near-infrared spectroscopy (NIRS) solution for routine analysis along the entire production chain. Its application of the latest technologies and its integration in the modern OMNIS Software are reflected in its speed, operability, and flexible utilization of this NIR spectrometer.

Overview of the advantages of the OMNIS NIR Analyzer Liquid:

- Measurements of liquid samples in less than 10 seconds
- Temperature control on the sample from 25–80 °C
- Automatic detection of the insertion and removal of the sample vessel
- Simple integration in an automation system or link with additional analysis technologies (titration)
- Supports numerous sample vessels with different path lengths

NIRS 12.5 mm quartz cuvette flow 2 mm

The flow quartz cuvettes enable continuous monitoring, for example of tablet disintegration processes and reaction kinetics. The high pressure resistance and a special bubble capturing system make all measurements particularly easy.

Windows made of quartz glass of maximum purity and homogeneity ensure a transmission of more than 80% in the wavelength range of 200 nm - 2,500 nm.

A variety of pathlengths are available:

0.5 mm pathlength and a volume = 175 µL (order number: 67401300)

1 mm pathlength and a volume = 350 µL (order number: 67401310)

2 mm pathlength and a volume = 700 µL (order number: 67401320)

5 mm pathlength and a volume = 1,750 µL (order number: 67401330)

10 mm pathlength and a volume = 3,500 µL (order number: 67401340)

Dimensions h x l x w = 35 mm x 12.5 mm x 12.5 mm

Window height = 8.5 - 15 mm

Compatible with the NIRS spacer for the XDS RapidLiquid Analyzer and the DS2500 holder for the DS2500 Liquid Analyzer.

Holder OMNIS NIR, flow-through cells

Cuvette holder for the OMNIS NIR Analyzer for flow-through cells

(6.7401.300; 6.7401.310; 6.7401.320; 6.7401.330; 6.7401.340).

OMNIS

A WHOLE NEW LEVEL OF PERFORMANCE

OMNIS Stand-Alone license

Enables stand-alone operation of the OMNIS software on a WindowsTM computer.

Features:

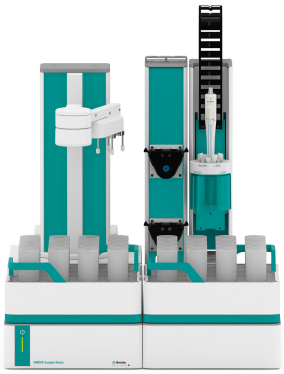
- The license already includes one OMNIS instrument license.
- Must be activated via the Metrohm licensing portal.

OMNIS

A WHOLE NEW LEVEL OF PERFORMANCE

Software license Quant Development

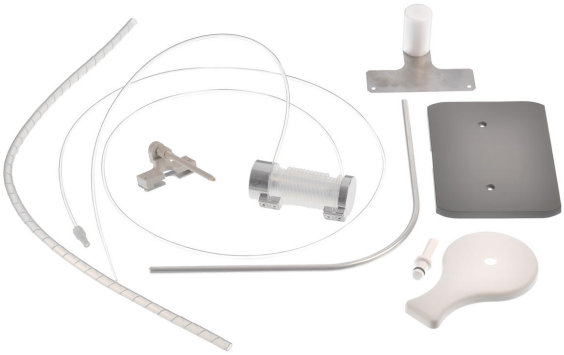
Software license for the creation and editing of quantification models in a stand-alone OMNIS Software installation.



OMNIS Sample Robot S Pick and Place

OMNIS Sample Robot S with a "Peristaltic" (2-channel) pump module and a Pick&Place module in addition to extensive accessories for the direct transition to fully automatic titration. The system provides space in two sample racks for 32 sample beakers of 120 mL each. This modular system is supplied completely installed and can thus be put into operation in a very short time.

The system can also be extended upon request to include two additional peristaltic pumps and another Pick&Place module, thus doubling the throughput. If additional workstations are required, then this Sample Robot is already able to be expanded to become an L-sized OMNIS Sample Robot, thus enabling samples from seven racks to be processed in parallel on up to four Pick&Place modules and quadrupling the sample throughput.



OMNIS pipetting equipment

Complete accessory set for converting the OMNIS Sample Robot Pick&Place into a version with pipetting options. The set can be mounted on all versions of the OMNIS Sample Robot (S,M and L).