Measuring Brix and individual sugars in fruit juices with NIR spectroscopy

Xác định nhanh đa thông số của đường với NIRS

Nước trái cây được sản xuất và tiêu thụ nhờ đặc tính giải khát, lợi ích dinh dưỡng và khả năng cung cấp năng lượng nhanh chóng. Việc xác định các thành phần đường khác nhau trong loại đồ uống ngọt này có vai trò rất quan trọng trong ngành công nghiệp thực phẩm. Đặc biệt, fructose, glucose và sucrose là những chỉ tiêu được theo dõi và kiểm soát chặt chẽ. Phân tích hàm lượng đường trong nước trái cây thường sử dụng các phương pháp như đo độ phân cực, chỉ số khúc xạ hoặc sắc ký lỏng hiệu năng cao

(HPLC). Những phương pháp này tiêu tốn nhiều thời gian và đòi hỏi nhiều loại thiết bị phòng thí nghiệm khác nhau. Trong khi đó, quang phổ cận hồng ngoại (NIRS) là một kỹ thuật phân tích không dùng hóa chất, có thể đồng thời đo glucose, fructose, sucrose và độ Brix trong nước trái cây chỉ trong vài giây. Phương pháp này không yêu cầu bước chuẩn bị mẫu, và việc tự động hóa bằng thiết bị OMNIS Sample Robot giúp quy trình phân tích trở nên đơn giản và hiệu quả hơn.

Ω Metrohm

THIẾT BỊ THỰC NGHIỆM

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.

KẾT QUẢ

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).
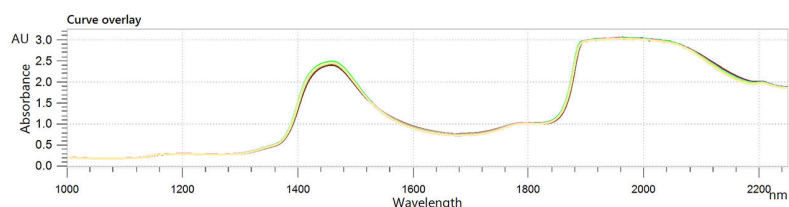

Figure 2. NIR spectra of a mixture of glucose, fructose, and sucrose in water analyzed on an OMNIS NIR Analyzer Liquid.

Ω **Metrohm**
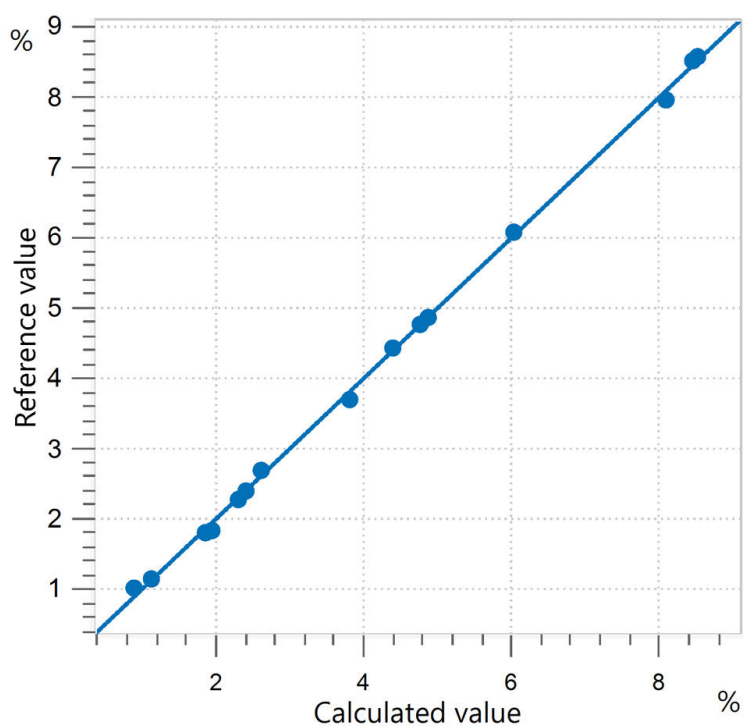
KẾT QUẢ HÀM LƯỢNG FRUCTOZA

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

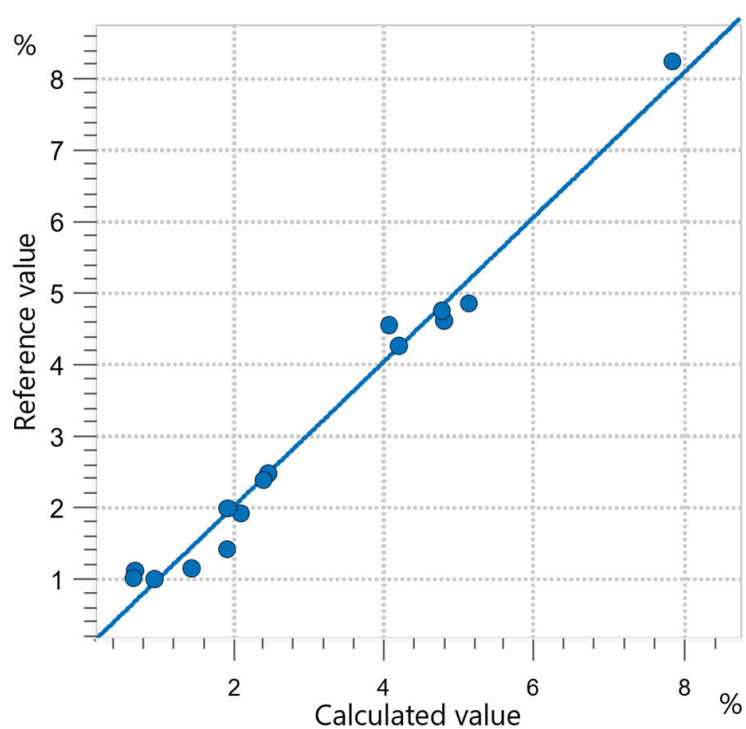Ω Metrohm

KẾT QUẢ HÀM LƯỢNG GLUCOSE

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	0.28	0.21

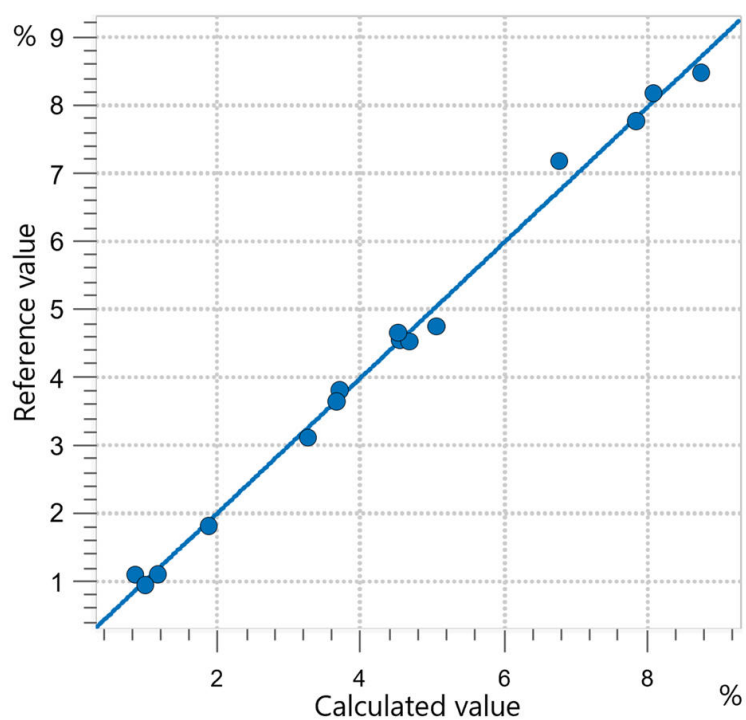Ω Metrohm

KẾT QUẢ HÀM LƯỢNG SUCROSE

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

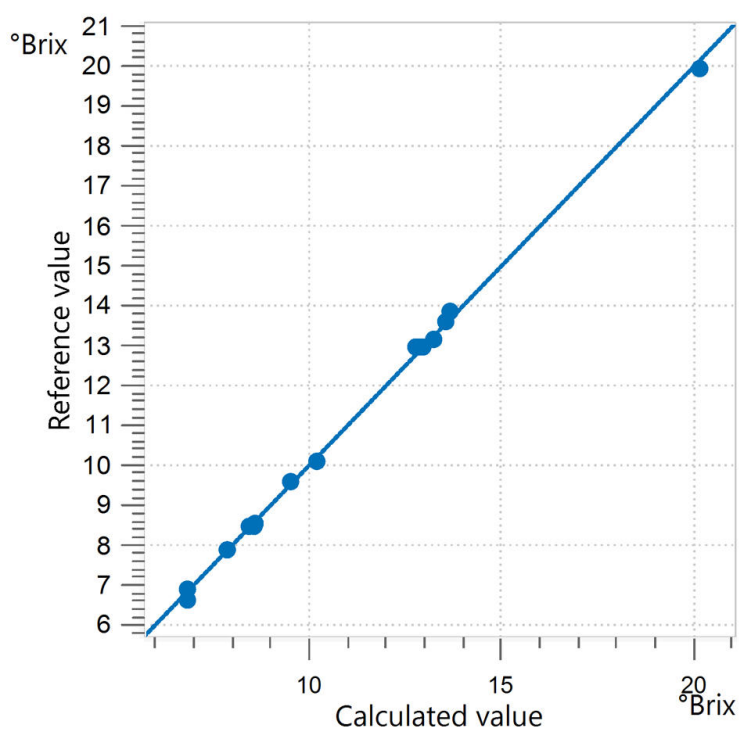Ω Metrohm

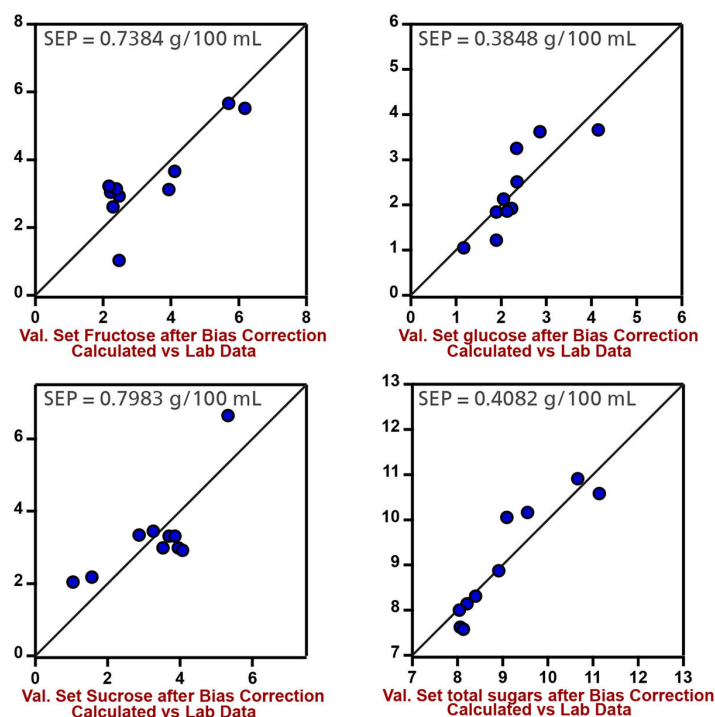# KẾT QUẢ TỔNG HÀM LƯỢNG ĐƯỜNG

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

Ω Metrohm

KẾT QUẢ TỔNG HÀM LƯỢNG ĐƯỜNG

Hình 7. Biểu đồ xác thực của fructose, glucose, sucrose và tổng lượng đường trong nước trái cây từ mẫu 1 đến 10 với SEP (Sai số Chuẩn Dự đoán).

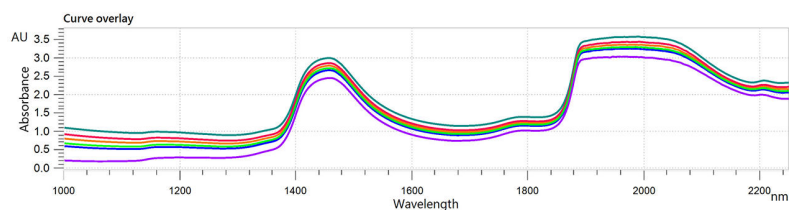## PREDICTED VALUES OF COMMERCIAL FRUIT JUICES

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**.

Ω Metrohm

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

Ω Metrohm

KẾT LUẬN

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

Internal reference: AW NIR CH-0071-042023

CONTACT

CÔNG TY TNHH METROHM
VIỆT NAM

Tòa nhà Park IX, số 08
Đường Phan Đình Giót,
Phường Tân Sơn Hòa
null Thành phố Hồ Chí Minh

info@metrohm.vn

Ω Metrohm

CẤU HÌNH

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

Ω Metrohm

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).

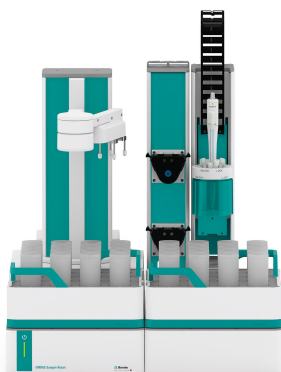### OMNIS Stand-Alone license

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.
- Not transferable to another computer.

OMNIS
A WHOLE NEW LEVEL OF PERFORMANCE

Ω Metrohm

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.
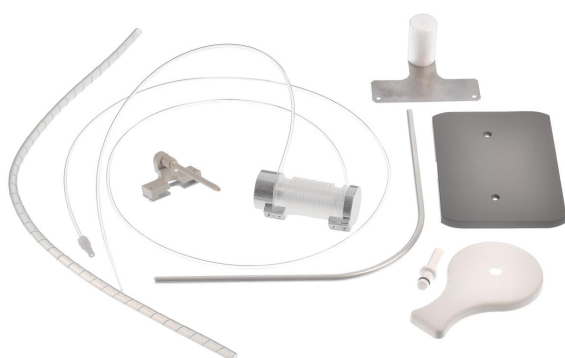
OMNIS pipetting equipment

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).

Ω Metrohm