Application Note AN-NIR-145

Coconut water analysis by NIRS

Determination of Brix, salinity, conductivity, and pH with one instrument

Fresh coconut water is the main edible part of the coconut (aside from the coconut meat) and has gained popularity as a health drink in recent years. Multiple factors influence the quality, such as harvesting time, growth location, and storage duration. This poses a challenge for industrial producers to achieve and maintain the desired product quality.

Testing the properties of coconut water with standard laboratory methods can be challenging, since trained lab personnel are needed. In contrast, near-infrared spectroscopy (NIRS) is fast, chemical-free, and does not require sample preparation. This Application Note explains how NIRS is used for the multiparameter analysis of coconut water. The NIRS solution is easy to use and can be implemented either atline or in a quality control lab.

EXPERIMENTAL EQUIPMENT

An OMNIS NIR Analyzer Liquid with a 1 mm flow-through cell (Figure 1) was used to analyze 206 coconut samples from a commercial supplier. In this configuration, a peristaltic pump injects the sample into the flow-through cell, which is inserted into the cuvette holder. The cell is rinsed with water after each measurement.

Figure 1. The OMNIS NIR Analyzer Liquid from Metrohm featured with a flow-through cell and holder.

RESULT

The obtained NIR spectra (Figure 2) were used to create prediction models for the different reference parameters (i.e., Brix, salinity, conductivity, and pH). An independent validation set of 25% was used to validate the calibration models. Correlation diagrams which display the relation between the NIR prediction and the reference values are shown in Figures 3–7 together with the respective figures of merit (FOM). The displayed standard errors of cross validation (SECV) and standard errors of prediction (SEP) show the expected accuracy during routine analysis in QC laboratories. The pH value FOM data indicate that the model can be used for classification or trend monitoring because of the limited NIRS correlation.

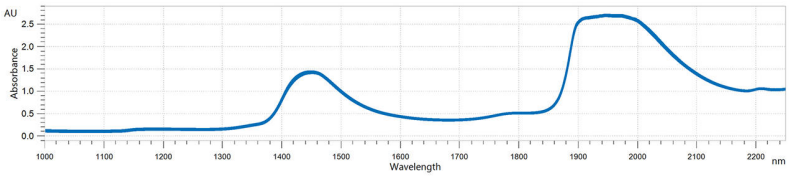

Figure 2. Selection of NIR spectra of coconut water samples measured with a 1 mm flow-through cell on an OMNIS NIR Analyzer Liquid.

RESULT BRIX VALUE

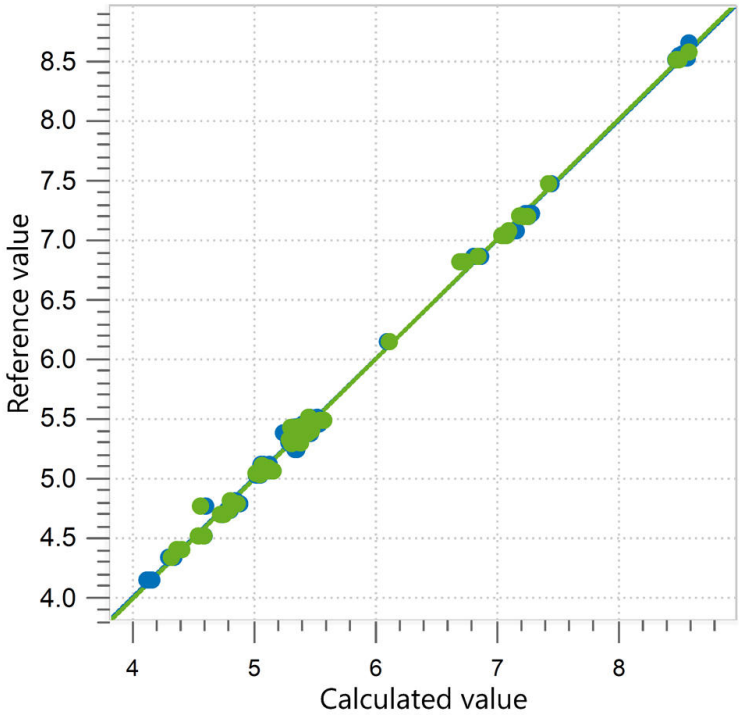

Figure 3. Correlation diagram and the respective FOMs for the prediction of Brix in coconut water using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2	SEC (°Bx)	SECV (°Bx)	SEP (°Bx)
0.997	0.04	0.04	0.05

RESULT SALINITY

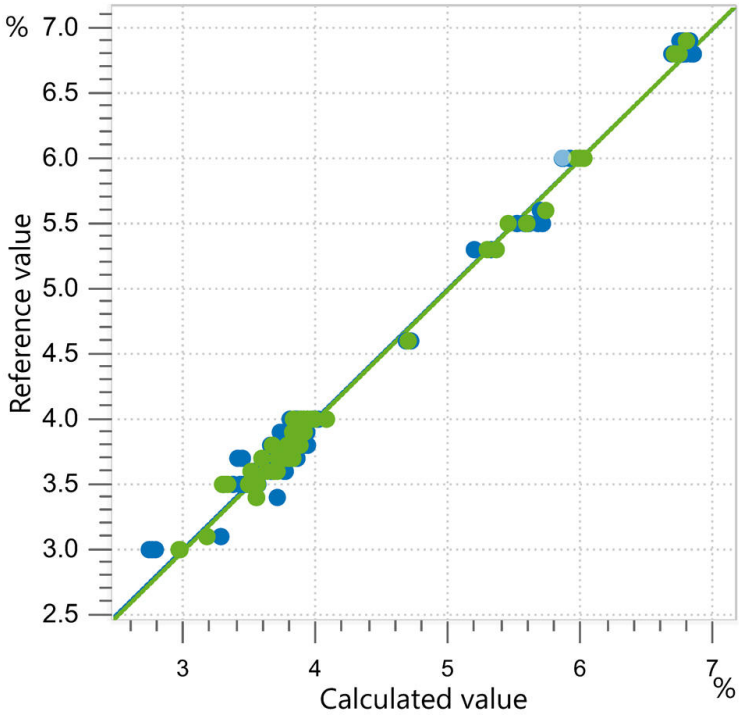

Figure 4. Correlation diagram and the respective FOMs for the prediction of coconut water salinity using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2	SEC (%)	SECV (%)	SEP (%)
0.992	0.08	0.10	0.09

RESULT PH VALUE

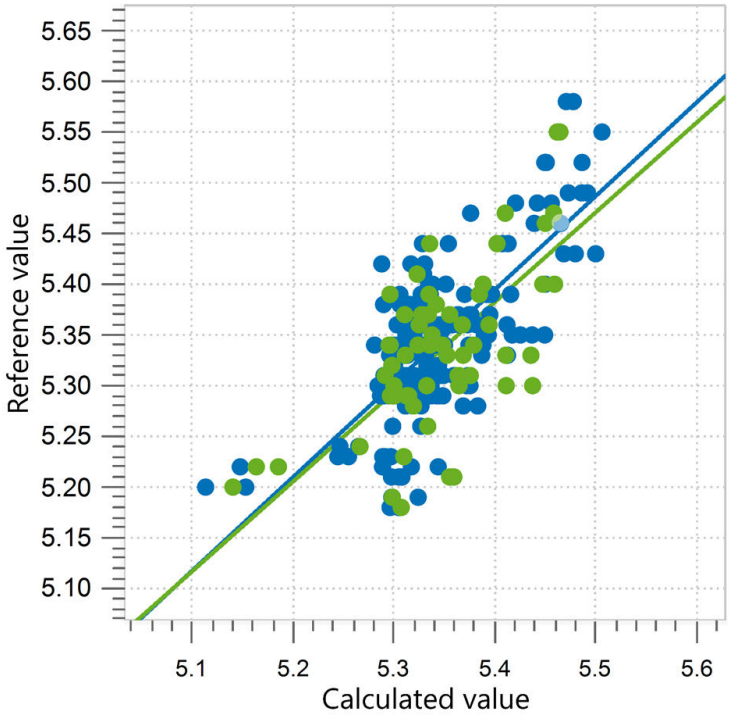

Figure 5. Correlation diagram and the respective FOMs for the prediction of coconut water pH value using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2	SEC	SECV	SEP
0.658	0.05	0.05	0.06

RESULT CONDUCTIVITY

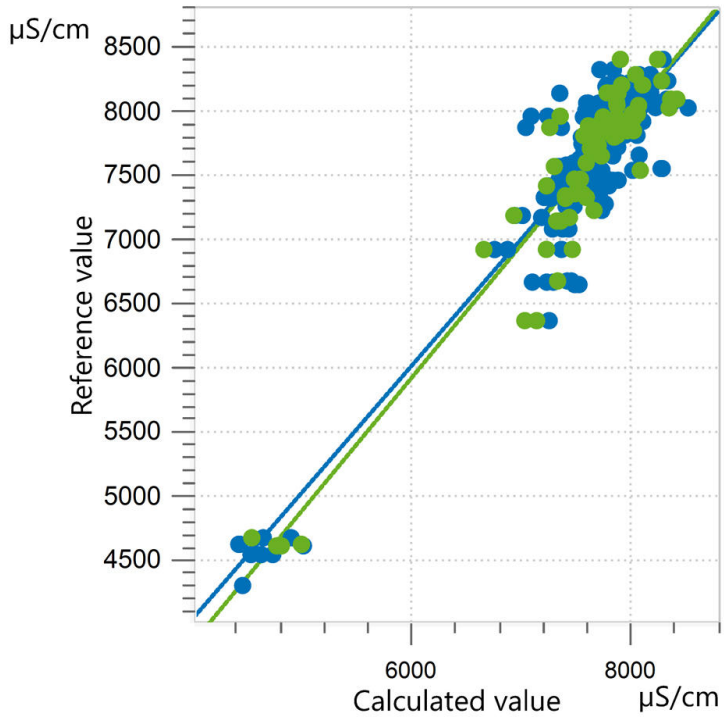

Figure 6. Correlation diagram and the respective FOMs for the prediction of coconut water conductivity using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2	SEC (µS/cm)	SECV (µS/cm)	SEP (µS/cm)
0.892	250	286	285

RESULT TURBIDITY

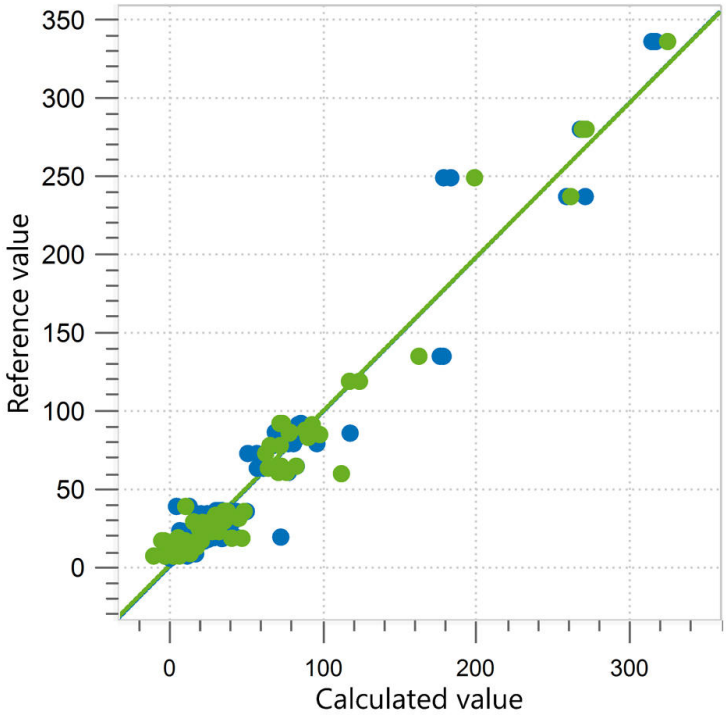

Figure 7. Correlation diagram and the respective FOMs for the prediction of coconut water turbidity using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2	SEC (ppm)	SECV (ppm)	SEP (ppm)
0.956	10.05	13.04	14.90

CONCLUSION

This Application Note shows the feasibility of using NIR spectroscopy for the quality control of coconut water. The parameters Brix, conductivity, turbidity, pH value, and salinity can be monitored by NIRS in seconds without any sample preparation. The presented setup with a flow-through cell not only simplifies sample handling but also allows full automation when using an OMNIS Sample Robot.

In addition to coconut water, the coconut fruit itself can also be analyzed using near-infrared spectroscopy.

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

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).

Flow-through cell, 1 mm

Flow quartz cuvettes with an optical path length of 1.0 mm suitable for near-infrared spectroscopy (NIRS) analyses.

Compatible with:

- Holder OMNIS NIR, flow-through cell (6.07401.100)
- DS2500 holder for flow cells (6.7493.000)

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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.

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Software license Quant Development

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