



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.

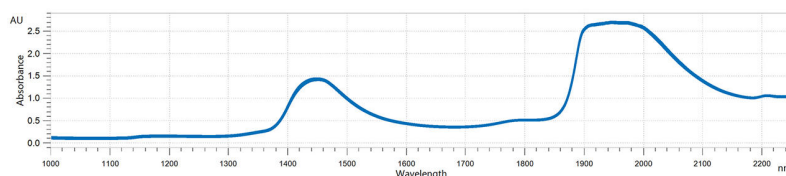


Figure 2. Selection of NIR spectra of coconut water samples measured with a 1 mm flow-through cell on an OMNIS NIR Analyzer Liquid.

RESULT BRIX VALUE

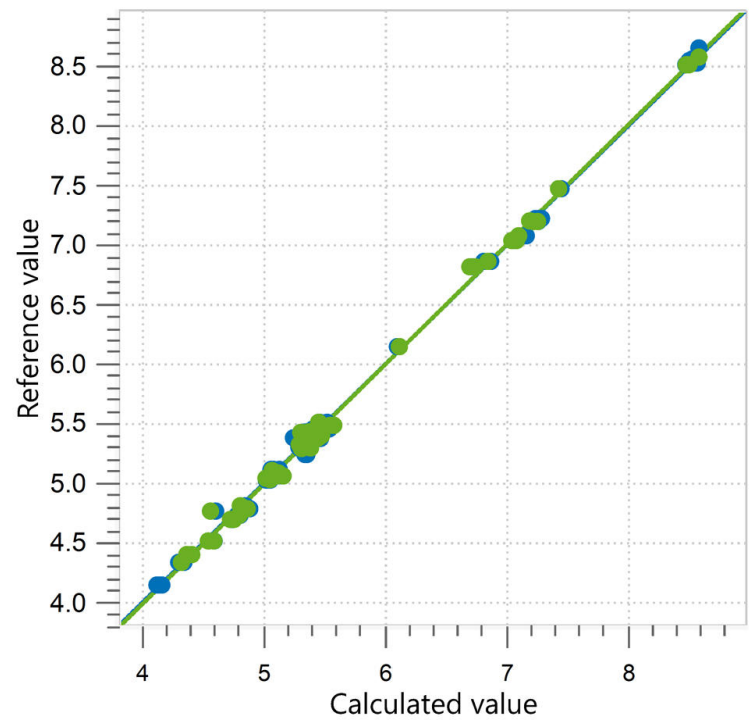


Figure 3. Correlation diagram and the respective FOMs for the prediction of Brix in coconut water using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

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

RESULT SALINITY

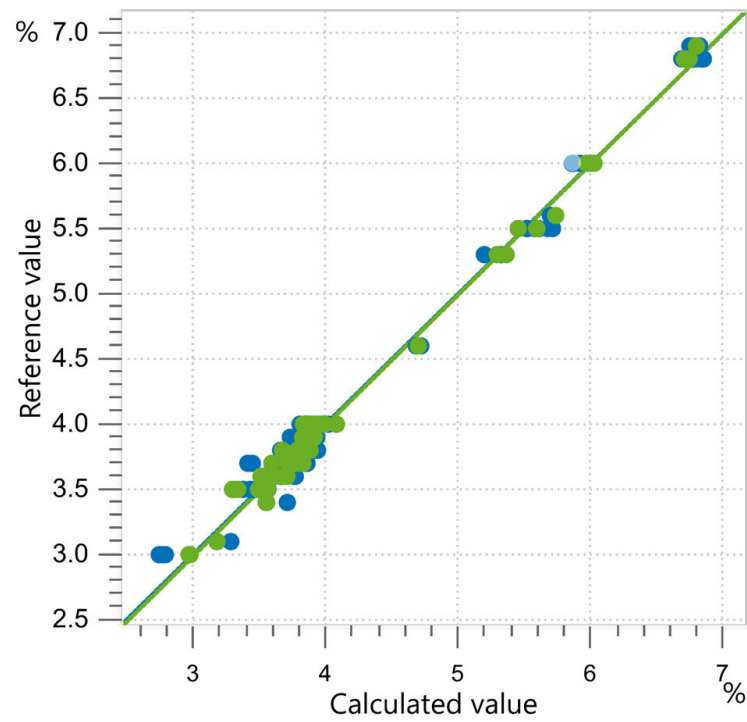


Figure 4. Correlation diagram and the respective FOMs for the prediction of coconut water salinity using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

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

RESULT PH VALUE

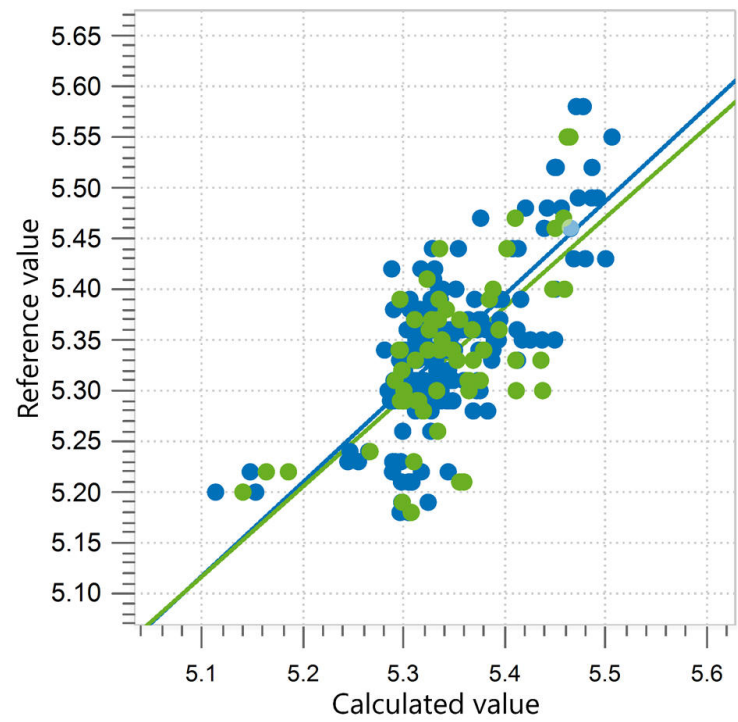


Figure 5. Correlation diagram and the respective FOMs for the prediction of coconut water pH value using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2	SEC	SECV	SEP
0.658	0.05	0.05	0.06

RESULT CONDUCTIVITY

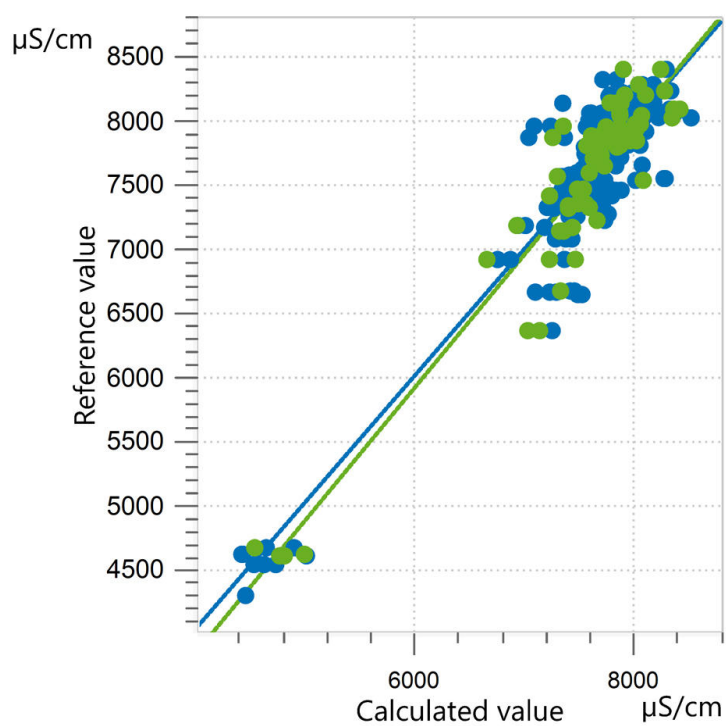


Figure 6. Correlation diagram and the respective FOMs for the prediction of coconut water conductivity using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2	SEC ($\mu\text{S/cm}$)	SECV ($\mu\text{S/cm}$)	SEP ($\mu\text{S/cm}$)
0.892	250	286	285

RESULT TURBIDITY

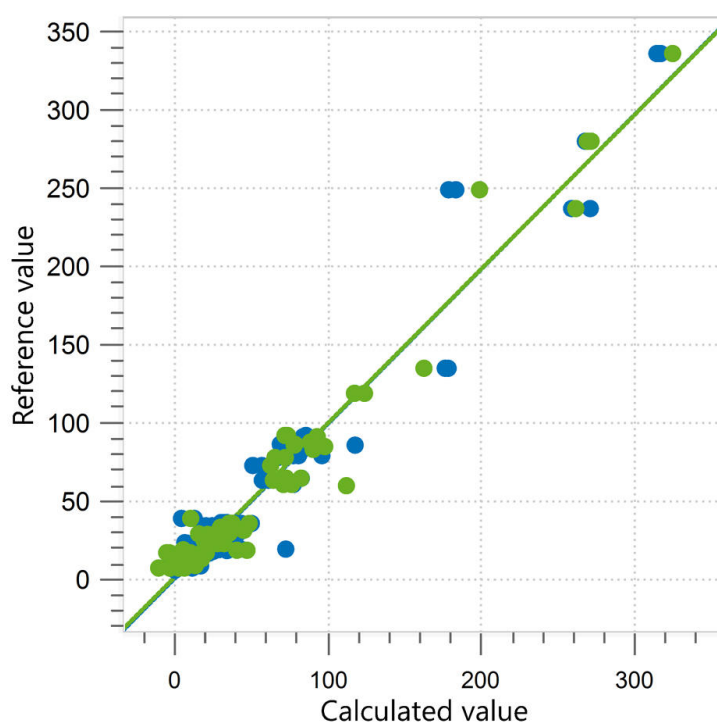


Figure 7. Correlation diagram and the respective FOMs for the prediction of coconut water turbidity using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

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

Metrohm Inula
Shuttleworthstraße 25
1210 Wien

office@metrohm.at

CONFIGURATION



OMNIS NIR Analyzer Liquid

Nahinfrarot-Spektrometer für Flüssigproben.

Der OMNIS NIR Analyzer ist die nach Schweizer Qualitätsstandards entwickelte und produzierte Nahinfrarotspektroskopie(NIRS)-Lösung für die Routineanalytik entlang der gesamten Produktionskette. Die Nutzung neuester Technologien und die Einbindung in die moderne OMNIS Software spiegeln sich in der Geschwindigkeit, der Bedienbarkeit und dem flexiblen Einsatz dieser NIR-Spektrometer wider.

Die Vorteile des OMNIS NIR Analyzer Liquid im Überblick:

- Messungen von Flüssigproben in weniger als 10 Sekunden
- Temperaturregelung an der Probe von 25 °C – 80 °C
- Automatische Erkennung des Einsetzens und der Entnahme des Probengefäßes
- Einfache Einbindung in ein Automationssystem oder Verknüpfung mit weiteren Analysentechniken (Titration)
- Unterstützung zahlreicher Probengefäße mit unterschiedlicher Pfadlänge



Halter OMNIS NIR, Durchfluszellen

Küvettenhalter für den OMNIS NIR Analyzer für Durchfluszellen

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



OMNIS
A WHOLE NEW LEVEL OF PERFORMANCE

OMNIS
A WHOLE NEW LEVEL OF PERFORMANCE

Durchflusszelle, 1 mm

Durchflussquarzküvetten mit einer optischen Pfadlänge von 1.0 mm geeignet für Nahinfrarotspektroskopie (NIRS) Analysen.

Kompatibel mit:

- Halter OMNIS NIR, Durchflusszelle (6.07401.100)
- DS2500 Halter für Durchflussküvetten (6.7493.000)

OMNIS Stand-Alone Lizenz

Ermöglicht den Stand-Alone Betrieb der OMNIS Software auf einem Windows™ Computer.

Merkmale:

- Die Lizenz enthält bereits eine OMNIS Geräte Lizenz.
- Muss über das Metrohm Lizenzierungsportal aktiviert werden.

Softwarelizenz Quant Development

Softwarelizenz für die Erstellung und Bearbeitung von Quantifizierungsmodellen in einer Stand-Alone OMNIS Software Installation.