



Application Note AN-NIR-105

Roasted coffee analysis by near-infrared spectroscopy

NIRS determines caffeine and moisture without any chemicals

For coffee roasters, the continuous analysis of roasted coffee beans can have significant financial impacts. Continuous analysis allows improvement of the roasting settings for more energy-efficient procedures and highly consistent final products. Tedious methods such as HPLC (high-performance liquid chromatography) for the determination of caffeine concentration require detailed knowledge to operate

the instrument, involve chemicals, and can take substantial time to run the analysis.

Near-infrared spectroscopy (NIRS) is a fast and chemical-free alternative for caffeine and moisture analysis in roasted coffee beans. The NIRS solution is easy to use, does not require any sample preparation, and such analyzers are operational either nearby the roaster or in a quality control laboratory.

EXPERIMENTAL EQUIPMENT

Up to 168 roasted coffee samples were analyzed on a Metrohm OMNIS NIR Analyzer Solid with the small cup OMNIS NIR, 60 mm (**Figure 1**). Samples of either whole or ground beans were placed in the small cup and analyzed in diffuse reflection mode. Reference values for caffeine and moisture were obtained with the respective primary methods. Caffeine analysis conducted with an ion chromatograph (IC) followed ISO 20481 guidelines, and moisture analysis followed AOAC 979.12 guidelines.



Figure 1. OMNIS NIR Analyzer Solid with roasted coffee beans in the small cup OMNIS NIR, 60 mm.

Table 1. Hardware and software equipment overview.

Equipment	Article number
OMNIS NIR Analyzer Solid	2.1071.0010
Small holder OMNIS NIR, 60 mm	6.07402.200
Small cup OMNIS NIR, 60 mm	6.07402.210
OMNIS Stand-Alone license	6.06003.010
Quant Development software license	6.06008.002

RESULT

The obtained NIR spectra (**Figure 2**) were used to create prediction models for the different reference parameters. Correlation diagrams which display the

relation between the NIR prediction and the reference values are shown in **Figures 3–4** together with the respective figures of merit (FOM).

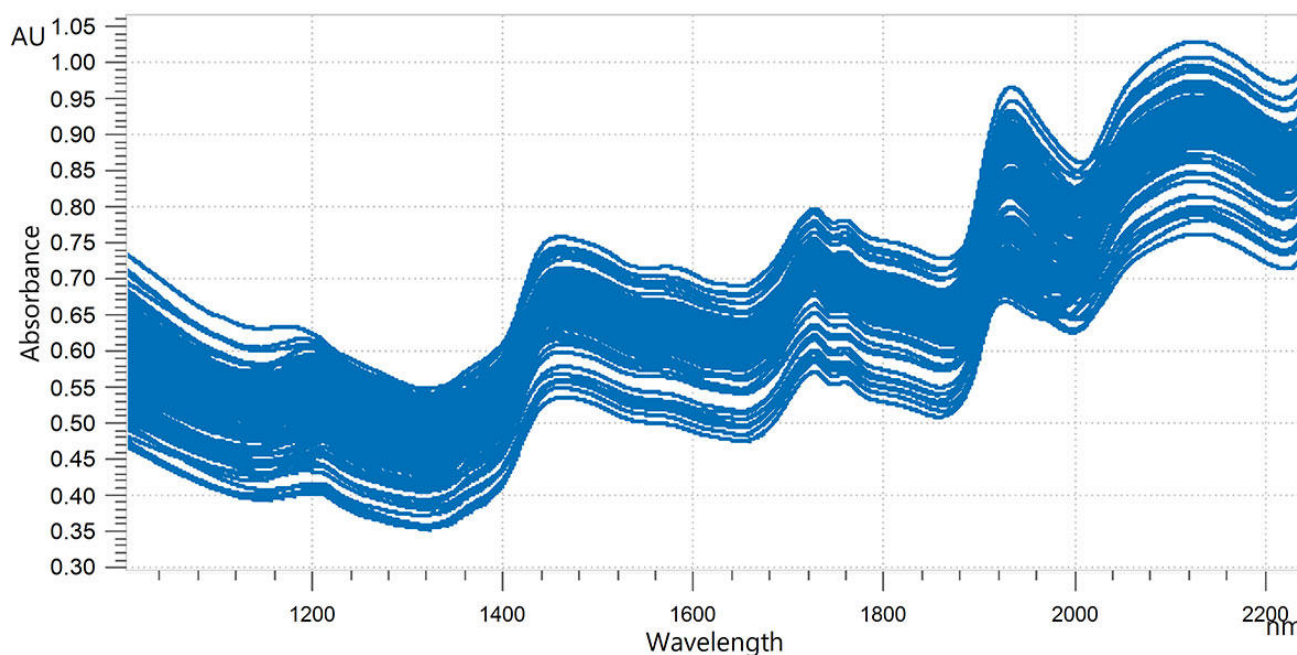


Figure 2. Overlaid NIR spectra of roasted coffee bean samples (whole beans). Data was obtained with an OMNIS NIR Analyzer Solid.

RESULT MOISTURE IN ROASTED COFFEE BEANS

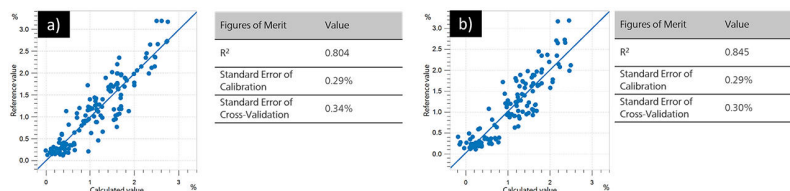


Figure 3. Correlation diagram and the respective FOMs for the prediction of moisture a) for whole coffee beans and b) for ground coffee beans.

RESULT CAFFEINE IN ROASTED COFFEE BEANS

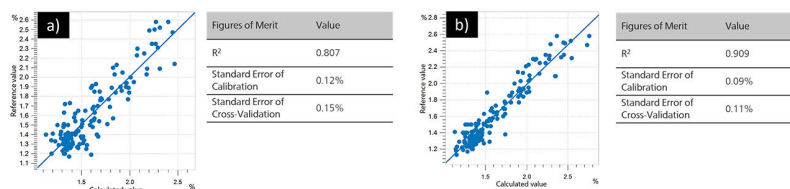


Figure 4. Correlation diagram and the respective FOMs for the prediction of caffeine a) for whole coffee beans and b) for ground coffee beans.

CONCLUSION

This Application Note shows the feasibility of using NIR spectroscopy for the fast analysis of roasted ground and whole coffee beans (**Table 2**). With no chemicals involved, the OMNIS NIR Analyzer allows

measurement of both parameters (caffeine and moisture content) with good accuracy. As expected, the prediction values are slightly better for the ground coffee samples which are more homogeneous.

Table 2. Time to result comparison for different methods used to analyze coffee.

Parameter	Method	Time to result
Caffeine	IC System (ISO 20481)	120 min (sample preparation and measurement)
Moisture	Oven – Loss on drying (AOAC 979.12)	13 hours (sample preparation and measurement)

Internal references: AW NIR CH-0069-042023; AW NIR CH-0070-042023

CONTACT

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CONFIGURATION



OMNIS NIR Analyzer Solid

Nahinfrarot-Spektrometer für feste und viskose Proben.

Der OMNIS NIR Analyzer ist die nach Schweizer Qualitätsstandards entwickelte und produzierte Nahinfrarot-Spektroskopie (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 Solid im Überblick:

- Messungen von Feststoffen und viskosen Proben in weniger als 10 Sekunden
- Automatisierte Mehrpositionenmessungen für reproduzierbare Ergebnisse auch bei inhomogenen Proben
- Einfache Einbindung in ein Automationssystem oder Verknüpfung mit weiteren Analysetechnologien (Titration)
- Unterstützung zahlreicher Probengefäße.



Kleiner Halter OMNIS NIR, 60 mm

Kleiner Halter für Kleines Probengefäß OMNIS NIR, 60 mm (6.07402.210).

Erlaubt eindeutige Positionierung des Probengefäßes und die Rotation des Probengefäßes.



Kleine Schale OMNIS NIR, 60 mm

Kleines Probengefäß für die Spektrenaufnahme von Pulvern und Granulaten in Reflexion an unterschiedlichen Probenstellen.

Kompatibel mit:

- Kleiner Halter OMNIS NIR, 60 mm (6.07402.200)

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Softwarelizenz Quant Development

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

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.



Vorkalibrierung, Kaffee, fest

OMNIS Vorkalibrierung für die Bestimmung der Feuchtigkeit und des Koffeingehalts in geröstetem Kaffee mittels NIR-Spektroskopie.