

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).

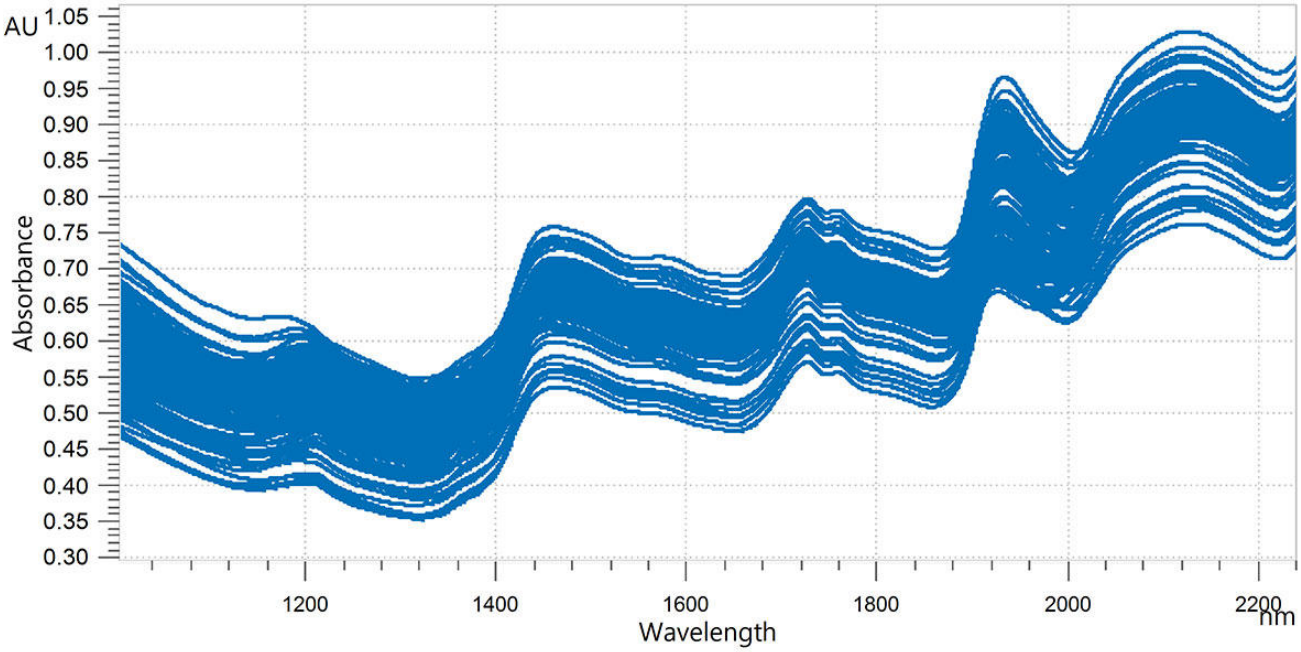
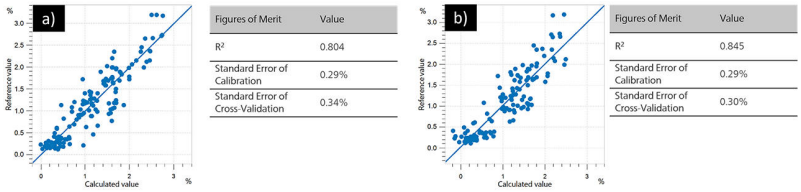


Figure 2. Overlaid NIR spectra of roasted coffee bean samples (whole beans). Data was obtained with an OMNIS NIR Analyzer Solid.

RESULT MOISTURE IN ROASTED COFFEE BEANS

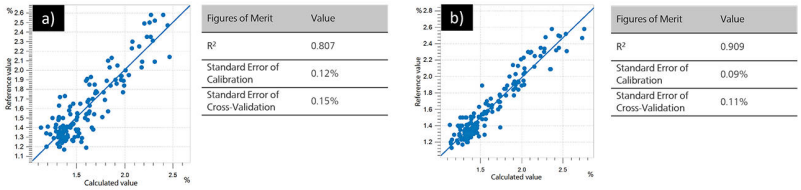


Figures of Merit	Value
R^2	0.804
Standard Error of Calibration	0.29%
Standard Error of Cross-Validation	0.34%

Figures of Merit	Value
R^2	0.845
Standard Error of Calibration	0.29%
Standard Error of Cross-Validation	0.30%

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



Figures of Merit	Value
R^2	0.807
Standard Error of Calibration	0.12%
Standard Error of Cross-Validation	0.15%

Figures of Merit	Value
R^2	0.909
Standard Error of Calibration	0.09%
Standard Error of Cross-Validation	0.11%

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

Metrohm Romania
Str. Emil Racoviță nr. 25
041753 București
office@metrohm.ro

CONFIGURATION



OMNIS NIR Analyzer Solid

Near-infrared spectrometer for solid and viscous 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 Solid:

- Measurements of solids and viscous samples in less than 10 seconds
- Automated multi-position measurements for reproducible results, even with nonhomogeneous samples
- Simple integration in an automation system or link with additional analysis technologies (titration)
- Supports numerous sample vessels



Small holder OMNIS NIR, 60 mm

Small holder for small sample vessel OMNIS NIR, 60 mm (**6.07402.210**).

Permits unambiguous positioning of the sample vessel and the rotation of the sample vessel.



Small cup OMNIS NIR, 60 mm

Small sample vessel for the spectra acquisition of powders and granulates in reflection at various sample positions.

The glass bottom is made of resistant Gorilla® Glass.

Compatible with:

- Small holder OMNIS NIR, 60 mm (**6.07402.200**)

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
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.



Pre-calibration, coffee, solid

OMNIS pre-calibration for determination of moisture and caffeine content in roasted coffee using NIR spectroscopy.