Application Note AN-NIR-105

Roasted and ground coffee analysis by near-infrared spectroscopy

Fast determination of caffeine, water activity, and moisture

Continuous analysis of roasted coffee beans allows roasteries to improve their roasting settings, leading to higher energy efficiency and more consistent final products. Not only is flavor affected by the roasting degree, but caffeine content can also change. Conventional analytical methods such as HPLC (high-performance liquid chromatography) for caffeine concentration determination require technical skills to operate, chemical reagents, and take from several minutes to hours to obtain the results.

In contrast, near-infrared spectroscopy (NIRS) is a fast and chemical-free alternative for caffeine, water activity, and moisture analysis in roasted coffee beans and ground coffee. The NIRS solution is easy to use and does not require any sample preparation. These analyzers can be operated nearby the roaster or in a quality control lab.

Up to 35 roasted ground coffee bean samples were analyzed on a Metrohm DS2500 Solid Analyzer with the DS2500 Holder and NIRS mini sample cups (Figure 1). Samples were positioned into the NIRS mini sample cups for the analysis in diffuse reflection mode. Data acquisition and prediction model development were performed with the software package Vision Air Complete (Table 1).

Reference values for caffeine, water activity, and moisture were obtained with the respective primary methods. Caffeine analysis followed the ISO 20481 guideline and was conducted with an ion chromatograph (IC), water activity determination followed the ISO 18787 norm, and moisture determination was performed according to DIN 10772-1.

Table 1. Hardware and software equipment overview.

Equipment	Article number
DS2500 Solid Analyzer	2.922.0010
DS2500 Holder	6.7430.040
NIRS mini sample cups	6.7402.030
Vision Air 2.0 Complete	6.6072.208

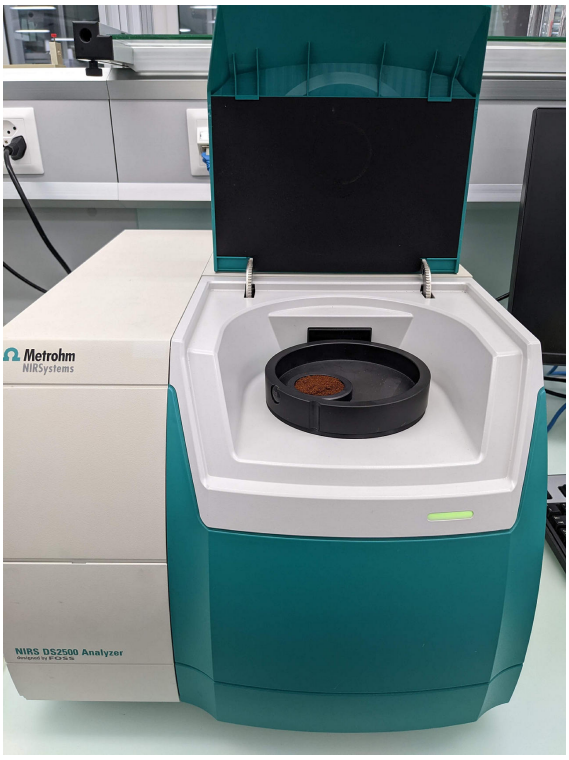


Figure 1. A Metrohm DS2500 Solid Analyzer with ground coffee beans held in a NIRS mini sample cup.

RESULT

The obtained Vis-NIR spectra (Figure 2) were used to create prediction models for the different reference parameters. Correlation diagrams which display the relation between the Vis-NIR prediction and the reference values are shown in Figures 3–5 together with the respective figures of merit (FOM).

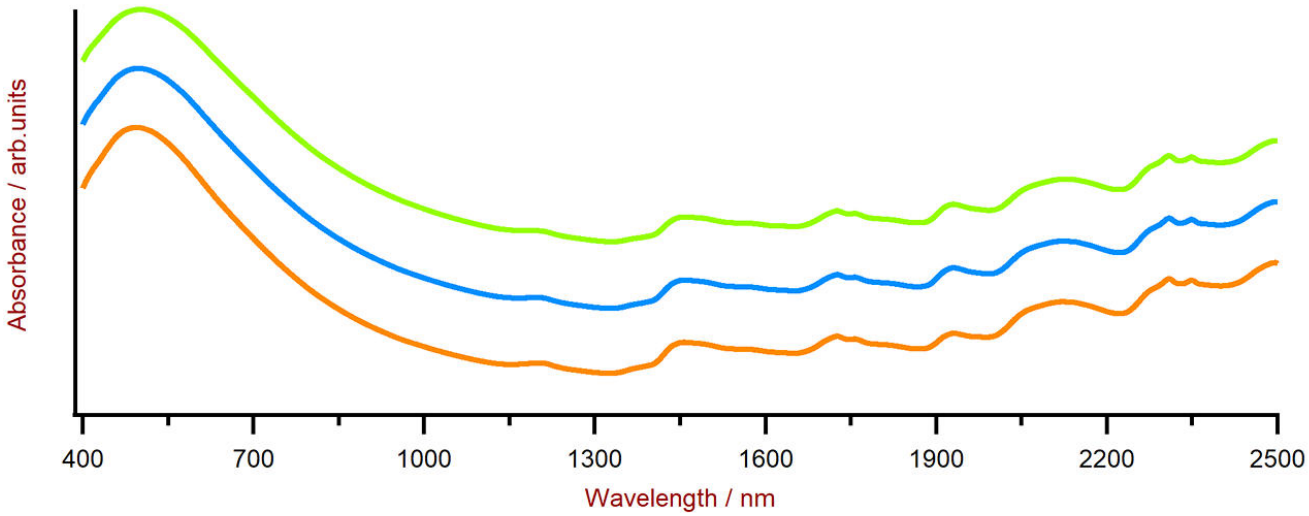
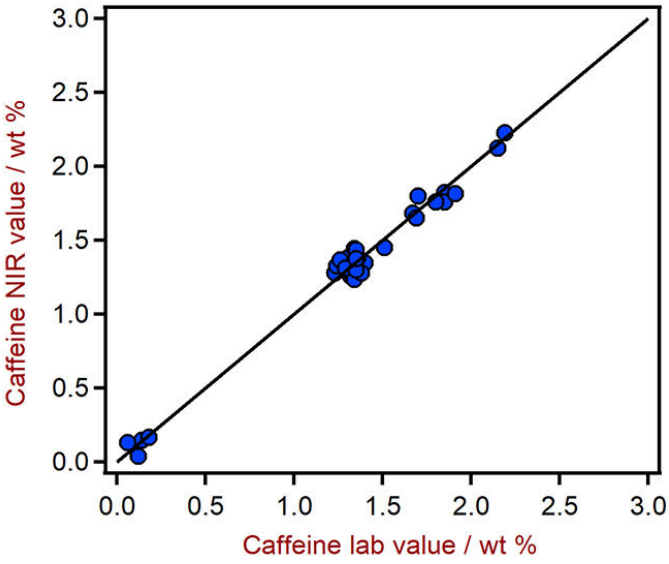


Figure 2. Selection of Vis-NIR spectra of roasted and ground coffee bean samples. Data was obtained with a DS2500 Solid Analyzer. A spectra offset was applied for visualization purposes.

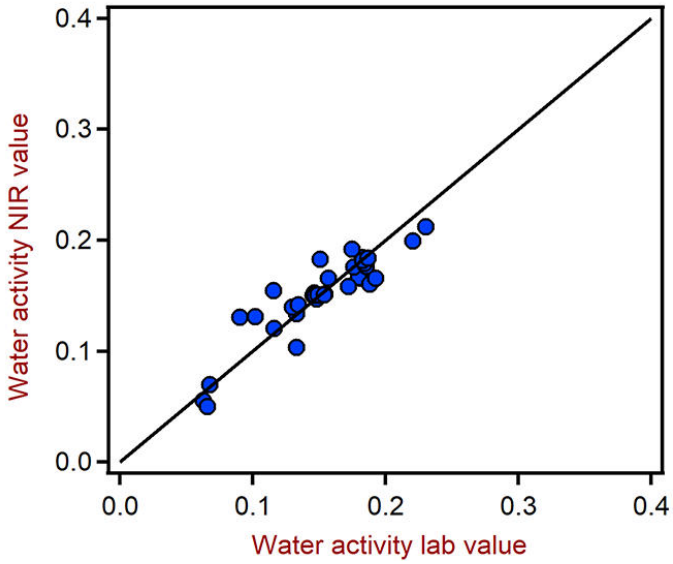
RESULT CAFFEINE IN ROASTED COFFEE



Figures of Merit	Value
R^2	0.986
Standard Error of Calibration	0.0742 wt%
Standard Error of Cross-Validation	0.0721 wt%

Figure 3. Correlation diagram and the respective FOMs for the prediction of caffeine in roasted ground coffee samples using a DS2500 Solid Analyzer. The lab values were determined by following the guidelines in ISO 20481.

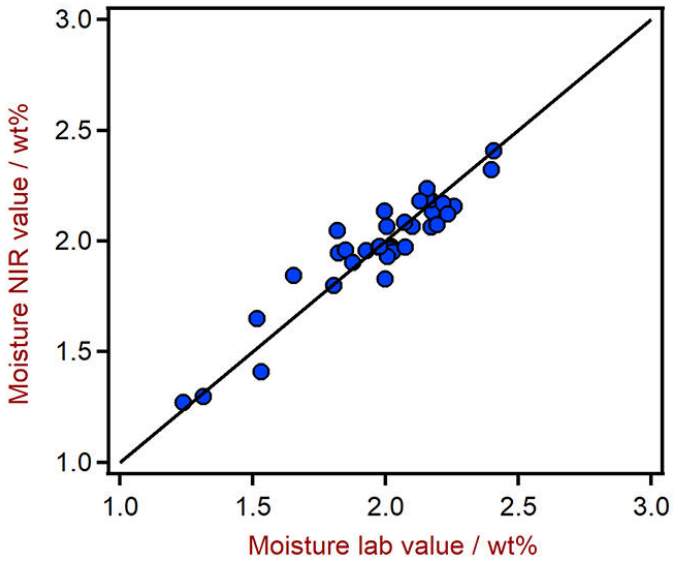
RESULT WATER ACTIVITY IN ROASTED COFFEE



Figures of Merit	Value
R^2	0.82
Standard Error of Calibration	0.018
Standard Error of Cross-Validation	0.021

Figure 4. Correlation diagram and the respective FOMs for the prediction of water activity in roasted ground coffee samples using a DS2500 Solid Analyzer. The lab values were determined according to the guidelines in ISO 18787.

RESULT MOISTURE IN ROASTED COFFEE



Figures of Merit	Value
R^2	0.88
Standard Error of Calibration	0.099 wt%
Standard Error of Cross-Validation	0.109 wt%

Figure 5. Correlation diagram and the respective FOMs for the prediction of moisture in roasted ground coffee samples using a DS2500 Solid Analyzer. The lab values were determined according to the guidelines in DIN 10772-1.

CONCLUSION

This Application Note shows the feasibility of near-infrared spectroscopy for the analysis of several quality parameters in roasted ground coffee. One NIRS analyzer can determine the caffeine concentration (0.1–2.5 wt%) in addition to water activity and moisture content in a single measurement. Not only are results delivered in less than a minute, but no chemical reagents are required for the analysis. The time savings by using NIRS compared to the traditional analytical methods (Table 2) is immense.

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)
Water activity	Water Activity System (ISO 18787)	15–30 min
Moisture	Oven – Loss on drying (DIN 10772-1)	13 hours (sample preparation and measurement)

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

CONTACT

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CONFIGURATION

DS2500 Solid Analyzer

Robust near-infrared spectroscopy for quality control, not only in laboratories but also in production environments.

The NIRS DS2500 Analyzer is the tried and tested, flexible solution for routine analysis of solids, creams, and optionally also liquids along the entire production chain. Its robust design makes the NIRS DS2500 Analyzer resistant to dust, moisture, vibrations, and temperature fluctuations, which means that it is eminently suited for use in harsh production environments.

The NIRS DS2500 covers the full spectral range from 400 to 2500 nm and delivers accurate, reproducible results in less than one minute. The NIRS DS2500 Analyzer meets the demands of the pharmaceutical industry and supports users in their day-to-day routine tasks thanks to its simple operation.

Thanks to accessories tailored perfectly to the instrument, optimum results are achieved with every sample type, no matter how challenging it is, e.g. coarse-grained solids such as granulates or semi-solid samples such as creams. The MultiSample Cup can help improve productivity when measuring solids, as it enables automated measurements of series containing up to nine samples.