Application Note AN-NIR-104

Analysis of green coffee beans by near-infrared spectroscopy

Reliable density, water activity, and moisture results in seconds

Before they are made suitable for consumption, raw (green) coffee beans must be roasted. For roasters, the continuous analysis of green coffee beans allows the improvement of warehouse management. This information helps roasters prioritize the order of lots to process and to optimize roasting settings for more consistency and energy efficiency. However, the time, effort, and somewhat complex workflows required when using traditional analytical methods (e.g., densimeters, water activity analyzers) can be an inconvenience.

Near-infrared spectroscopy (NIRS) is a fast, multiparameter analytical method suitable for the analysis of density, water activity, and moisture content of green coffee beans. Neither chemicals nor sample preparation are required, making NIRS easy to use in the warehouse, nearby the roaster, or in a quality control laboratory.

EXPERIMENTAL EQUIPMENT

Up to 31 samples of green coffee beans were analyzed on a Metrohm DS2500 Solid Analyzer with the DS2500 Holder and NIRS mini sample cups (Figure 1). Green coffee beans 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 density, water activity, and moisture content were obtained with the respective primary methods. Water activity analysis followed the guideline of ISO 18787, moisture content was determined according to ISO 6673, and density was determined with a density determination set for a Precisa balance.

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

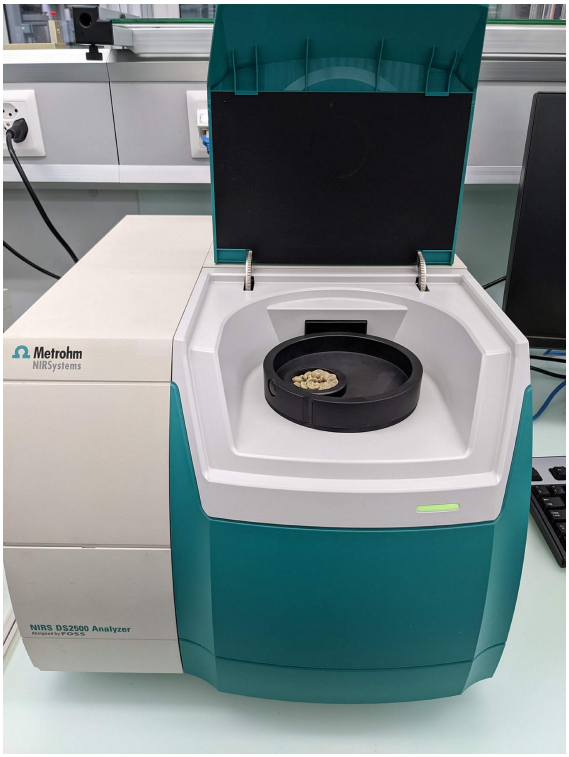


Figure 1. A Metrohm DS2500 Solid Analyzer with green coffee beans held in a NIRS mini sample cup.

RESULT

The obtained Vis-NIR spectra (Figure 2) were used to create prediction models for the different reference parameters. To verify the quality of the prediction models, the data sets for water activity and moisture were split into calibration and validation sets. A leave one out validation procedure was used for density. 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).

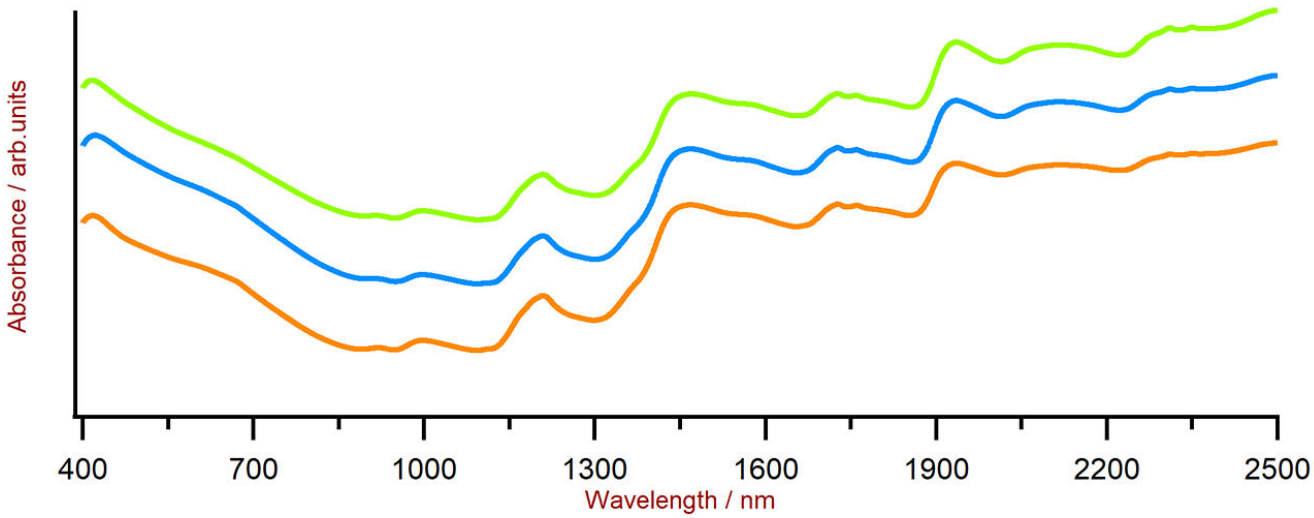
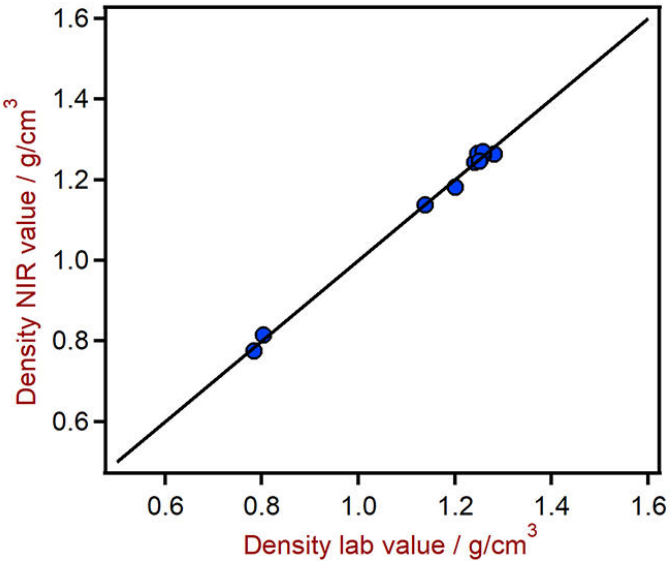


Figure 2. Selection of Vis-NIR spectra of green coffee bean samples. Data was obtained with a DS2500 Solid Analyzer. A spectra offset was applied for visualization purposes.

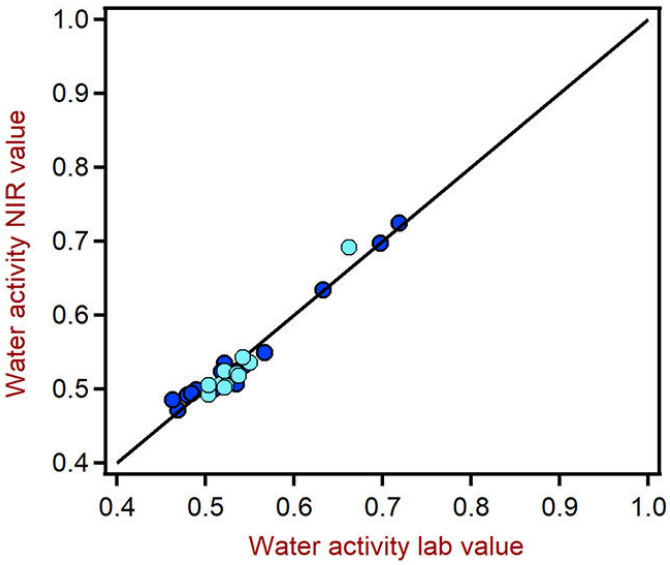
RESULT DENSITY IN GREEN COFFEE BEANS



Figures of Merit	Value
R^2	0.99
Standard Error of Calibration	0.015 g/cm³
Standard Error of Cross-Validation	0.042 g/cm³

Figure 3. Correlation diagram and the respective FOMs for the prediction of the density of green coffee beans using a DS2500 Solid Analyzer. The lab values were determined using density determination set for a balance.

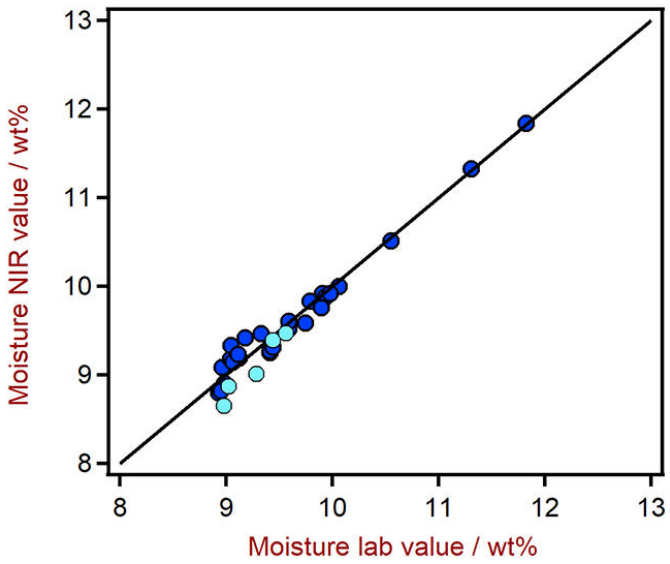
RESULT WATER ACTIVITY IN GREEN COFFEE BEANS



Figures of Merit	Value
R^2	0.97
Standard Error of Calibration	0.014
Standard Error of Cross-Validation	0.017
Standard Error of Prediction	0.015

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

RESULT MOISTURE IN GREEN COFFEE BEANS



Figures of Merit	Value
R^2	0.97
Standard Error of Calibration	0.133
Standard Error of Cross-Validation	0.149
Standard Error of Prediction	0.205

Figure 5. Correlation diagram and the respective FOMs for the prediction of moisture in green coffee beans using a DS2500 Solid Analyzer. The lab values were determined according to the guidelines in ISO 6673.

CONCLUSION

This Application Note shows the feasibility of near-infrared spectroscopy for the analysis of density, water activity, and moisture content in green coffee beans. Without using any chemicals, these quality parameters can be measured with results obtained in less than a minute. This easy-to-use method allows roasters to improve warehouse management by selecting raw beans to roast based on indicators of shelf life. Additionally, roast settings can be optimized for better product consistency and higher energy efficiency.

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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 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 DS2500 Analyzer resistant to dust, moisture, vibrations, and temperature fluctuations, which means that it is eminently suited for use in harsh production environments.

The DS2500 covers the full spectral range from 400 to 2500 nm and delivers accurate, reproducible results in less than one minute. The 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 9 samples.