



Application Note AN-NIR-104

利用近红外光谱分析绿咖啡豆

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

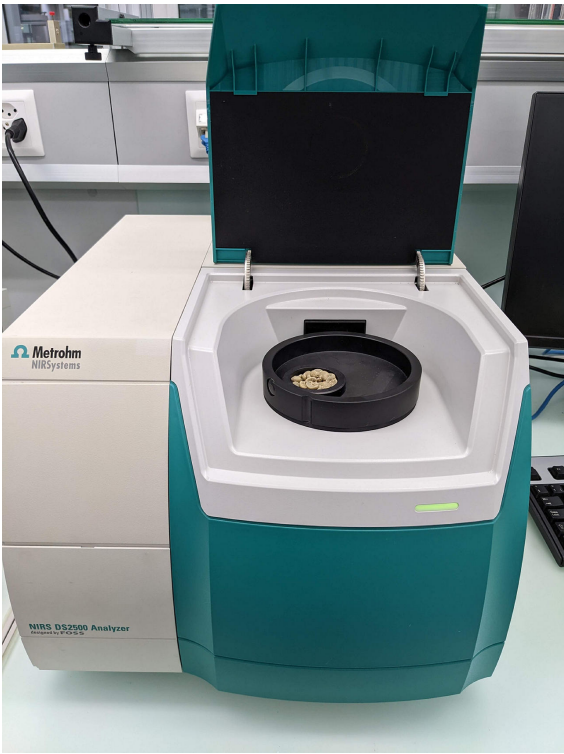


Figure 1. A Metrohm DS2500 Solid Analyzer with green coffee beans held in a NIRS mini sample cup.

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).

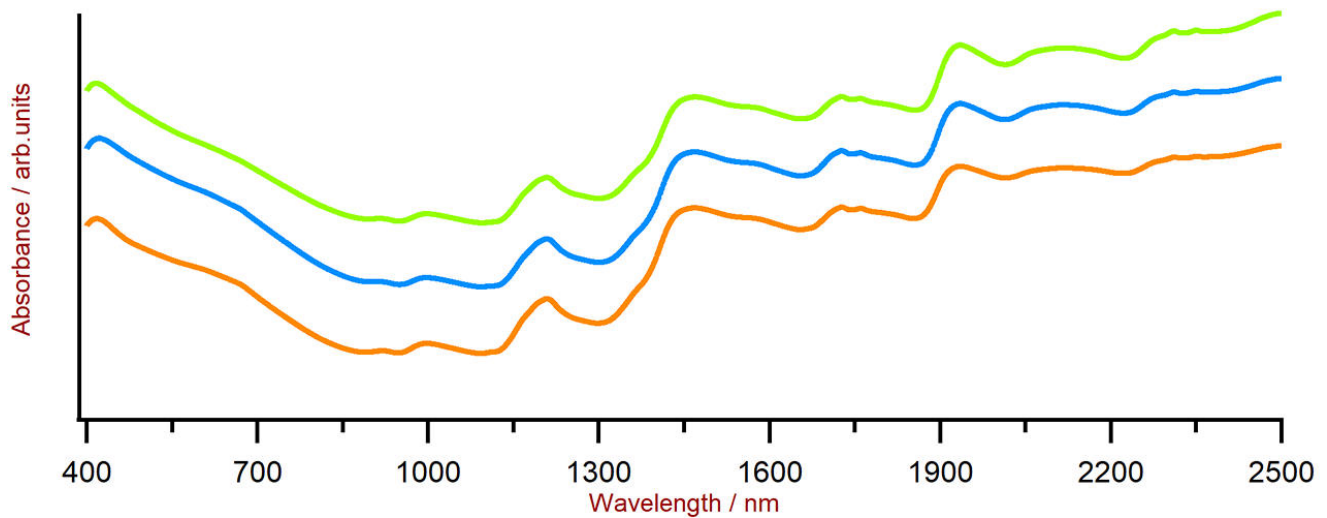
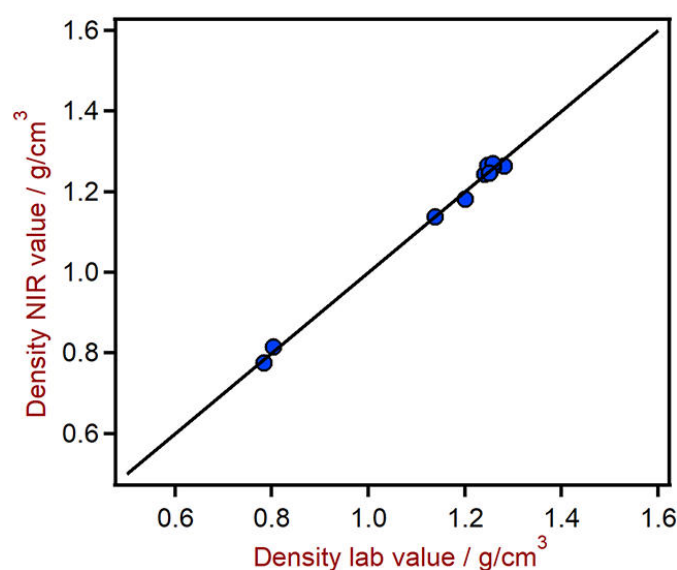


Figure 2. Selection of Vis-NIR spectra of green coffee bean samples. Data was obtained with a DS2500 Solid Analyzer. A spectra offset was applied for visualization purposes.

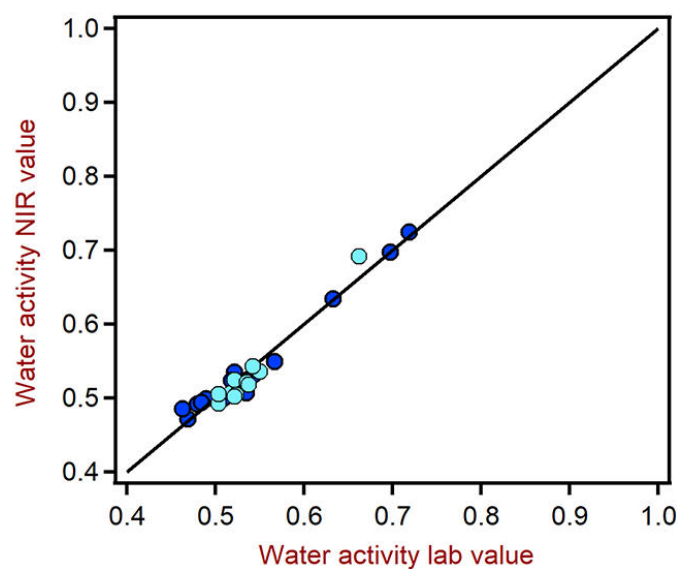
RESULT DENSITY IN GREEN COFFEE BEANS



Figures of Merit	Value
R^2	0.99
Standard Error of Calibration	0.015 g/cm ³
Standard Error of Cross-Validation	0.042 g/cm ³

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.

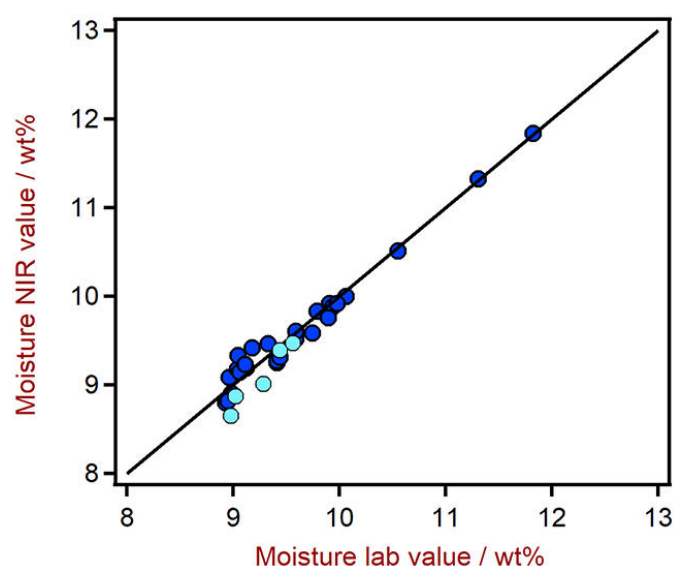
RESULT WATER ACTIVITY IN GREEN COFFEE BEANS



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

坚固结实的近红外光谱仪,用于生产环境和试验室中的质量检查。

DS2500 分析仪是经过验证的灵活解决方案,用于对整个生产链过程中的固体、乳膏和液体进行常规分析。其坚固结实的设计使 DS2500 Analyzer 分析仪不受灰尘、湿度、振动和温度波动的影响,因此非常适用于在恶劣的生产环境中使用。

DS2500 涵盖了从 400 到 2500 nm 的整个光谱范围,并能在不到一分钟时间内提供准确和可再现的结果。DS2500 Analyzer 满足制药行业的要求,并由于操作简便而能帮助用户完成其日常工作任务。

由于与设备匹配,附件可以承受任何具有挑战性的样品类型,例如:粒料之类的粗颗粒固体或乳膏之类的半固体样品,可获得结果。测量固体的时候,使用 MultiSample Cup 可以提高生产率,可以自动批量测量多 9 个样品。