



Application Note AN-NIR-105

用近外光分析焙和研磨

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

EXPERIMENTAL EQUIPMENT

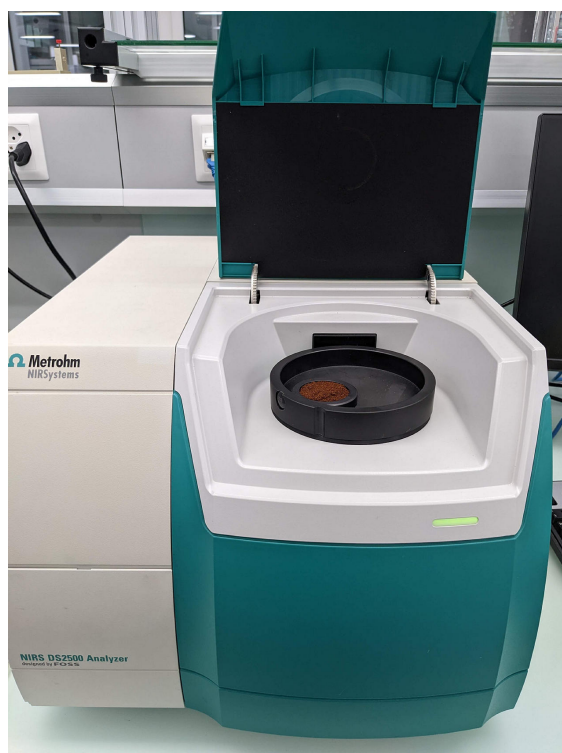


Figure 1. A Metrohm DS2500 Solid Analyzer with ground coffee beans held in a NIRS mini sample cup.

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).

RESULT

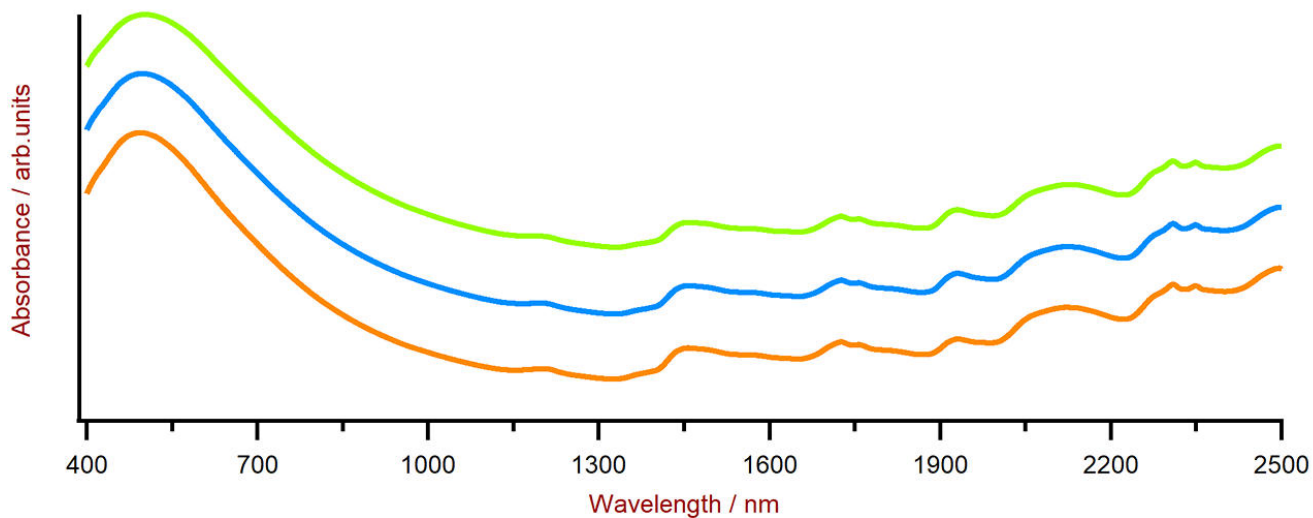
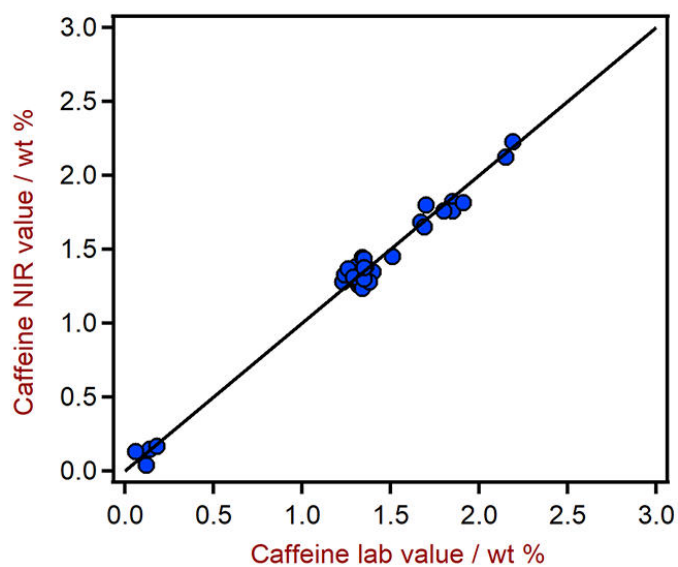


Figure 2. Selection of Vis-NIR spectra of roasted and ground coffee bean samples. Data was obtained with a DS2500 Solid Analyzer. A spectra offset was applied for visualization purposes.

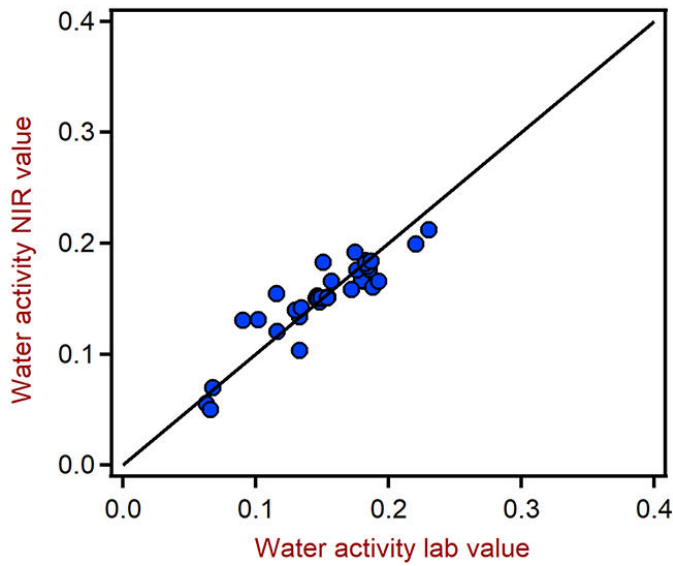
RESULT CAFFEINE IN ROASTED COFFEE



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 using ion chromatography according to the guidelines in ISO 20481.

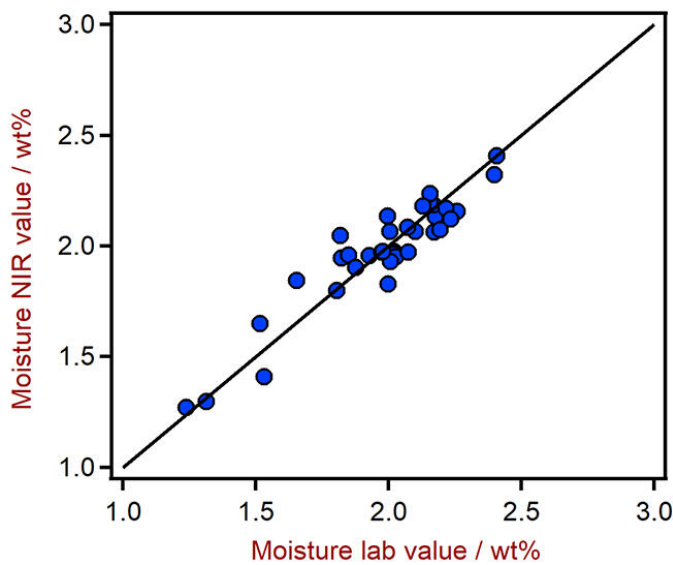
RESULT WATER ACTIVITY IN ROASTED COFFEE



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.

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

固的近外光,用于生境和室中的量。

DS2500 分析是的活解决方案,用于整个生程中的固体、乳膏和液体行常分析。其固的使 DS2500 Analyzer 分析不受灰、湿度、振和温度波的影,因此非常用于在劣的生境中使用。

DS2500 涵盖了从 400 到 2500 nm 的整个光范,并能在不到一分内提供准和可再的果。DS2500 Analyzer 足制行的要求,并由于操作便而能助用完成其日常工作任。

由于与匹配,附件可以承受任何具有挑性的品型,例如:粒料之的粗粒固体或乳膏之的半固体品,可得果。量固体的候,使用 MultiSample Cup 可以提高生率,可以自批批量多 9 个品。