



Application Note AN-NIR-105

## 用近红外光谱分析烘焙咖啡

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.

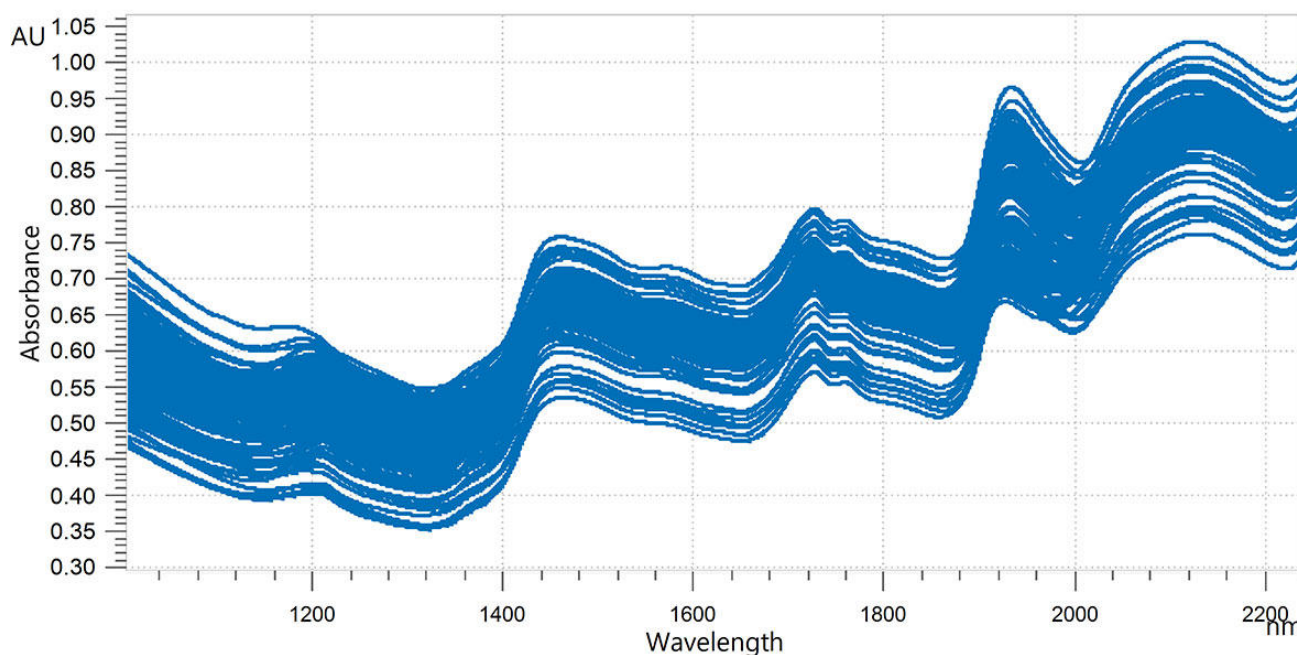
**Table 1.** Hardware and software equipment overview.

| 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

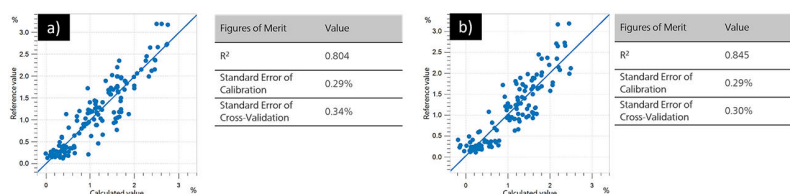
The obtained NIR spectra (**Figure 2**) were used to create prediction models for the different reference parameters. Correlation diagrams which display the relation between the NIR

prediction and the reference values are shown in **Figures 3–4** together with the respective figures of merit (FOM).



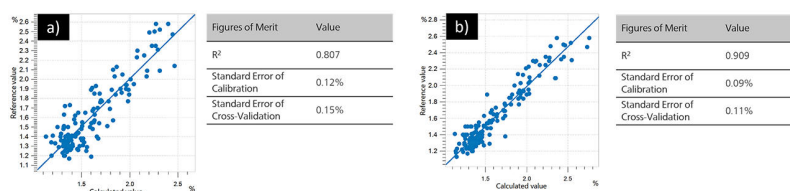
**Figure 2.** Overlaid NIR spectra of roasted coffee bean samples (whole beans). Data was obtained with an OMNIS NIR Analyzer Solid.

## RESULT MOISTURE IN ROASTED COFFEE BEANS



**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



**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

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## CONFIGURATION



### OMNIS NIR Analyzer Solid

适合固体和粘性样品的近红外光谱仪。

OMNIS NIR Analyzer 是一种按照瑞士质量标准开发和生产的近红外光谱 (NIRS) 解决方案,用于整个生产链的常规分析。使用新技术和嵌入先进 OMNIS Software 反应在该 NIR 光谱仪的速度、可操作性和灵活使用上。

OMNIS NIR Analyzer Solid 的优点概览:

- 在 10 秒以内测量固体和粘性样品
- 自动化多位置测量,即使在样品不均匀时,也能够获得可重现的结果
- 方便地嵌入自动系统,或者与其它分析技术(滴定)关联
- 支持大量样品容器



### OMNIS NIR60 mm

适合小样品容器的小支架 OMNIS NIR,60 mm (6.07402.210)。

允许明确地定位样品容器和旋转样品容器。



### OMNIS NIR60 mm

用于在不同样品位置处通过反射采集粉末和颗粒反射光谱的小样品容器。

兼容:

- 小支架 OMNIS NIR,60 mm (6.07402.200)

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## Quant Development

用于在独立 OMNIS Software 安装套件中编写和编辑量化模型的软件许可证。

## OMNIS

允许单机版 OMNIS 软件在一台 Windows™ 计算机上运行。

### 特性:

- 该许可证已含有一份 OMNIS 设备许可证。
- 须通过万通许可授权平台进行激活。

通过 NIR 光谱测定烘焙后咖啡中湿度和咖啡因含量的 OMNIS 预校准。