



Application Note AN-NIR-105

Roasted coffee analysis by near-infrared spectroscopy

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

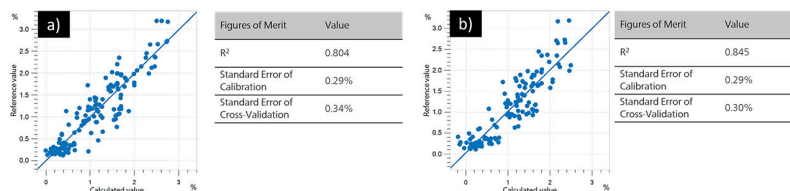


Figure 3. Correlation diagram and the respective FOMs for the prediction of moisture a) for whole coffee beans and b) for ground coffee beans.

RESULT CAFFEINE IN ROASTED COFFEE BEANS

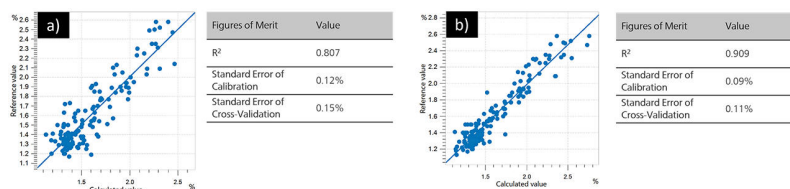


Figure 4. Correlation diagram and the respective FOMs for the prediction of caffeine a) for whole coffee beans and b) for ground coffee beans.

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

Spectromètre proche infrarouge pour échantillons solides et visqueux.

L'OMNIS NIR Analyzer est la solution de spectroscopie proche infrarouge (NIRS) développée et produite selon les normes de qualité suisses pour les analyses de routine tout au long de la chaîne de fabrication. L'utilisation des technologies les plus récentes et l'intégration dans le logiciel OMNIS moderne se reflètent dans la vitesse, la facilité d'utilisation et la flexibilité d'utilisation de ces spectromètres NIR.

Vue d'ensemble des avantages de l'OMNIS NIR Analyzer Solid :

- Mesures d'échantillons solides et visqueux en moins de 10 secondes
- Mesures multi-positions automatisées pour des résultats reproductibles même avec des échantillons non homogènes
- Intégration simple dans un système d'automatisation ou liaison avec d'autres technologies d'analyse (titrage)
- Prise en charge de nombreux récipients d'échantillon



Petit support OMNIS NIR, 60 mm

Petit support pour petit récipient d'échantillon OMNIS NIR, 60 mm (6.07402.210).

Permet un positionnement univoque du récipient d'échantillon et sa rotation.



Petite coupelle OMNIS NIR, 60 mm

Petit récipient d'échantillon pour l'enregistrement de spectre par réflexion de poudres et de granulés en différents points de l'échantillon.

Compatible avec :

- Petit support OMNIS NIR, 60 mm (6.07402.200)

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Licence logicielle Quant Development

Licence logicielle pour la création et l'édition de modèles de quantification dans une installation du logiciel OMNIS Stand-Alone.

Licence OMNIS autonome

Elle permet l'exploitation autonome du logiciel OMNIS sur un ordinateur Windows™.

Caractéristiques :

- La licence comprend déjà une licence pour appareils OMNIS.
- Elle doit être activée via le portail d'octroi de licences Metrohm.



Pré-calibration, café, solide

Pré-calibration OMNIS pour la détermination de l'humidité et de la teneur en caféine dans le café torréfié par spectroscopie NIR.