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.

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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.

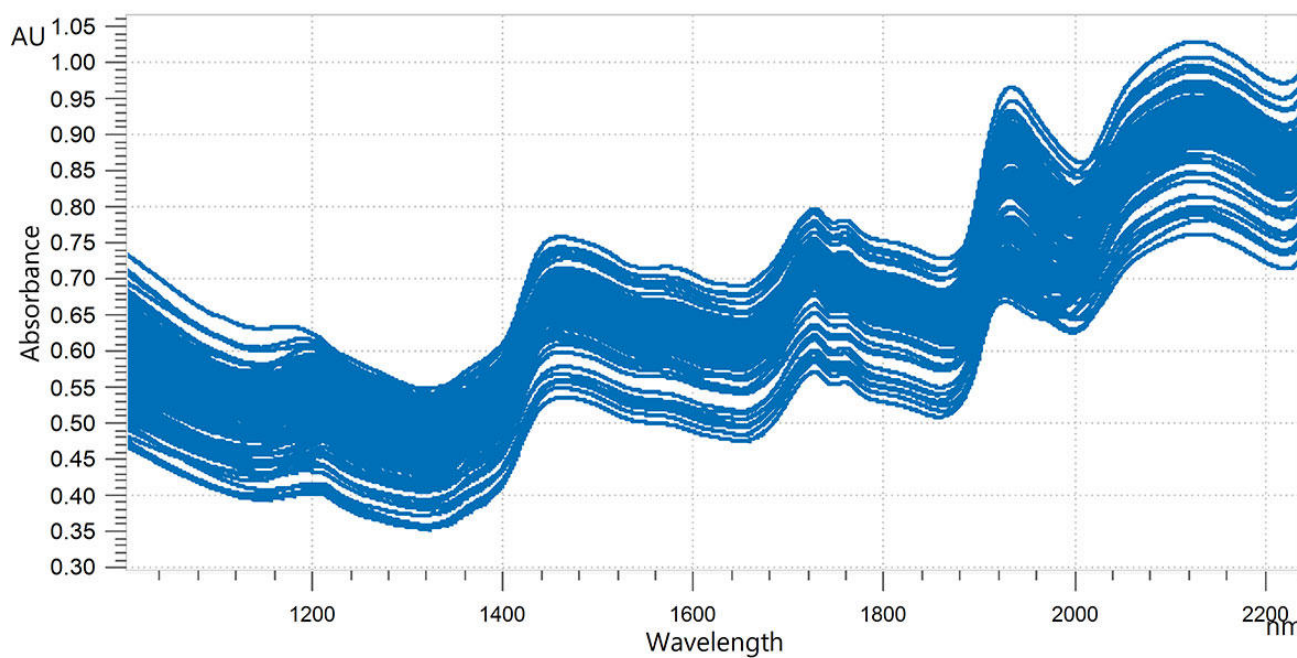**Figure 1.** OMNIS NIR Analyzer Solid with roasted coffee beans in the small cup OMNIS NIR, 60 mm.

Table 1. Hardware and software equipment overview.

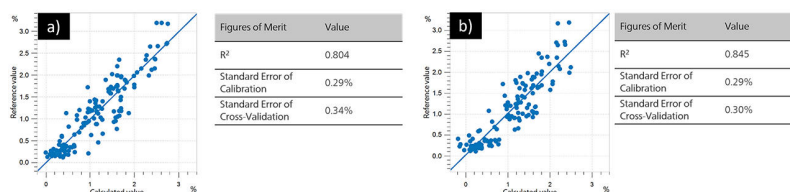| Equipment	Article number
OMNIS NIR Analyzer Solid	2.1071.0010
Small holder OMNIS NIR, 60 mm	6.07402.200
Small cup OMNIS NIR, 60 mm	6.07402.210
OMNIS Stand-Alone license	6.06003.010
Quant Development software license	6.06008.002

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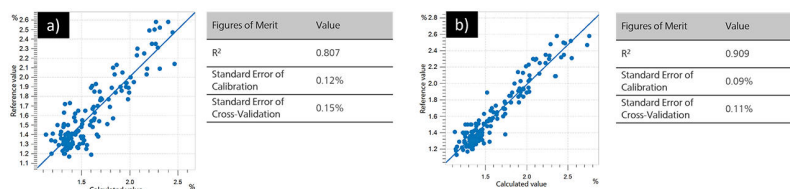
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Figure 2. Overlaid NIR spectra of roasted coffee bean samples (whole beans). Data was obtained with an OMNIS NIR Analyzer Solid.

Figures of Merit	Value
R²	0.804
Standard Error of Calibration	0.29%
Standard Error of Cross-Validation	0.34%

Figures of Merit	Value
R²	0.845
Standard Error of Calibration	0.29%
Standard Error of Cross-Validation	0.30%

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

Figures of Merit	Value
R²	0.807
Standard Error of Calibration	0.12%
Standard Error of Cross-Validation	0.15%

Figures of Merit	Value
R²	0.909
Standard Error of Calibration	0.09%
Standard Error of Cross-Validation	0.11%

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

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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)

CONCLUSION

Internal references: AW NIR CH-0069-042023; AW NIR CH-0070-042023

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CONFIGURATION

OMNIS NIR Analyzer Solid
固体および粘性のサンフルのための近赤外スヘクトロメーター。
OMNIS NIR Analyzer は、スイスの品質基準に従って開発・製造された、生産チェーン全体に沿ったルーチン分析のための近赤外分光法 (NIRS) ソリューションてす。最新技術の適用と最新の OMNIS Software への統合は、この NIR スヘクトロメーターの速度、ユーサヒリティ、柔軟な使用に反映されています。
OMNIS NIR Analyzer Solid の利点の概要:
- 10秒未満て固体サンフルと粘性サンフルを測定
- 不均質なサンフルても再現性のある結果を得るための自動マルチホシション測定
- オートメーションシステムへの統合、またはその他の分析技術 (滴定) との連結か容易
- 多数のサンフル容器に対応

OMNIS NIR60 mm
小型サンフル容器 OMNIS NIR、60 mm (**6.07402.210**) 用小型ホルター。
サンフル容器の確実な配置と回転を可能にします。

OMNIS NIR60 mm

:
- OMNIS NIR60 mm (**6.07402.200**)

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