Application Note AN-NIR-019

Human stool analysis by near-infrared spectroscopy

Determination of moisture, fat, and nitrogen

Several diseases like pancreatic insufficiency or hepatic disorders cause malabsorption or maldigestion. The resulting changes in stool composition (e.g., in moisture, nitrogen content, or fat content) provide important information for medical diagnostics.

Time-consuming lab methods which require a significant amount of sample preparation can be replaced by near-infrared spectroscopy (NIRS) for fast screening of human stool samples with no sample preparation. The NIRS method is easy to use – no chemicals are required and results are given for several parameters within one minute.

EXPERIMENTAL EQUIPMENT

522 human stool samples were analyzed on a Metrohm DS2500 Solid Analyzer with a modified DS2500 Holder for petri dishes (Figure 1). Stool samples were positioned into the petri dishes for the analysis in diffuse reflection mode. Reference values for moisture, fat, and nitrogen content were obtained with the respective primary methods.

Figure 1. DS2500 Solid Analyzer with human stool samples.

Equipment	Metrohm number
DS2500 Solid Analyzer	2.922.0010
DS2500 Holder	6.7430.040
Vision Air 2.0 Complete	6.6072.208

RESULTS

The obtained Vis-NIR spectra (Figure 2) were used to create prediction models for the different reference parameters. The data set was split into calibration and validation sets to verify the quality of the prediction models. 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).

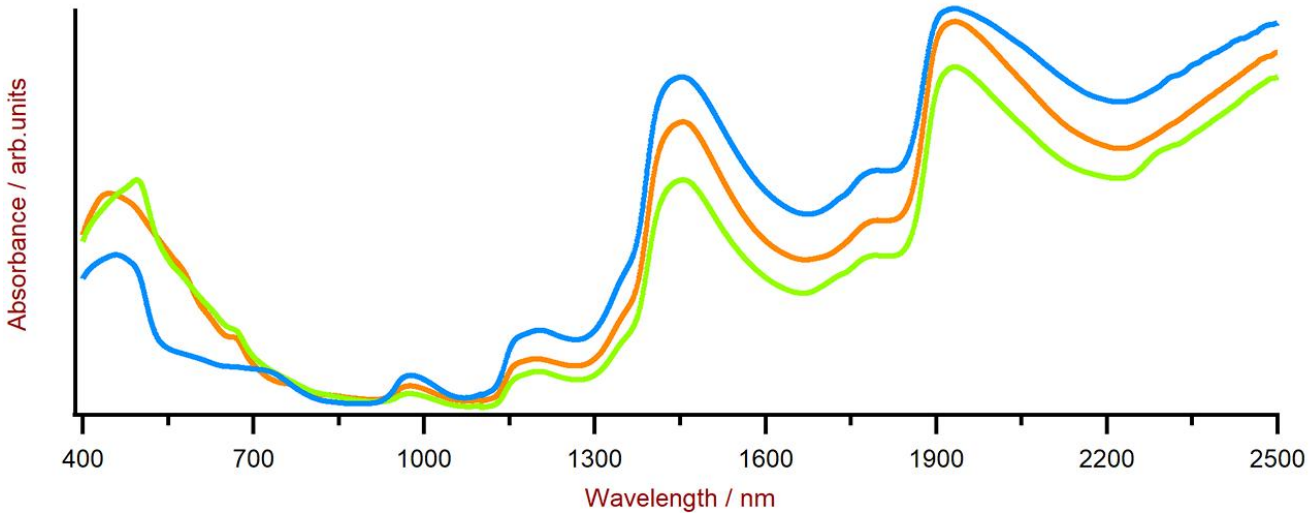
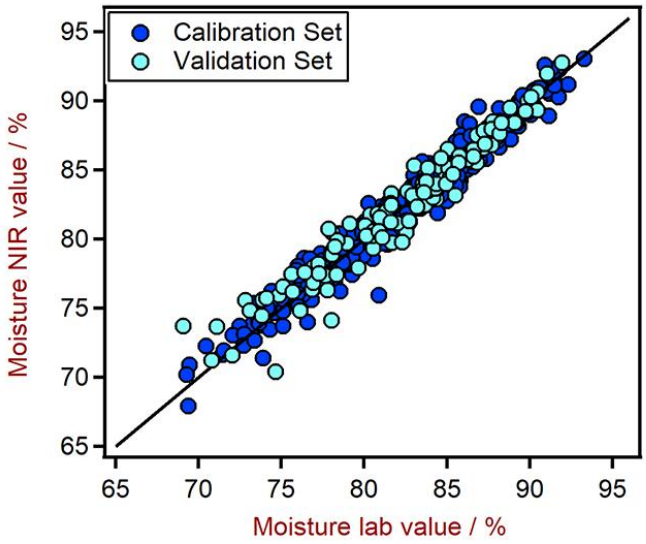
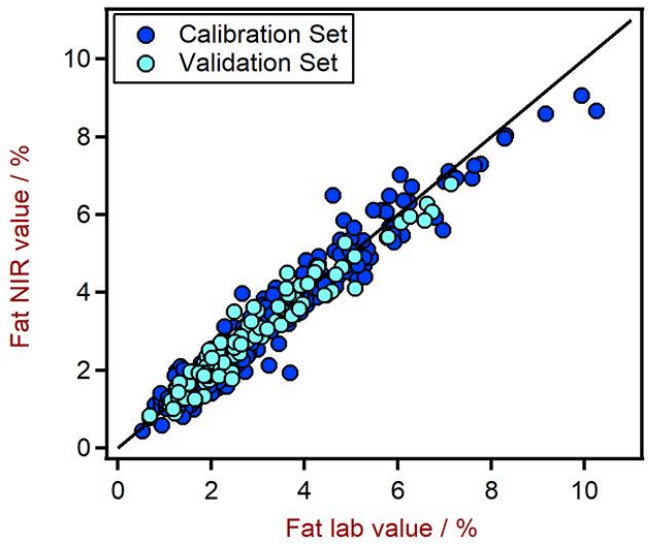


Figure 2. Selection of Vis-NIR spectra of human stool samples. Data was obtained with a DS2500 Solid Analyzer.



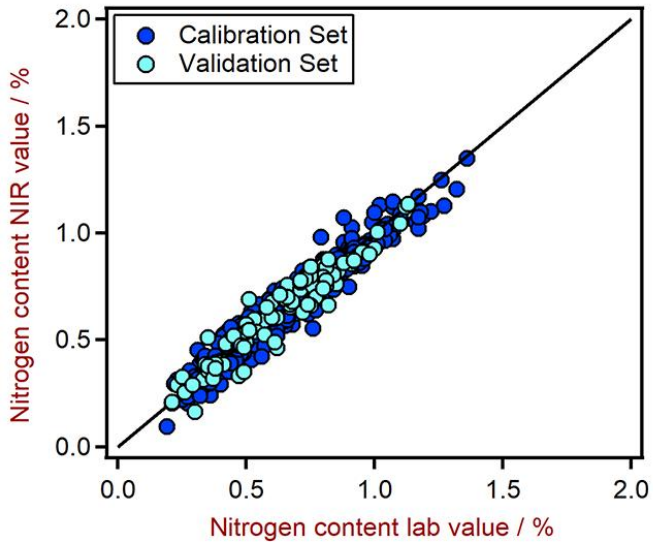
Figures of Merit	Value
R^2	0.962
Standard Error of Calibration	0.979%
Standard Error of Cross-Validation	1.103%
Standard Error of Prediction	1.266%

Figure 3.



Figures of Merit	Value
R^2	0.942
Standard Error of Calibration	0.3696%
Standard Error of Cross-Validation	0.3811%
Standard Error of Prediction	0.3523%

Figure 4.



Figures of Merit	Value
R^2	0.936
Standard Error of Calibration	0.057%
Standard Error of Cross-Validation	0.060%
Standard Error of Prediction	0.061%

Figure 5.

CONCLUSION

This Application Note shows the feasibility of NIR spectroscopy for the analysis of moisture, fat, and nitrogen content in human stool samples by NIRS, which can be conducted without chemicals or sample preparation.

CONTACT

Metrohm AG
Ionenstrasse
9100 Herisau

info@metrohm.com

CONFIGURATION

DS2500 Solid Analyzer

Robust near-infrared spectroscopy for quality control, not only in laboratories but also in production environments.

The DS2500 Analyzer is the tried and tested, flexible solution for routine analysis of solids, creams, and optionally also liquids along the entire production chain. Its robust design makes the DS2500 Analyzer resistant to dust, moisture, vibrations, and temperature fluctuations, which means that it is eminently suited for use in harsh production environments.

The DS2500 covers the full spectral range from 400 to 2500 nm and delivers accurate, reproducible results in less than one minute. The DS2500 Analyzer meets the demands of the pharmaceutical industry and supports users in their day-to-day routine tasks thanks to its simple operation.

Thanks to accessories tailored perfectly to the instrument, optimum results are achieved with every sample type, no matter how challenging it is, e.g. coarse-grained solids such as granulates or semi-solid samples such as creams. The MultiSample Cup can help improve productivity when measuring solids, as it enables automated measurements of series containing up to 9 samples.

DS2500 Holder

Holder for use with:

- Small sample vessels (6.7402.030)
- DS2500 Iris (6.7425.100)

Vision Air 2.0 Complete

Vision Air - Universal spectroscopy software.

Vision Air Complete is a modern and simple-to-operate software solution for use in a regulated environment.

Overview of the advantages of Vision Air:

- Individual software applications with adapted user interfaces ensure intuitive and simple operation
- Simple creation and maintenance of operating procedures
- SQL database for secure and simple data management

The Vision Air Complete version (66072208) includes all applications for quality assurance using Vis-NIR spectroscopy:

- Application for instrument and data management
- Application for method development
- Application for routine analysis

Additional Vision Air Complete solutions:

- 66072207 (Vision Air Network Complete)
- 66072209 (Vision Air Pharma Complete)
- 66072210 (Vision Air Pharma Network Complete)