

Application Note AN-NIR-146

Quality control of deodorant by near-infrared spectroscopy

Determination of pH, density, viscosity, and aluminum content in a few seconds

Personal care products like deodorants are tested using various time-consuming analytical methods during production as well as after the final product is made. This Application Note demonstrates how quality parameters such as viscosity, pH, density, and aluminum content in deodorant can be measured with near-infrared spectroscopy (NIRS) simultaneously and without any sample preparation. NIRS is a fast, chemical-free technology that is very user-friendly. NIR spectroscopy can be used either atline during the production process or offline in a quality control laboratory.

EXPERIMENTAL EQUIPMENT

Sixty samples of deodorant were measured in an OMNIS NIR Analyzer Solid (Figure 1). All measurements were performed in transflection mode (1000–2250 nm) using a 1 mm gap size large reflector and a transflection vessel.

Reference values of aluminum content were measured with titration (AN-T-228), pH values with a pH meter, and viscosity and density with a viscometer and density meter, respectively.

OMNIS Software was used for all data acquisition and prediction model development.



Figure 1. OMNIS NIR Analyzer Solid with transflection vessel and large reflector.

Table 1. Hardware and software equipment overview.

Equipment	Article number
OMNIS NIR Analyzer solid	2.1071.0010
Large reflector OMNIS NIR, 1mm	6.07402.940
Transflection vessel OMNIS NIR, 60mm	6.07402.260
OMNIS Stand-Alone license	6.06003.010
Software license Quant Development	6.06008.002

RESULT

The obtained NIR spectra of deodorant samples (Figure 2) were used to create prediction models for pH, viscosity, density, and aluminum content. The quality of the prediction models was evaluated using correlation diagrams which display a very high correlation between the NIR prediction and the reference values. The respective figures of merit (FOM) display the expected precision of a prediction during routine analysis (Figures 3–6).

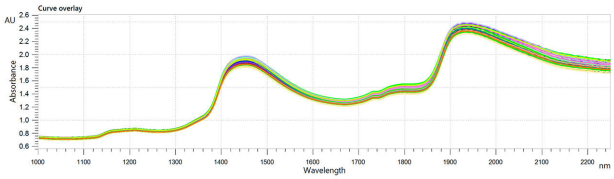


Figure 2. NIR spectra of various deodorant samples analyzed on an OMNIS NIR Analyzer Solid.

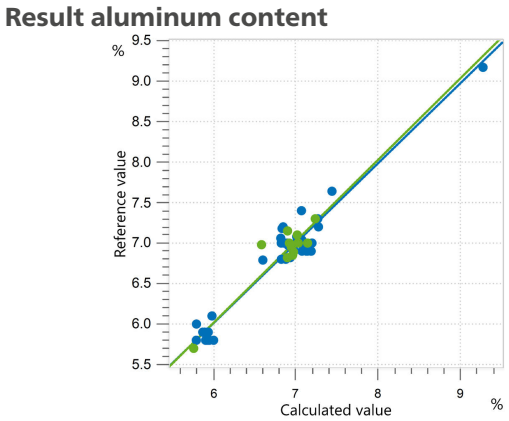


Figure 3. Correlation diagram and the respective figures of merit for the prediction of aluminum content in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. Titration was used as a reference method for the determination of aluminum in deodorant.

R^2	SEC (%)	SECV (%)	SEP (%)
0.908	0.12	0.16	0.14

Result density

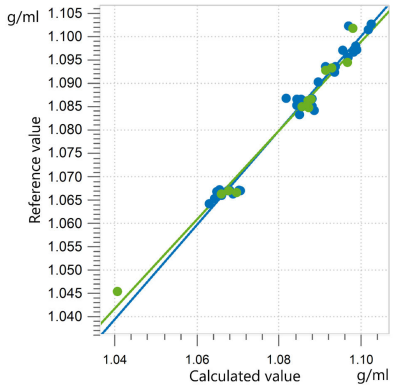


Figure 4. Correlation diagram and the respective figures of merit for the prediction of density in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. A density meter was used as the reference method.

R^2	SEC (g/mL)	SECV (g/mL)	SEP (g/mL)
0.979	0.0017	0.0020	0.0023

Result viscosity

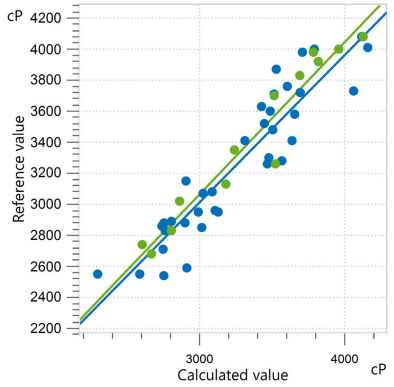


Figure 5. Correlation diagram and the respective figures of merit for the prediction of viscosity in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. Reference values were obtained with a viscometer.

R^2	SEC (cP)	SECV (cP)	SEP (cP)
0.941	147.05	176.05	133.74

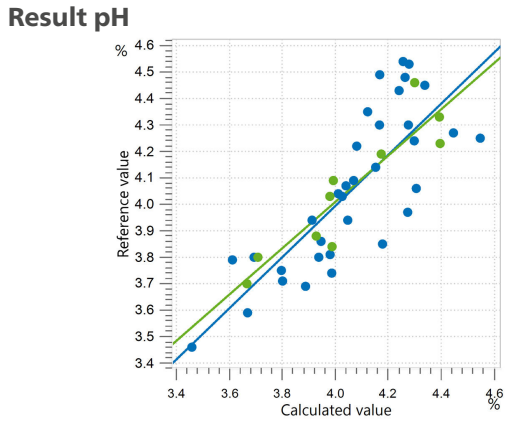


Figure 6. Correlation diagram and the respective figures of merit for the prediction of pH value in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. A pH meter was used as the reference method for the pH measurement of deodorant.

R^2	SEC	SECV	SEP
0.832	0.13	0.18	0.10

CONCLUSION

This Application Note shows the feasibility of using NIR spectroscopy for the analysis of aluminum content, pH, viscosity, and density in deodorants. With NIRS, the measurement can be conducted within seconds and requires no chemicals. This solution is easier, much faster than other conventional techniques, and can be used atline in several steps of the production chain or during quality control of the final product, saving manufacturers time and money.

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CONFIGURATION



OMNIS NIR Analyzer Solid

Near-infrared spectrometer for solid and viscous samples.

Developed and produced in accordance with Swiss quality standards, the OMNIS NIR Analyzer is the near-infrared spectroscopy (NIRS) solution for routine analysis along the entire production chain. Its application of the latest technologies and its integration in the modern OMNIS Software are reflected in its speed, operability and flexible utilization of this NIR spectrometer.

Overview of the advantages of the OMNIS NIR Analyzer Solid:

- Measurements of solids and viscous samples in less than 10 seconds
- Automated multi-position measurements for reproducible results, even with nonhomogeneous samples
- Simple integration in an automation system or link with additional analysis technologies (titration)
- Supports numerous sample vessels



Large reflector OMNIS NIR, 1 mm

Reflector with a gap size of 1 mm (optical path length of 2 mm) for the transflection measurement of liquids.

Suitable for transflection vessels (6.07402.260 and 6.7401.000).



Transflection vessel OMNIS NIR, 60 mm

Optically flat transflection vessel for the spectral measurement of liquids.

OMNIS
A WHOLE NEW LEVEL OF PERFORMANCE

OMNIS Stand-Alone license

Enables stand-alone operation of the OMNIS software on a WindowsTM computer.

Features:

- The license already includes one OMNIS instrument license.
- Must be activated via the Metrohm licensing portal.

OMNIS
A WHOLE NEW LEVEL OF PERFORMANCE

Software license Quant Development

Software license for the creation and editing of quantification models in a stand-alone OMNIS Software installation.