

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).

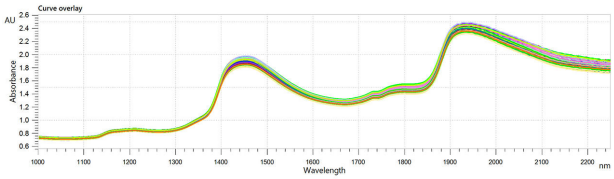


Figure 2. NIR spectra of various deodorant samples analyzed on an OMNIS NIR Analyzer Solid.

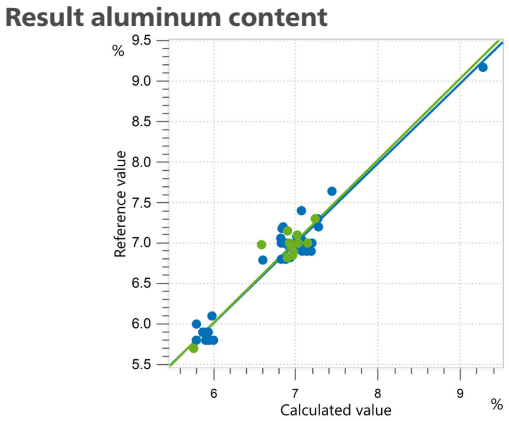


Figure 3. Correlation diagram and the respective figures of merit for the prediction of aluminum content in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. Titration was used as a reference method for the determination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

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

Result density

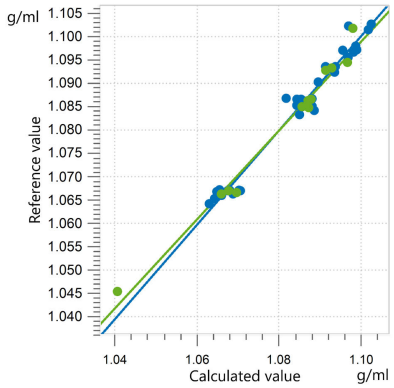


Figure 4. Correlation diagram and the respective figures of merit for the prediction of density in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. A density meter was used as the reference method.

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

Result viscosity

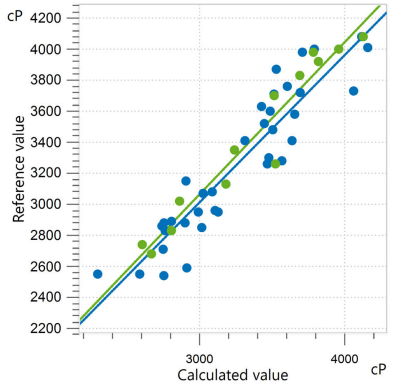


Figure 5. Correlation diagram and the respective figures of merit for the prediction of viscosity in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. Reference values were obtained with a viscometer.

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

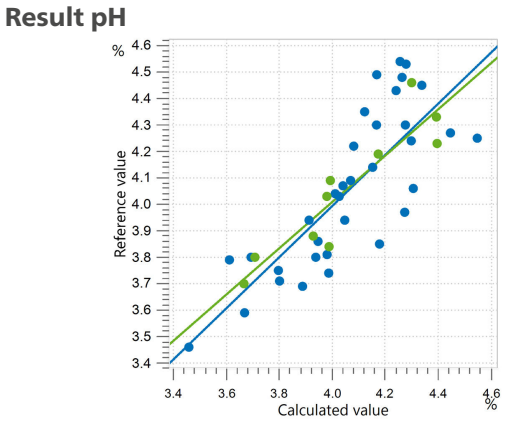


Figure 6. Correlation diagram and the respective figures of merit for the prediction of pH value in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. A pH meter was used as the reference method for the pH measurement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

CONTACT

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CONFIGURATION



OMNIS NIR Analyzer Solid

Nahinfrarotspektrometer für feste und viskose Proben.

Der OMNIS NIR Analyzer ist die nach Schweizer Qualitätsstandards entwickelte und produzierte Nahinfrarotspektroskopie(NIRS)-Lösung für die Routineanalyse entlang der gesamten Produktionskette. Die Anwendung neuester Technologien und die Integration in die moderne OMNIS Software spiegeln sich in der Geschwindigkeit, der Bedienbarkeit und dem flexiblen Einsatz dieser NIR-Spektrometer wider.

Die Vorteile des OMNIS NIR Analyzer Solid im Überblick:

- Messungen von Feststoffen und viskosen Proben in weniger als 10 Sekunden
- Automatisierte Mehrpositionenmessungen für reproduzierbare Resultate auch bei inhomogenen Proben
- Einfache Integration in ein Automationssystem oder Verknüpfung mit weiteren Analysentechniken (Titration)
- Unterstützung zahlreicher Probengefässe



Grosser Reflektor OMNIS NIR, 1 mm

Reflektor mit Spaltgrösse von 1 mm (optische Pfadlänge von 2 mm) für die Transflexionsmessung von Flüssigkeiten.

Passend für Transflexionsgefässe (6.07402.260 und 6.7401.000).



Transflexionsgefäss OMNIS NIR, 60 mm

Optisch planes Transflexionsgefäss für die spektrale Vermessung von Flüssigkeiten.

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OMNIS Stand-Alone Lizenz

Ermöglicht den Stand-Alone Betrieb der OMNIS Software auf einem WindowsTM Computer.

Merkmale:

- Die Lizenz enthält bereits eine OMNIS Geräte Lizenz.
- Muss über das Metrohm Lizenzierungsportal aktiviert werden.

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Softwarelizenz Quant Development

Softwarelizenz für die Erstellung und Bearbeitung von Quantifizierungsmodellen in einer Stand-Alone OMNIS Software Installation.