

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).

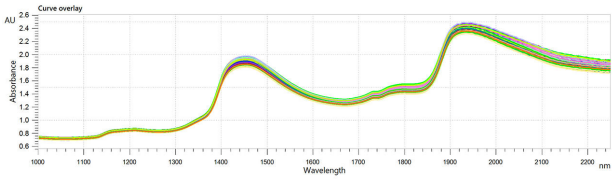


Figure 2. NIR spectra of various deodorant samples analyzed on an OMNIS NIR Analyzer Solid.

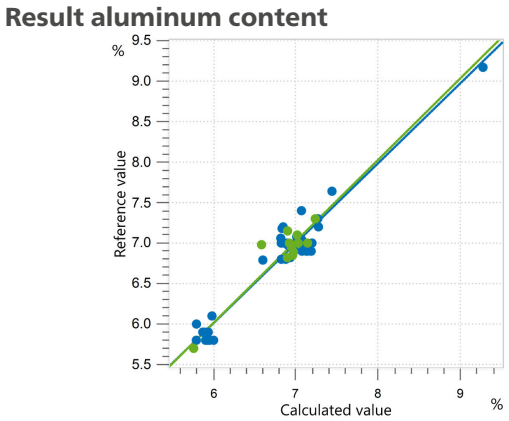


Figure 3. Correlation diagram and the respective figures of merit for the prediction of aluminum content in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. Titration was used as a reference method for the determination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

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

Result density

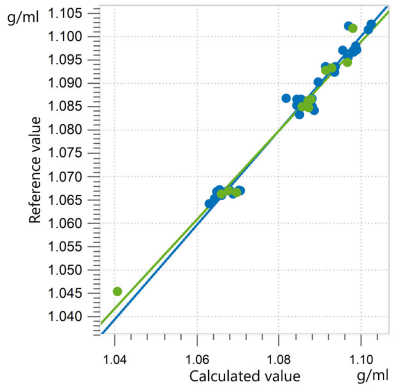


Figure 4. Correlation diagram and the respective figures of merit for the prediction of density in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. A density meter was used as the reference method.

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

Result viscosity

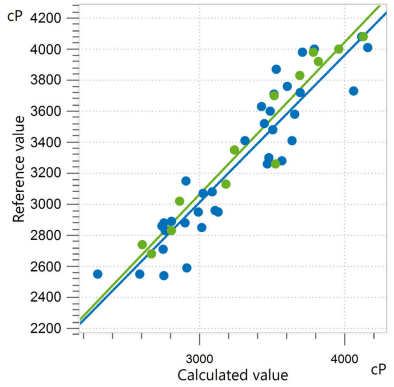


Figure 5. Correlation diagram and the respective figures of merit for the prediction of viscosity in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. Reference values were obtained with a viscometer.

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

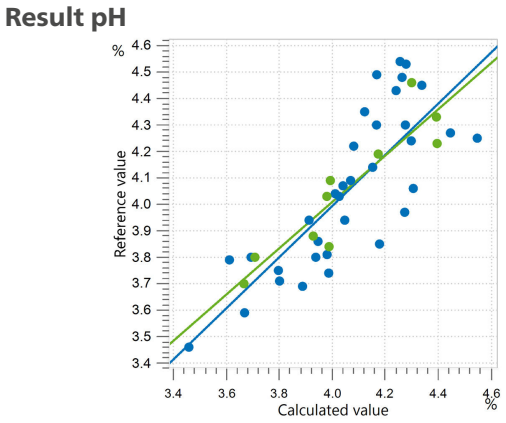


Figure 6. Correlation diagram and the respective figures of merit for the prediction of pH value in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. A pH meter was used as the reference method for the pH measurement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

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 chaine de fabrication. L'application des technologies les plus récentes et l'intégration dans le logiciel OMNIS moderne se reflètent dans la vitesse, la facilité du maniement et la flexibilité d'utilisation de ce spectromètre NIR.

Apercu 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



Grand réflecteur OMNIS NIR, 1 mm

Réflecteur avec une dimension de fente de 1 mm (longueur de chemin optique de 2 mm) pour la mesure par transflexion des liquides.

Compatible avec les récipients pour transflexion (6.07402.260 et 6.7401.000).



Récipient pour transflexion OMNIS NIRS, 60 mm

Récipient pour transflexion optiquement plan pour la mesure spectrale des liquides.

OMNIS
A WHOLE NEW LEVEL OF PERFORMANCE

Licence OMNIS autonome

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

Caractéristiques :

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

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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.