

Application Note AN-NIR-146

近红外光谱法在除臭剂质量控制中的应用

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).

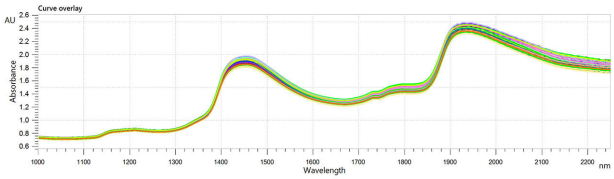


Figure 2. NIR spectra of various deodorant samples analyzed on an OMNIS NIR Analyzer Solid.

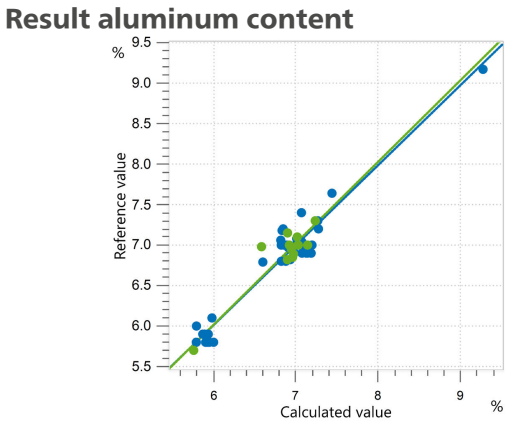


Figure 3. Correlation diagram and the respective figures of merit for the prediction of aluminum content in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. Titration was used as a reference method for the determination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

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

Result density

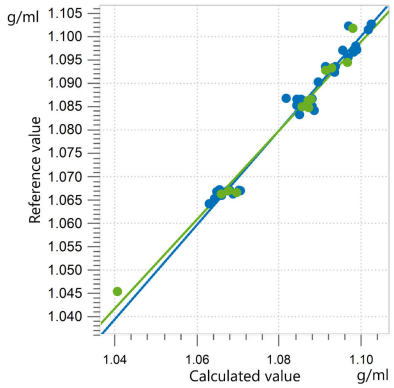


Figure 4. Correlation diagram and the respective figures of merit for the prediction of density in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. A density meter was used as the reference method.

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

Result viscosity

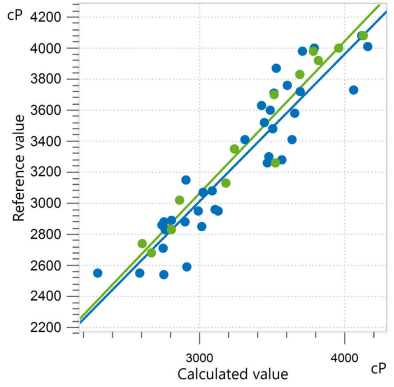


Figure 5. Correlation diagram and the respective figures of merit for the prediction of viscosity in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. Reference values were obtained with a viscometer.

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

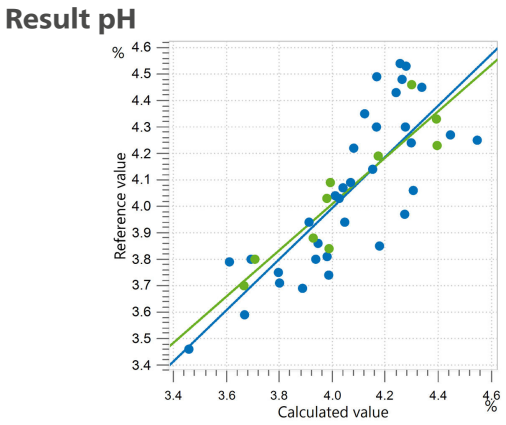


Figure 6. Correlation diagram and the respective figures of merit for the prediction of pH value in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. A pH meter was used as the reference method for the pH measurement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

Metrohm Taiwan Ltd.
開封街二段 46 號 5 樓
108 台北市
info@metrohm.com.tw

CONFIGURATION



OMNIS NIR Analyzer Solid

用于固体物质和粘稠样品的近红外光谱仪。

OMNIS NIR Analyzer 按照瑞士质量标准开发和制造,是用于整个生产链中常规分析的近红外光谱 (NIRS) 解决方案。最新技术的应用以及与现代 OMNIS Software 的集成,体现在这款 NIR 光谱仪的速度、操作性和灵活应用上。

OMNIS NIR Analyzer Solid 的优势概览:

- 固体物质和粘稠样品测量时间小于 10 秒
- 自动多位置测量,确保即使在非均质样品中也能获得可重现的结果
- 可轻松集成至自动系统,或与其它分析技术(滴定)联用
- 支持多种样品容器



OMNIS NIR1 mm

对液体进行透射反射测量的缝隙量 1 mm(光路长度 2 mm)的反射器。

适用于透射容器(6.07402.260 和 6.7401.000)。



OMNIS NIR60 mm

对液体进行光谱测量的光学平面透射反射器皿。



OMNIS

允许单机版 OMNIS 软件在一台 WindowsTM 计算机上运行。

特性:

- 该许可证已含有一份 OMNIS 设备许可证。
- 须通过万通许可授权平台进行激活。



Quant Development

用于在独立 OMNIS Software 安装套件中编写和编辑量化模型的软件许可证。