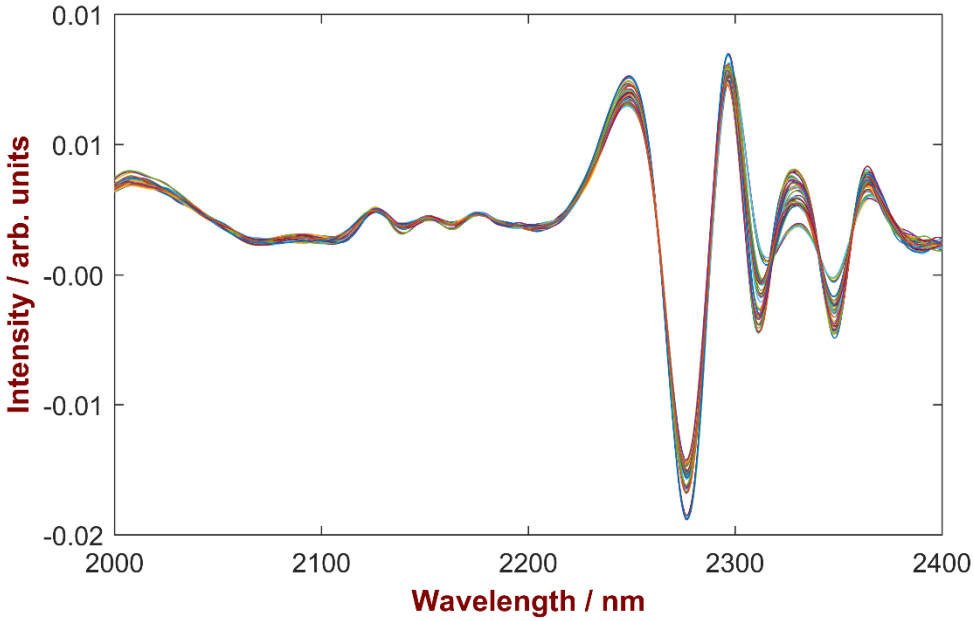
NIR Application Note NIR–069

Determination of sodium dodecyl sulfate in toothpaste using Vis-NIR spectroscopy



Rapid quality control for toothpaste is achieved by Metrohm`s Vis-NIR analyzers. Vis-NIR technology offers significant advantages compared to standard reference analysis. It is a cost effective and safe method because no hazardous chemicals are used.

Metrohm NIRSystems

Method description

Introduction

Toothpaste is the product of daily use, which needs to fulfill multiple quality requirements in order to ensure safe usage of this good. Parameters, which usually need to be determined, are content of additives, color, and content of active ingredients, if such components are present in the product. The determination of these parameters often requires sample preparation, complex analytical techniques, and chemicals. Alternatively, near-infrared spectroscopy (NIR) can be used for the determination of various quality parameters with minimal running costs. When using Vis-NIR, the sample can be analyzed without sample preparation and without cost-intensive chemicals. This enables significant time and costs savings.

This Application Note exemplifies the use of Vis-NIR for quality control of toothpaste. Vis-NIR was used for the determination of the sodium lauryl sulfate content (SLS, also known as sodium dodecyl sulfate (SDS)). This compound is often added as surfactant. The classical way of the analysis involves HPLC, which requires cost intensive chemicals as mobile phase in contrast to NIR.

Experimental

37 samples provided by a customer were used in the present study. Based on supplied reference values, all samples were grouped into six segments. The main difference within each group is attributed to content variation of further components i.e. flavoring agents. The spectra were collected in transflection mode on a NIRS XDS RapidContent Analyzer over the full wavelength range (400–2500 nm). The software package Vision Air 2.0 Complete was used for data acquisition, data management, and development of the quantification method. **Tab. 1/Fig. 1** lists the used equipment.

Tab. 1: Used equipment and software.

Equipment	Metrohm number
NIRS XDS RapidContent Analyzer	2.921.1110
NIRS Liquid Sample Kit Transflection	6.7400.010
Vision Air 2.0 Complete	6.6072.208

Fig. 1: The NIRS XDS RapidContent Analyzer was used for spectral data acquisition over the full range from 400 to 2500 nm.

Results

Fig. 2 shows Vis-NIR spectra of the provided samples. Redundant spectral information was excluded from the method development by the selection of analyte specific wavelength ranges combined with dedicated spectral pre-treatments. An example of such procedure is shown in **Fig. 3**, which displays spectra pretreated with a 2nd derivative.

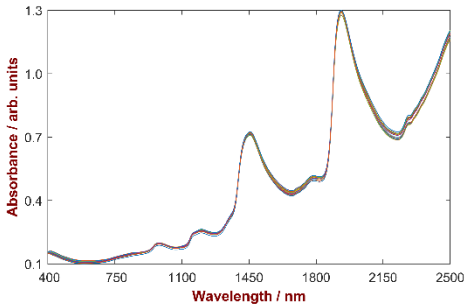


Fig. 2: Raw Vis-NIR spectra of 37 toothpaste samples over the full wavelength range.

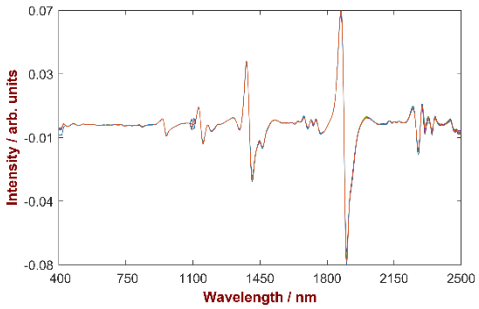


Fig. 3: Spectra pretreated with 2nd derivative over the full wavelength range.

The correlation plot (**Fig. 4**) shows high correlation between the SLS content determined by reference analytical method (x-axis) and the predicted values (y-axis) from Vis-NIR spectroscopy. Furthermore very low

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standard errors of calibration and cross-validation (SEC, SECV) were achieved (Tab. 2).

Tab. 2: Results of the quantitative method development for SLS content.

Range	0.5–1.8%
Regression model	PLS, 6 factors
Pre-treatment	2nd derivative
Wavelength ranges	1190–1298 nm 1626–1804 nm
R^2	0.996
SEC	0.021%
SECV	0.026%

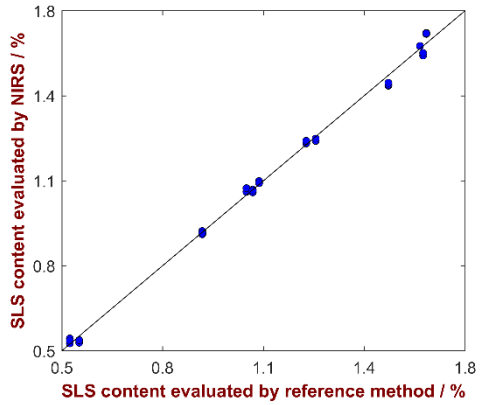

Fig. 4: Correlation plot of the SLS content predicted by NIRS versus the reference values. A high correlation is observable.

Summary

The combination of NIRS XDS RapidContent Analyzer and Vision Air 2.0 Complete is an ideal tool for the quality control of toothpaste. As an example this present Application Note demonstrates the determination of SLS content in toothpaste. For further quality parameters such as moisture content, color, or content of other additives i.e. sodium laureth sulfate (SLES), similar NIR methods can be developed.

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