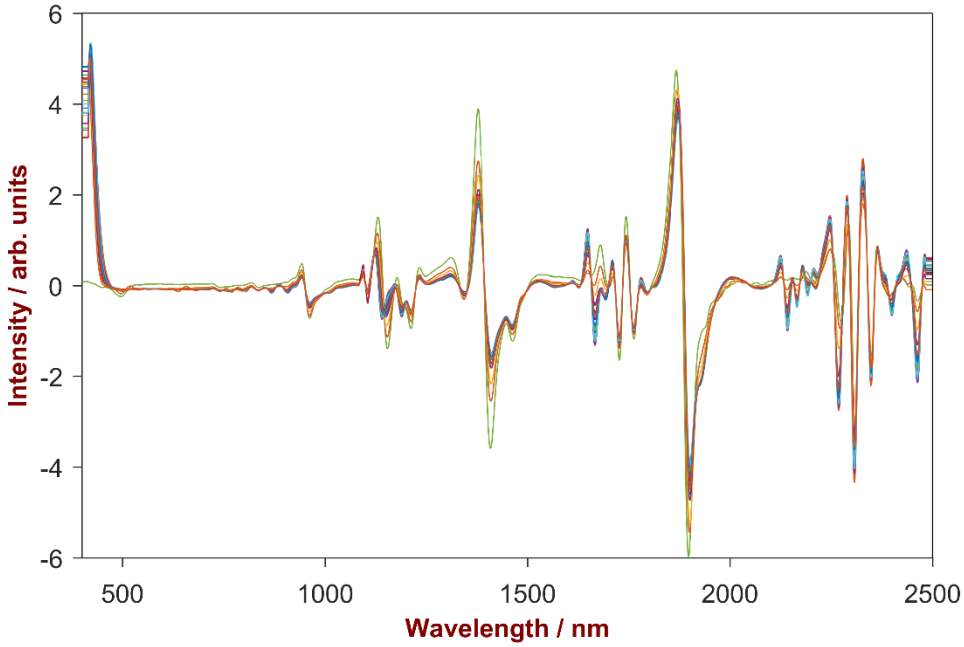
NIR Application Note NIR-062

Determination of sun protection factor in creams using visible near-infrared spectroscopy



This Application Note shows that visible near-infrared spectroscopy (Vis-NIRS) can determine the sun protection factor (SPF) of sunscreen products. Thanks to measurement durations of less than 30 seconds, NIR spectroscopy is ideally suited for rapid quality control.

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Method description

Introduction

Every year, over 2 million people are diagnosed with skin cancer, mostly on the areas of the body that are more frequently exposed to the sun. The harmful effects of solar radiation are predominantly caused by ultraviolet (UV)-B radiation, which is not completely filtered out by the ozone layer. Due to these facts, sunscreen substances are now incorporated into everyday products such as creams, moisturizers, and lotions. The efficiency of a sunscreen is expressed by the sun protection factor (SPF), which is a measure of the amount of UV radiation required to produce sunburn on protected skin relative to the amount of radiation required to produce sunburn on unprotected skin. The higher the SPF, the more effective the product is in preventing skin damage. Organic or inorganic chemicalfands are used as active ingredients, which attenuate the transmission of UV-rays to the skin. To provide the best protection across the whole UV wavelength range, a combination of different sunscreen filters is needed. However, sunscreen regulations vary from country to country leading to different sunscreen compositions across the world. Due to these facts, the determination of the SPF is important the ensure product quality. Commonly, UV-spectrophotometry and chromatography are the methods to determine SPF, however these techniques require sample preparation steps such as dilution and filtering before analysis. In contrast, visible near-infrared spectroscopy (NIRS) is a fast, non-destructive analysis method, which makes sample pretreatment redundant. The market for sunscreens is constantly evolving, requiring fast methods to guarantee quality control for personal care products.

Experimental

In this study, 14 specific sunscreen samples were provided by the customer. The sun protection factor ranged from 10 to 50. For sample analysis, approximately 1 g of cream was applied on the DS2500 Slurry Cup. The Gold diffuse reflector with 1mm path length was pressed on the sample to ensure even distribution and a constant path length. The Slurry Cup was placed in the Metrohm NIRS DS2500 Analyzer and the spectra were acquired in transflection mode over the full wavelength range from 400 nm to 2500 nm. (**Tab. 1, Fig. 1, Fig. 2**). After each measurement, both the gold stamp and the Slurry Cup were cleaned using paper towels. For data acquisition, data management, and developing the quantification method the software package Vision Air 2.0 Complete was used.

Tab. 1: Used equipment and software

Equipment	Metrohm order code
NIRS DS2500 Analyzer	2.922.0010
DS2500 Slurry Cup	6.7490.430
NIRS Gold diffuse reflectors, Gold 1 mm	6.7420.000
Vision Air 2.0 Complete	6.6072.208

Fig. 1: The Metrohm NIRS DS2500 Analyzer was used for spectral data acquisition over the full range from 400 to 2500 nm.

Fig. 2: Used accessories: DS2500 Slurry Cup and 1mm Gold Diffuse Reflector.

The spectra were pre-treated using 2nd derivative, standard normal variate (SNV), and a Partial Least Squares Regression (PLS) was performed over the entire spectral range.

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Results and discussion

Fig. 3 shows the Vis-NIR spectra of all analyzed samples, for which the correlation between absorbance change and SPF change is obvious. **Fig. 4** shows the sample spectra after 2nd derivative and SNV pretreatment.

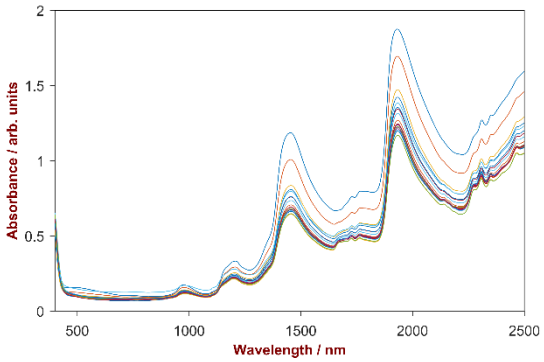

Fig. 3: Vis-NIR spectra of 12 sunscreen samples with differing SPF from 10 to 50.

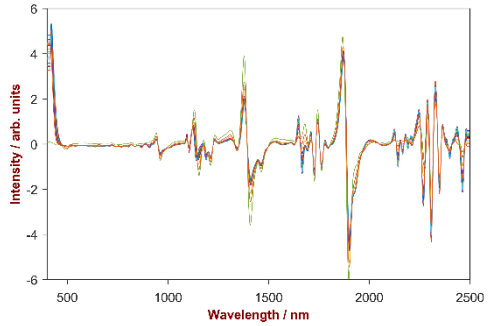

Fig. 4: 2- derivative and SNV pre-treatment of sample spectra.

Internal cross-validation was applied on the data set to verify the performance of the derived quantitative model. A high correlation between the reference values provided by the costumer (x-axis) and the predicted values (y-axis) from Vis-NIR spectroscopy was achieved, see **Fig. 5**. Furthermore, the results show low standard errors of calibration and cross-validation (SEC, SECV).

Tab. 2: Results of the quantitative method development

SPF range	10–50
Method	PLS
Number of factors	4
Wavelength range	400–2500 nm
Pretreatment	2nd derivative, SNV
SEC	1.30
SECV	2.20
R^2	0.9932

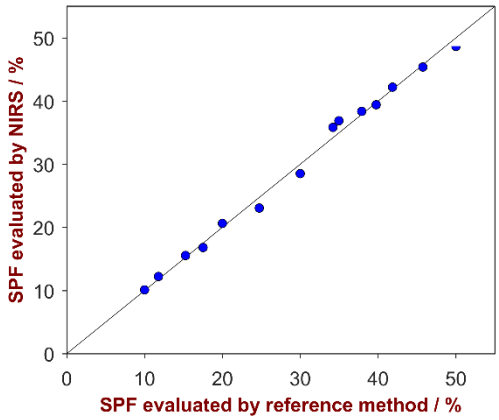

Fig. 5: Correlation plot of SPF predicted by Vis-NIRS versus the reference values. A high correlation is observable.

Summary

This Application note shows that Vis-NIR spectroscopy can be used to accurately determine SPF in creams in less than a minute with no sample preparation needed. The samples were successfully analyzed using a Metrohm NIRS DS2500 Analyzer. Therefore, near-infrared spectroscopy offers unique advantages over traditional analysis methods: it generates reliable results within seconds, but it does not need any sample preparation and it does not create chemical waste. After an easy cleaning process, the accessories are available for further measurements. Furthermore, this technique can be utilized not only for the determination of SPF but also for simultaneous determination of further quality parameters such as moisture and additive content.

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