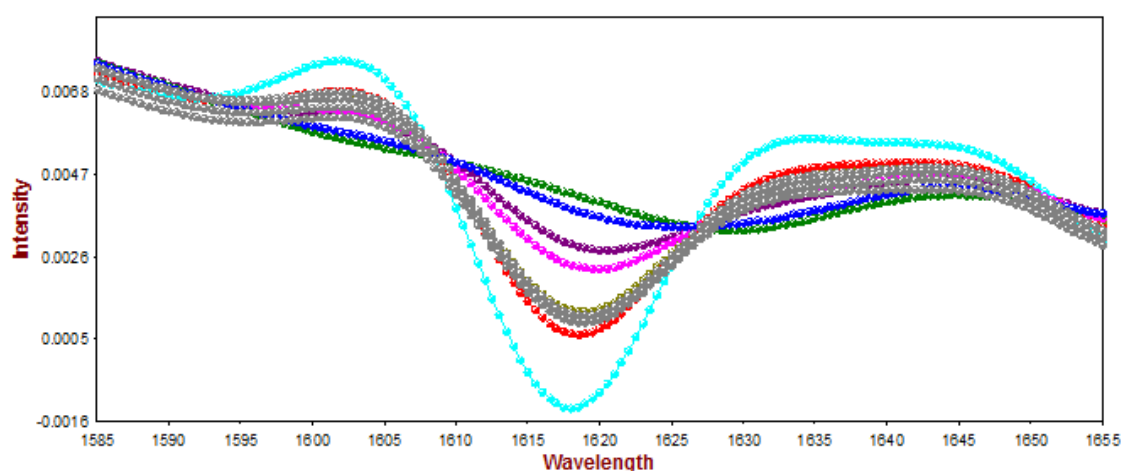


Quality control of an active ingredient in hair creams using near-infrared spectroscopy



Visible Near-infrared (Vis-NIR) spectroscopy is a valuable chemical analysis tool that can be used to determine quality parameters of hair creams. A qualitative method was developed in order to allow a fast out-of-spec analyses of an active antibacterial ingredient.

Method description

Introduction

Hair creams are cosmetic products used for styling, protecting and refining the look and feel of hair. To obtain the desired properties of hair creams many different ingredients are in interplay, which require that concentrations of each constituent is added precisely.

Reference methods to determine the active ingredients in hair creams are LC-MS or LC-MS/MS. However due to the complex matrix, single compounds need to be chemically extracted prior to the analysis. This has the drawback of generating waste and being a time consuming procedure of approximately 30 minutes.

In contrast, with the Vis-NIR spectroscopy technology sample preparation steps can be omitted, increasing the speed of analysis significantly. This application note presents the experimental procedure and the obtained results for an analysis performed with Vis-NIR spectroscopy to qualify the concentration amount of an anti-bacterial ingredient in hair creams.

Experimental

For this feasibility study a total of 14 hair cream samples and one reference sample were used. The concentration of the active ingredient (AI) ranged between 0.0% and 3.1%. The reference sample consisted of pure AI to identify inherent regions in the spectra. The analysis was performed with the Metrohm DS2500 using approximately 3 g of hair cream per measurement positioned on the Metrohm NIRS SlurryCup (see Figure 1). To improve the signal output all measurement were performed in transfection over the full wavelength range using Metrohm gold reflectors. The data acquisition and method development was performed with the Vision Air Complete software.



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

Results

Figure 2 displays the obtained spectra. A qualification model was developed by conducting a 2nd derivative pretreatment to correct for multiplicative effects and using a maximum distance in wavelength space algorithm over the two inherent region of the pure AI (1554-1750 nm and 2210-2340 nm). The set quality acceptance criteria for the model were defined to concentration ranges between 1.8% and 2.5%.

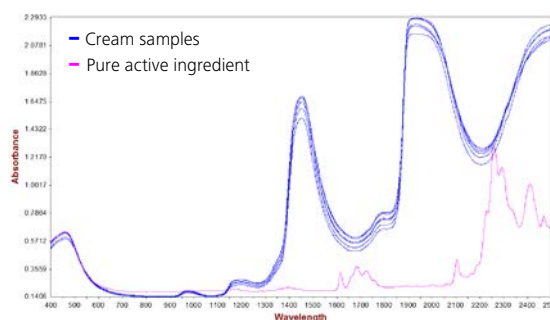


Fig. 2: Spectra of hair cream samples with various concentrations of active ingredient (0.0% to 3.1%). The pure AI is displayed in pink, which was used to specify bands of interest for the active ingredient (1550 nm - 1750 nm and 2210 nm - 2340 nm).

A testing procedure performed according to the defined limits performed satisfyingly, displaying hair cream samples with AI concentration ranges of 1.8% to 2.5% as within specification and samples with lower and higher AI concentration as out of specification.

Summary

The results obtained from this feasibility study show that Vis-NIR spectroscopy is a suitable technology for the qualification of active ingredients in hair creams. With the help of the hereby developed quality prediction model, a preparation and chemical free analysis can be performed to detect easily out-of-specification batches.

Tab.1: Used equipment and software.

Equipment	Order code
NIRS DS2500 Analyzer	2.922.0010
NIRS SlurryCup	6.7490.430
NIRS Diffuse Reflectors, Gold 2 mm	6.7420.020
Vision Air 2.0 Complete	6.6072.208