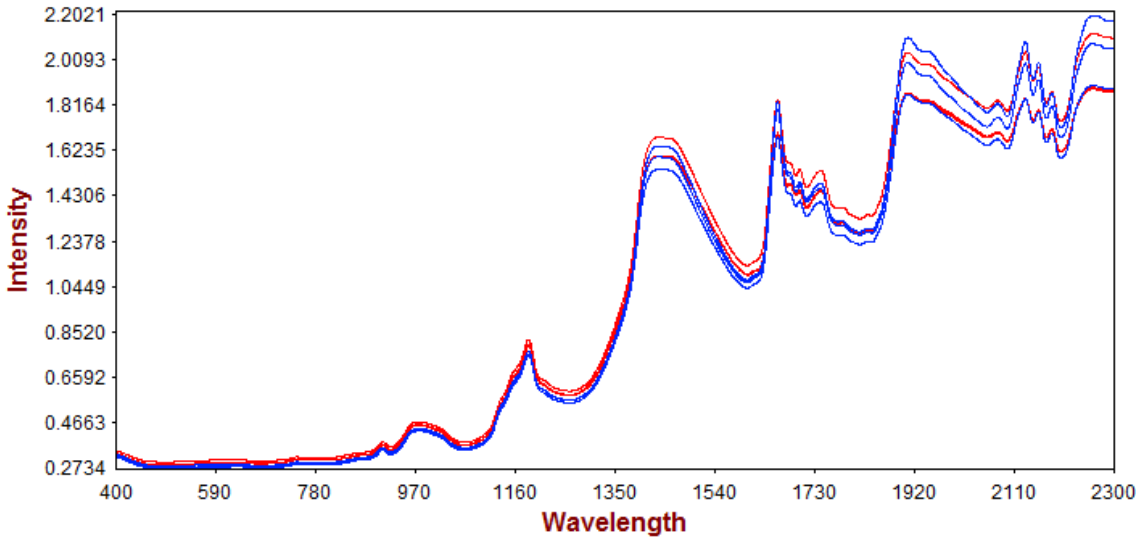
NIR Application Note NIR–46

Qualification of droplet morphology in hair conditioner by Vis-NIR spectroscopy



Vis-NIR spectroscopy is used to determine the droplet morphology in hair conditioner. This Application Note shows that near-infrared (NIR) spectroscopy can be used to distinguish between unprocessed and processed hair conditioner and to qualify quality parameters such as the droplet size.

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Method description

Introduction

Hair conditioners are used to enrich the look and refine the feel of hair. These cosmetic products are composed of water and hydrophobic ingredients, thus forming an emulsion with a specified droplet size. The droplet size varies throughout different processing steps. This parameter is of great importance, since this affects the efficacy of the conditioner. Therefore, the droplet size is a quality parameter and needs to be determined on a regular base.
There are several ways to determine the droplet size. This can be achieved mainly by microscopy or laser diffraction particle sizing techniques.
Vis-NIR spectroscopy is a fast alternative quality analytics technique that can be used as well to determine droplet sizes.

Experimental

Two products were provided by the customer. One contained the unprocessed hair conditioner (A), the other contained the processed conditioner (B). In both products, droplet size of the formulation ranged from 5-20 µm and 5-50 µm, respectively.
The spectral data acquisition was performed over the full range of 400 nm to 2500 nm using the Metrohm NIRS DS2500 Analyzer (see Figure 1) with variable spot size. The samples were filled into disposable vials and analyzed in diffuse reflectance mode.

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

Tab.1: Used equipment and software.

Equipment	Order code
NIRS DS2500 Analyzer	2.922.0010
NIRS DS2500 Iris	6.7425.100
Vision Air 2.0 Complete	6.6072.208

The identification and qualification methods were developed based on parameters seen in Tables 2 and 3 using the Vision Air Complete software.

Tab. 2: Identify method parameters.

Method	Correlation in Wavelength Space
Wavelength regions	416-1080 nm, 1120-2480 nm
Pre-treatments	2nd derivative, Segment=10.0 nm, Gap=0.0 nm

Tab. 3: Qualification method parameters.

Method	Maximum Distance in Wavelength Space
Regions	1380-1404 nm
Pre-treatments	2nd derivative, Segment=10.0 nm, Gap=0.0 nm

The purpose of the identification method is to distinguish whether an unknown sample is an unprocessed (A) or a processed (B) hair conditioner. If the sample could be allocated to one of those products, the qualification step determines whether the droplet size either exceeds or is below the threshold size.
The methods were validated by using an independent set of samples. The predefined identification and qualification analysis was completed automatically by the Vision Air software after each measurement and results were given in seconds.

Results and discussion

Figure 2 shows the raw spectra of both products (A) in red and (B) in blue. By computation of the 2nd derivatives of the spectra, spectral variations can be distinguished independent of baseline shifts.

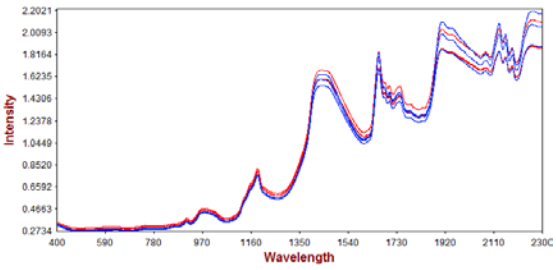

Fig. 2: Raw spectra of the unprocessed (red) and processed (blue) products.

Method description

In Figure 3, the 2nd derivative spectra are shown. The products (A) and (B) can be distinguished clearly, allowing identification. The spectral variation within a product arises due to different droplet sizes. This variation is used for the qualification of the different droplet sizes.

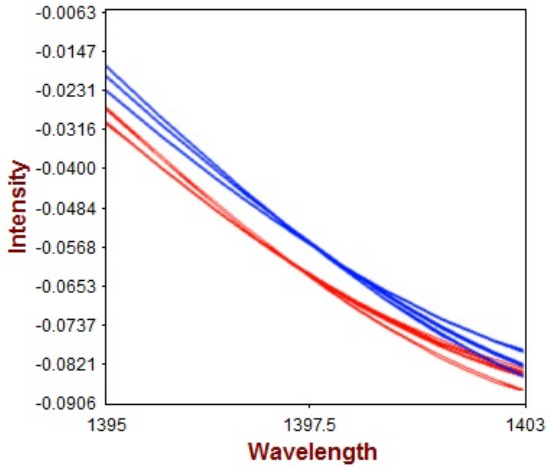

Fig. 3: 2nd derivative spectra of the unprocessed (red) and the processed (blue) product. The spectral variations observed within the products arise due to different droplet sizes.

As expected, the unprocessed samples passed the identification step (since they are the correct formulation), but failed qualification (since the predicted droplet size clearly exceeded the limits). However, the processed samples both passed the identification and qualification step, showing reliable differentiation between out-of-specification products and such with desired quality.

Summary

In this feasibility study, Vis NIR methods were developed to identify formulation and to qualify the droplet morphology. The primary goal was to distinguish between two different intermediate products with droplet sizes ranging from 5-50 microns and 5-20 microns, respectively. Qualitative models were developed based on the collected spectra. The models were tested with an external validation and were consistently able to distinguish between the two different types of sample (A and B). It could be shown that Vis NIR spectroscopy is an excellent method to relieve the primary methods.

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