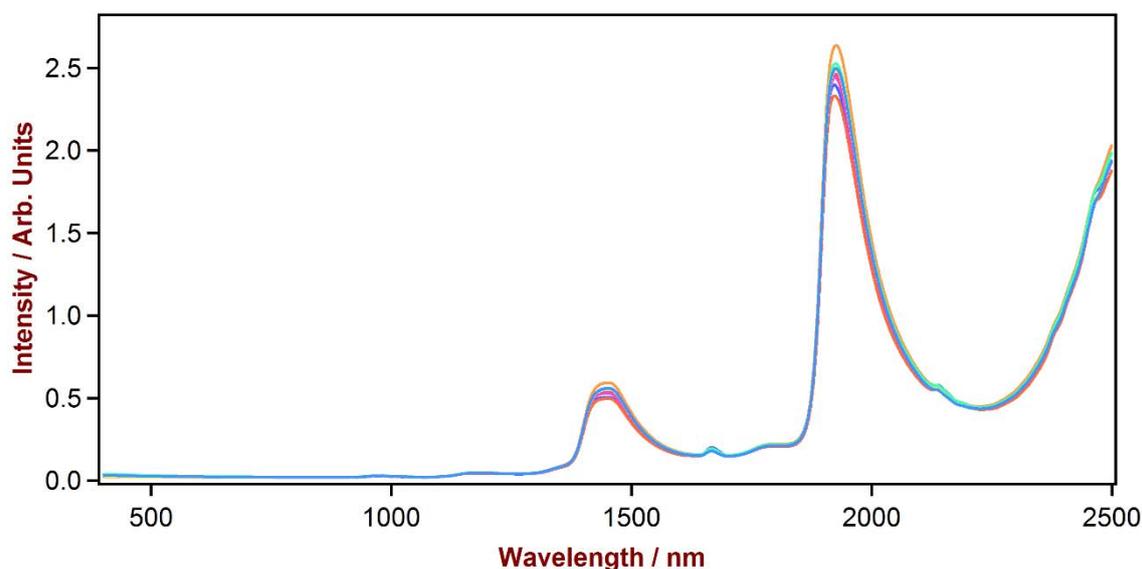


Quantification of active ingredients in shampoo using near-infrared spectroscopy (NIR)



Near-infrared spectroscopy (NIRS) was used in a preliminary study as a fast and accurate method for the quantification of different preservatives and active ingredients in liquid shampoo. This Application Note shows how this analytical method allows the simultaneous determination of several constituents in shampoo in a single measurement.

Method description

Introduction

Shampoo hair care products are not only used for cleaning, but also for refining the look and feel of hair. Shampoos are complex multi-constituent mixtures, containing detergents, preservatives and active substances, such as anti-dandruff actives. For the quantification of the ingredients, HPLC is generally the method of choice. However, this primary method can be time consuming, requires chemicals and generates wastes. Furthermore, expensive chromatography columns need to be replaced when separation criteria are not met anymore and/or retention times differ significantly from reference values.

In contrast, near-infrared spectroscopy (NIRS) is an alternative method that does not have these drawbacks. As shown herein, it is excellently suited to perform non-destructive quantitative multi-constituent analyses of shampoo hair care products in a matter of seconds requiring no additional chemicals like solvents or standards.

Experimental

In this feasibility study, shampoo samples were tested for their content of one preservative A and two active ingredients B and C. Raw-materials and crude shampoo were made available for preparation of in total 48 samples with differing concentrations of A, B and C. Spectra were acquired using a Metrohm NIRS XDS RapidLiquid Analyzer with NIRS Quartz Cuvette Open Top 0.5 mm and the associated NIRS Spacer for Quartz Cuvette 0.5 mm. Data acquisition and quantification method development was performed using the software package Vision Air 2.0 Complete (see Table 1 and Figure 1).

Tab. 1: Used equipment for this shampoo application.

Equipment	Metrohm order code
NIRS XDS RapidLiquid Analyzer	2.921.1410
NIRS Quartz Cuvette Open Top 0.5 mm	6.7401.110
NIRS Spacer for Quartz Cuvette 0.5 mm	6.7403.110
Vision Air 2.0 Complete	6.6072.208



Fig. 1: The Metrohm NIRS XDS RapidLiquid Analyzer with used cuvettes and cuvette spacer.

Various spectral regions were taken into account depending on the analyte. A partial least squares regression (PLS) was performed using 2nd derivative as data pre-treatment.

Preservative A

For the quantification of the preservative A in shampoo, 4 factors were used, resulting in a Standard Error of Calibration (SEC) of 0.111% over the typical range of 0-4% (see Figure 2).

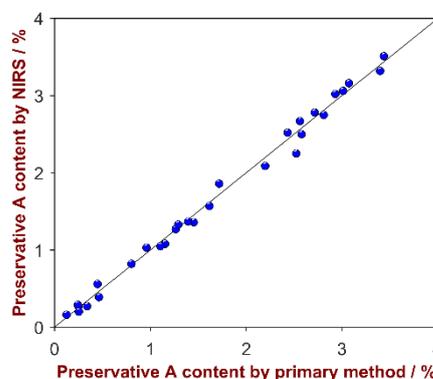


Fig. 2: Correlation plot of the predicted values by NIRS versus the laboratory values of the preservative A.

Method description

Active ingredient B

For the quantification of the active ingredient B, 4 factors were used, and yielding a SEC of 0.147% over the range of 0-4% (see Figure 3).

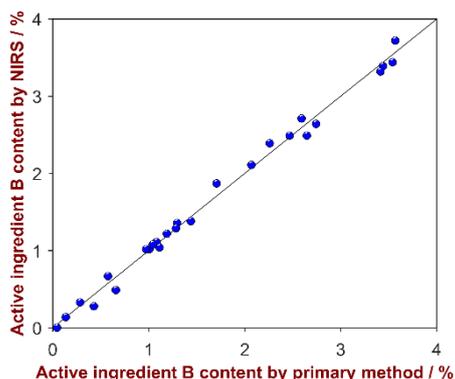


Fig. 3: Correlation plot of the predicted values by NIRS versus the laboratory values of the active ingredient B.

Results

This application note shows that Vis-NIR spectroscopy can be used for simultaneous determination of different ingredients in shampoo such as a preservative and two active ingredients with time to results of less than one minute. As the calculated standard errors are small, near-infrared spectroscopy is an excellent analysis method to detect out-of-specification batches. Short measurement times, the possibility to determine several constituents simultaneously and the fact that no further chemicals are required make this method an economic choice compared to other analysis methods.

Active ingredient C

For quantitative analysis of the active ingredient C, 2 factors were used. The SEC was found to be 0.026% over the typical range of 0-1%. The correlation plot is displayed in Figure 4.

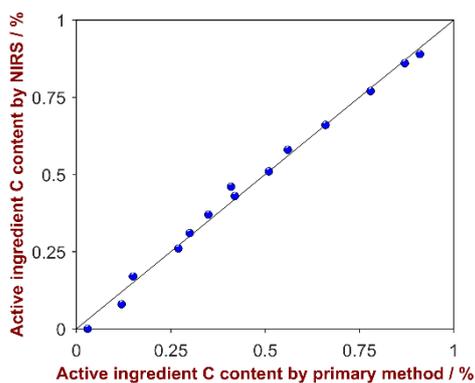


Fig. 4: Correlation plot of the predicted values by NIRS versus the laboratory values of the active ingredient C.