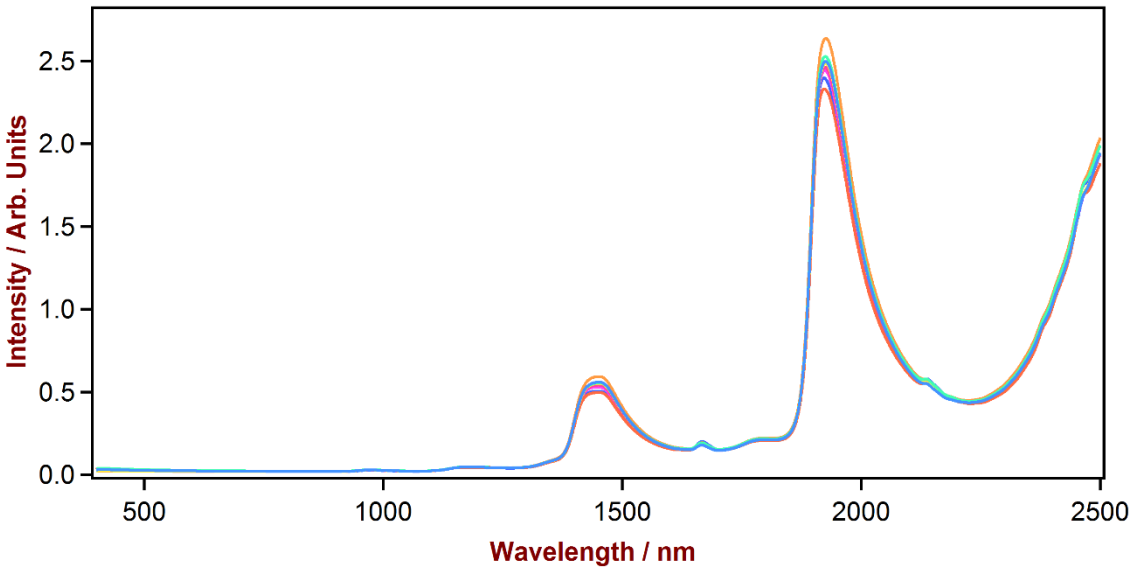
Near-infrared spectroscopy Application Note NIR–49

Quantification of TAED, PCS and protease enzyme in detergents using Near-infrared spectroscopy



Visible Near-infrared (Vis-NIR) spectroscopy can be used as a fast and accurate analytical method for the quantification of different analytes and active ingredients in detergents, such as Tetraacetylethylendiamin (TAED), Sodium percarbonate (PCS), and enzymes. This Application Note shows how NIRS can be used for multi-constituent analyses in detergents in a single measurement.

Metrohm NIRSystems

Method description

Introduction

Detergents are products with cleaning properties. The complexity of the formulation of detergents depends heavily on the application field. Laundry detergents contain water softeners, surfactants, bleachers as well as enzymes. In order to guarantee claimed cleaning power at all times, the products are analyzed as part of final product quality controls: only if the contents of ingredients meet the specifications, the products can be released.
The quantification of the ingredients is performed in quality control laboratories, using primary methods such as HPLC. Therefore, sample preparation is necessary, such as extraction and/or dilution steps. This leads to time consumption, consumption of chemicals and production of wastes. Chromatography columns need to be replaced when separation criteria are not met and/or retention times differ heavily from reference values.
In contrast, near-infrared spectroscopy (NIRS) is able to perform non-destructive quantitative multi-constituent analyses of detergent products in a matter of seconds without any additional chemicals like solvents or standards.

Experimental

In this study, laundry detergent samples were tested for their content of two active bleaching ingredients TAED and PCS, such as a common protease enzyme. From 8 samples, spectra were acquired using the Metrohm NIRS DS2500 Analyzer in combination with the Large Sample Cup in pure reflectance mode. This accessory allows spectral data acquisition at multiple points of the Sample Cup in order to capture and average inhomogeneity. For data acquisition and method development, the software Vision Air 2.0 Complete was used (see Table 1 and Figure 1).

Tab. 1: Used equipment and software for this application.

Equipment	Metrohm order code
NIRS DS2500 Analyzer	2.921.1410
NIRS DS2500 Large Sample Cup	6.7402.050
Vision Air 2.0 Complete	6.6072.208

For all quantification methods the spectra were derived by 2nd order and normalized using Standard Normal Variate (SNV). The wavelength region 1120-2300 nm was taken into account for the Partial Least Squares (PLS) algorithm.

Fig. 1: The Metrohm NIRS DS2500 Analyzer with used DS2500 Large Sample Cup.

TAED:

For the quantification of TAED, 2 factors were used with a Standard Error of Calibration (SEC) of 0.32% and a Standard Error of Cross Validation (SECV) of 0.37% over the range of 0-10% (see Figure 2). These figures of merit show clear applicability of Vis-NIR spectroscopy to determine the TAED content in detergents.

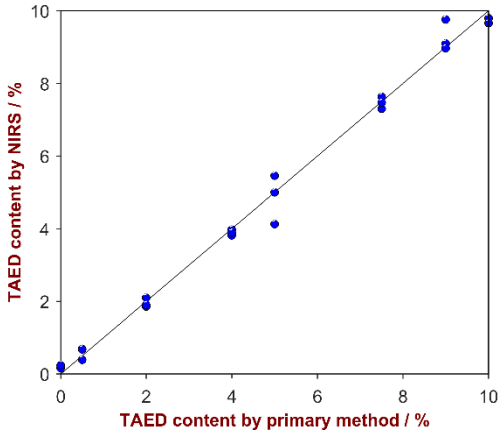


Fig. 2: Correlation plot of the predicted values by NIRS versus the laboratory values of TAED.

PCS:

For the quantification of PCS, 4 factors were used and yielded to SEC of 0.19% and a SECV of 0.27% over the range of 0.0-2.6% (see Figure 3). These figures of merit show that PCS can be quantified using Vis-NIR spectroscopy.

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Version 1, first published in December, 2017

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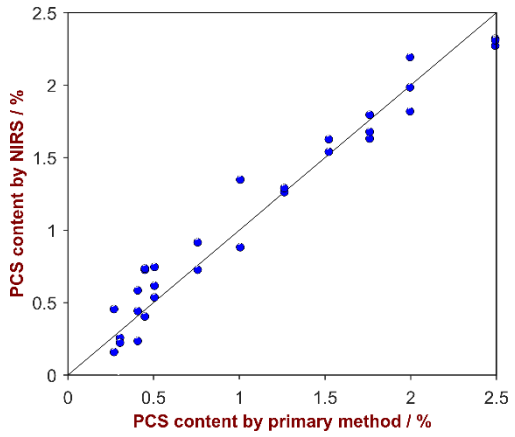

Fig. 3: Correlation plot of the predicted values by NIRS versus the laboratory values of PCS.

Protease:

For quantitative analysis of the protease enzyme, 3 factors were used. The SEC is found to be 0.06% and SECV is 0.07% over the range of 0.0-0.5%. The calibration plot is displayed in Figure 4.

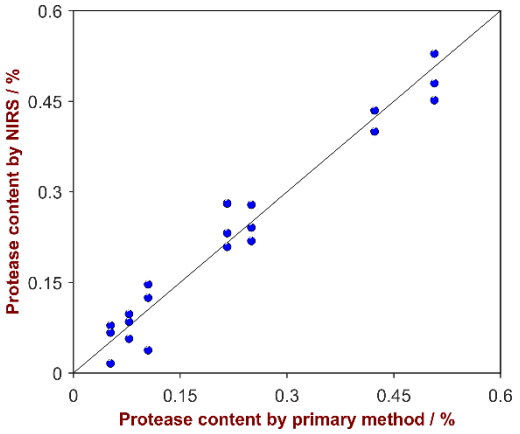

Fig. 4: Correlation plot of the predicted values by NIRS versus the laboratory values of the protease enzyme.

Results

Vis-NIR spectroscopy can be successfully used for quantification of additives in washing powders. Therefore, it can be used as high-throughput quality control analysis method to determine the composition of intermediate and final products. Vis-NIR spectroscopy solutions offer a number of unique advantages over traditional analysis methods, most notably: it generates reliable results within seconds, it does not need any sample preparation, it generates no waste and its non-destructive nature allows the sample to be re-used.

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