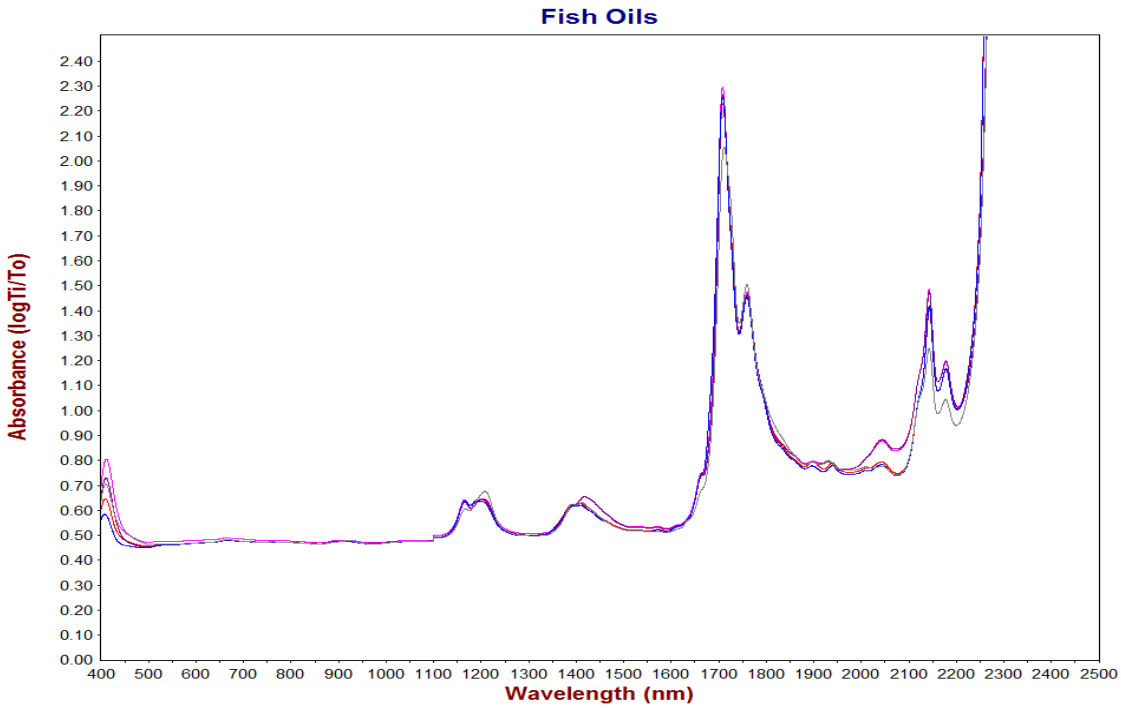
NIR Application Note NIR–US–002

Rapid qualitative analysis of fish oil blends using near-infrared spectroscopy (NIR)



The nutraceutical industry has experienced strong growth in recent years, and FDA regulations have added more stringent requirements. Near-Infrared Spectroscopy (NIRS) can differentiate between fish oil blends of similar composition, and determine if each blend meets specifications. This technology is a faster alternative to conventional lab methods and therefore accelerates raw material inspection, process monitoring and final product control.

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Method description

Introduction

Near-infrared (NIR) spectroscopy has been successfully used for identification of several closely related fish oil blends, with measurements taking 30 seconds per sample. Some samples varied only in triglyceride concentration, while other blends contained different components. By developing a library of NIR spectral variation for each unique product and running samples against the database of libraries, identification of fish oil blends was effective by NIR to a high degree.

Experimental

Spectra were collected via transmission in 4 mm disposable vials (Tab. 1) using the Metrohm NIRS XDS RapidLiquid Analyzer (Fig. 1). After collection of the spectra, pre-math treatments such as 2nd derivative were used to accentuate the spectral variation and dampen the effects of scattering. Once a valid approach was established, libraries of desired parameters were prepared using the provided samples. Identification methods were then developed by modeling of the spectra. Details of these methods are described below. The models were validated by analyzing additional samples not used in creation of the libraries.

Tab. 1: Used equipment for this application.

Equipment	Item Number
Metrohm NIRS XDS RapidLiquid Analyzer (RLA)	2.921.1410
NIRS disposable glass vials, 4 mm diameter	6.7402.010
NIRS XDS spacer for 4 mm vials	6.7403.010
Vision Pharma 4.1	6.6069.413

In Vision (Metrohm chemometric software), using the algorithm of Maximum Distance in Wavelength Space with a match value threshold of 20 (Fig. 3), a library for the named substances was developed. The data was pretreated using 2nd derivative to reduce scatter effects and accentuate changes in the spectra caused by chemical differences. One of the two used regions of math pretreated spectra is shown in Fig. 2. Internal cross-validation was applied to verify the performance of the derived library.

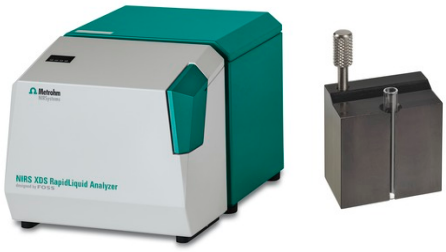
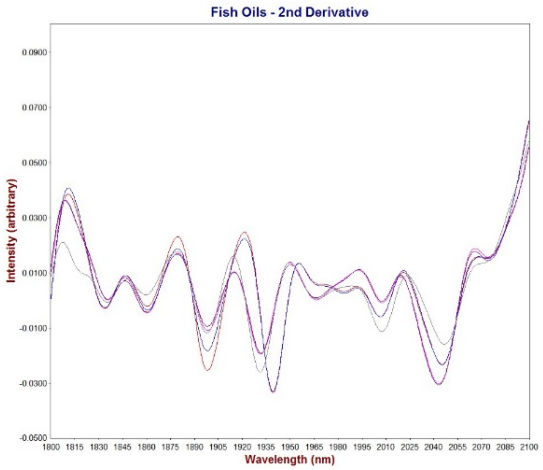


Fig. 1: The NIRS XDS RapidLiquid Analyzer was used with 4 mm diameter disposable vials to collect transmission spectra over the full wavelength range (400 – 2500 nm).

Fig. 2: 2nd derivative was applied on the raw spectra. One usable wavelength region (1800 – 2100 nm) is displayed, where the different fish oils show the largest differences.



Method	Maximum Distance in Wavelength Space
Wavelength Regions	400-1700 & 1720-2250 nm
Math Pretreatments	2nd Derivative
Match Value Threshold	20

Fig. 3: Details of the qualitative method developed for identification of fish oil blends.

Conclusion

The acquired NIR spectra can be successfully used in qualitative identification of fish oil blends.

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