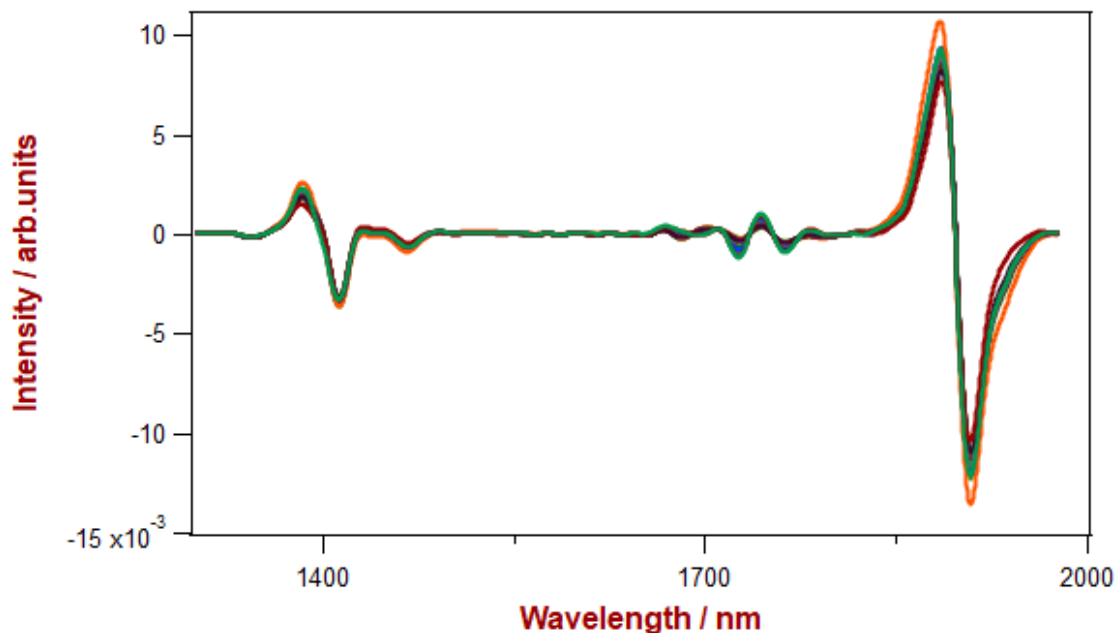


NIR Application Note AN-NIR-075

Naphtha in soil by Vis-NIR spectroscopy

A straightforward solution for testing laboratories



Naphtha is the first petroleum product during the distillation process of crude oil or coal tar. It is primarily used as a base material for the production of gasoline or as a solvent. Accidental spills occur regularly at many locations throughout the world, leading to soil contamination. Investigation of contaminated sites is usually performed using gas chromatography, for which the soil sample has to be frozen, grinded, and subsequently extracted prior to the analysis. Using Visible-Near Infrared Spectroscopy such sample preparation steps are not necessary at all, making this method a viable, fast, and simple to use alternative.

Method description

Samples & Sample preparation

To develop a calibration model 52 soil samples were spiked with varying Naphtha concentrations from 700–35000 ppm. The VIS-NIR spectra were measured in reflection mode using a Metrohm NIRS DS2500 Analyzer without any sample preparation.

Configuration

NIRS DS2500 Analyzer	2.922.0010
DS2500 large sample cup	6.7402.050
Vision Air 2.0 Complete	6.6072.208

Experimental

Spectral data was acquired by using the large sample cup in moving mode, to cover spectral variation caused by inhomogeneity of the samples. The software package Vision Air 2.0 Complete was used for data acquisition, data management, and development of the quantification method.



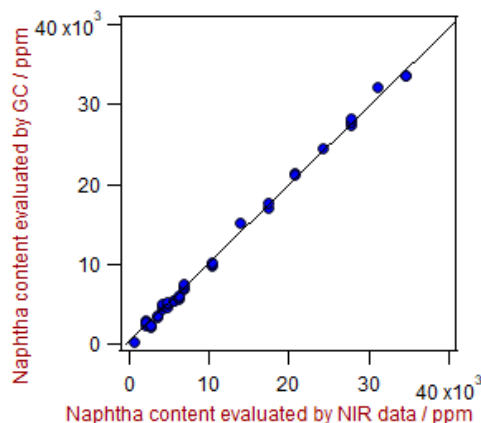
Method development

39 soil samples were used to create a calibration set. 13 soil samples were used as an independent sample set for validation. Baseline drift was corrected using 2nd derivative as a pre-treatment. The calibration model was established using the following settings:

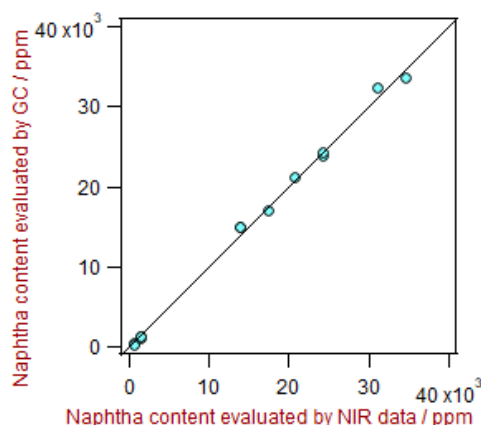
Regression model	PLS
Pretreatment	2 nd derivative
Validation	Validation set

Results

Naphtha content calibration set



Naphtha content validation set



Range	700–35000 ppm
No. of factors	3
R ²	0.99
SEC	563 ppm
SECV	653 ppm

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