Application Note AN-NIR-113

体中研究辛(RON)的定

NIRS offers users fast, efficient analysis with low running costs

Light naphtha isomerization is used by refineries to produce high-octane isomerate products which meet current gasoline specifications. Isomerization increases the octane value of light naphtha by increasing the degree of branching of paraffin molecules. The research octane number (RON) of the target product is dependent on various plant production parameters (e.g., temperature or hydrogen to hydrocarbon ratio). To optimize the plant process, a reliable and quick analytical method is key.

The standard method to determine RON in isomerate is with expensive and maintenance-intensive engines. In contrast to this, the research octane number can also be analyzed by near-infrared spectroscopy (NIRS). NIRS provides accurate results within one minute without the need for any sample preparation or chemicals.

63 different isomerate samples with varying RON values were measured with the Metrohm DS2500 Liquid Analyzer (**Figure 1**) in transmission mode over the full wavelength range of 400–2500 nm. The built-in temperature controller ensured measurement stability with a constant sample temperature of 35 °C. For convenience, disposable vials with a pathlength of 8 mm were used which made a cleaning procedure obsolete. The Vision Air Complete software package from Metrohm was used for data acquisition and prediction model development.

Table 1. Hardware and software equipment overview.

Equipment	Article number
DS2500 Liquid Analyzer	2.929.0010
DS2500 Holder 8 mm vials	6.7492.020
Vision Air 2.0 Complete	6.6072.208

Figure 1. Metrohm DS2500 Liquid Analyzer used for the determination of research octane number (RON) in isomerate samples.

RESULT

The obtained Vis-NIR spectra (**Figure 2**) were used to create a prediction model for the quantification of research octane number in isomerate. The quality of the prediction models was evaluated using correlation diagrams based on the cross-validation algorithm. A value of R^2 > 0.98 displays a high correlation between the Vis-NIR prediction and the reference ASTM method. The respective figures of merit (FOM) display the expected precision during routine analysis (**Figure 3**).

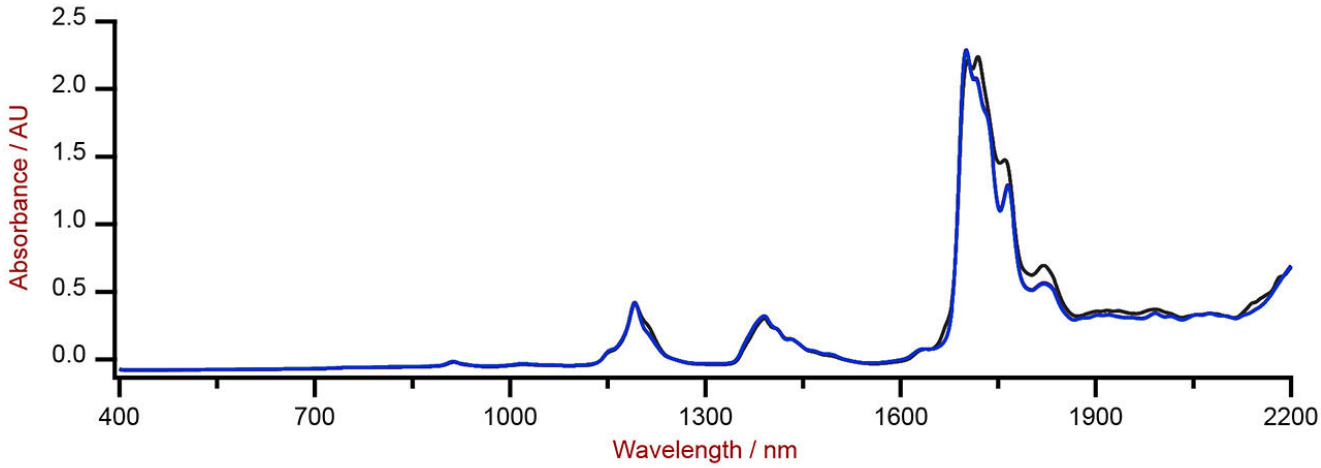

Figure 2. Selection of Vis-NIR spectra of isomerate samples analyzed on a DS2500 Liquid Analyzer with 8 mm vials.

RESULT RON VALUE

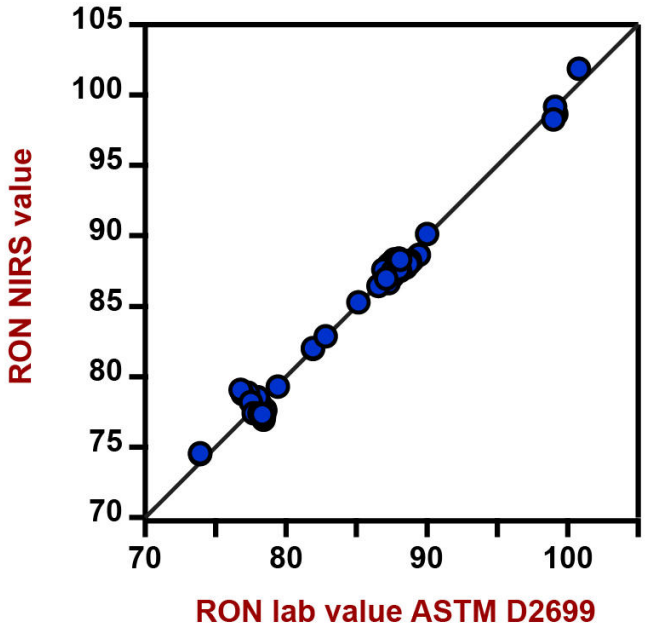

Figure 3. Correlation diagram and the respective figures of merit for the prediction of RON value using a DS2500 Liquid Analyzer. The lab value was evaluated according to ASTM D2699.

Figures of Merit	Value
R^2	0.986
Standard Error of Calibration	0.73
Standard Error of Cross-Validation	0.76

CONCLUSION

This Application Note demonstrates the feasibility of NIR spectroscopy for the analysis of RON in isomerate samples. In comparison to the conventional method, the time to result (**Table 2**) is a major advantage of Vis-NIR spectroscopy. With NIRS, a single measurement is performed within one minute, while the CFR engine test is much longer.

Table 2. Time to result for the determination of RON value with the standard reference method ASTM D2699.

Parameter	Method	Time to result
RON	CFR engine test	30 minutes per sample

CONTACT

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CONFIGURATION

DS2500 Liquid Analyzer

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DS2500 Liquid Analyzer , DS2500 Liquid Analyzer ,

DS2500 Liquid Analyzer 400 2500 nm , 80°C , ,DS2500 Liquid Analyzer , Vision Air ,

, Metrohm

DS2500 8 mm

8 mm

Vision Air 2.0 Complete

Vision Air –

Vision Air Complete

Vision Air :

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- SQL ,

Vision Air Complete (66072208) :

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Vision Air Complete :

- 66072207 (Vision Air Network Complete)
- 66072209 (Vision Air Pharma Complete)
- 66072210 (Vision Air Pharma Network Complete)