Application Note AN-NIR-114

Determination of RON, aromatics, benzene, olefins, and density in reformate by NIRS

Multiparameter analysis with results delivered in one minute

SUMMARY

Refiners use the catalytic reforming process to produce high-octane reformate. This reformate is used for premium gasoline blends or petrochemical feedstock. The determination of key quality parameters of reformate—namely research octane number (RON, ASTM D2699), aromatic content (ASTM D5769), benzene content, olefin content, and density—requires time-consuming and laborious conventional methods.

In contrast, all of these parameters (and more) can be measured by near-infrared (NIR) spectroscopy. The Metrohm DS2500 Liquid Analyzer, operating in the visible and near-infrared spectral region (Vis-NIR), provides results within one minute without any sample preparation.

EXPERIMENTAL EQUIPMENT

507 different reformate samples were measured on the Metrohm DS2500 Liquid Analyzer (Figure 1). All measurements were performed in transmission mode from 400–2500 nm using 8 mm disposable vials. The temperature control of the analyzer was set to 35 °C for all measurements to ensure the best performance and highest quality data. Data acquisition and prediction model development was performed with the Metrohm software package Vision Air Complete.

Figure 1. Metrohm DS2500 Liquid Analyzer used for the determination of research octane number (RON), aromatics, benzene, olefins, and density in reformate.

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

RESULT

The measured Vis-NIR spectra (Figure 2) were used to create a prediction model for quantification of all five parameters. The quality of the prediction models was evaluated using correlation diagrams which display a high correlation (R^2 > 0.98) between the Vis-NIR prediction and the reference methods for all parameters. The respective figures of merit (FOM) display the expected precision and confirm the feasibility during routine analysis (Figures 3–7).

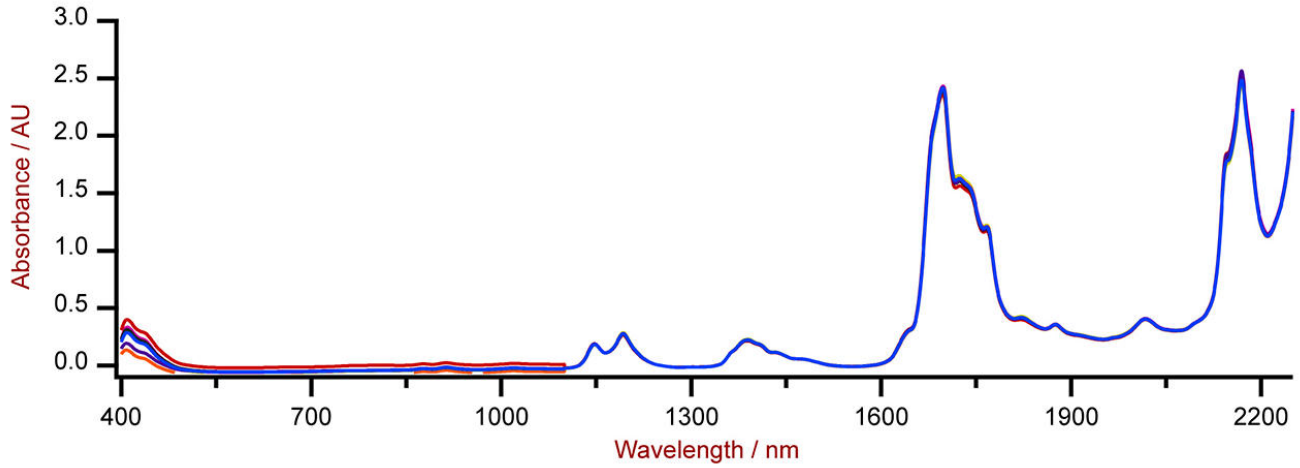

Figure 2. Selection of Vis-NIR spectra of reformate samples analyzed on a Metrohm DS2500 Liquid Analyzer with 8 mm vials.

RESULT RON VALUE

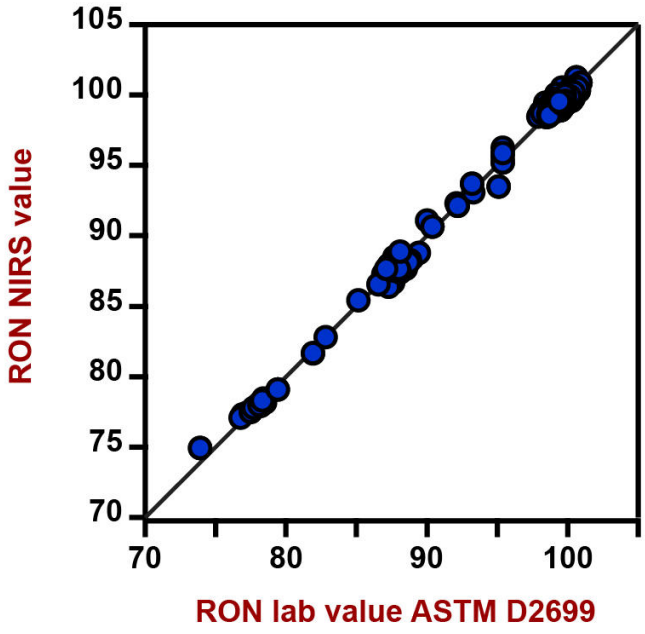

Figure 3. Correlation diagram and the respective figures of merit for the prediction of RON value using a DS2500 Liquid Analyzer. The lab value was evaluated according to ASTM D2699.

Figures of Merit	Value
R^2	0.996
Standard Error of Calibration	0.34
Standard Error of Cross-Validation	0.36

RESULT AROMATIC CONTENT

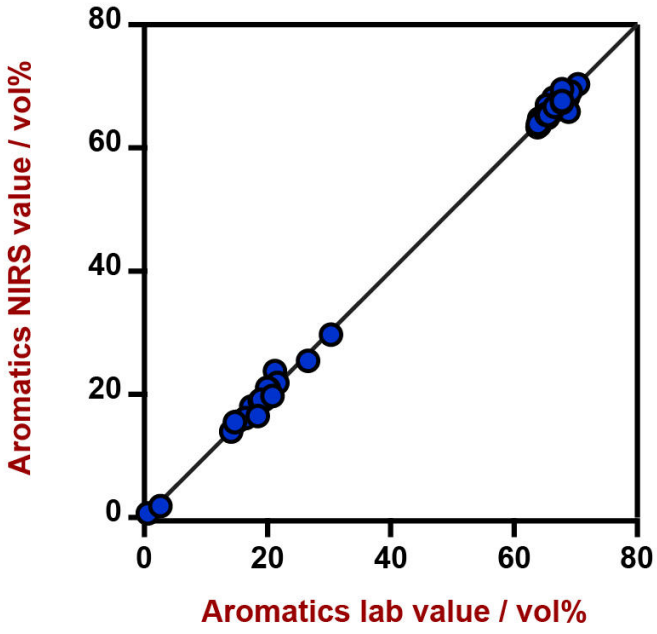

Figure 4. Correlation diagram and the respective figures of merit for the prediction of aromatic content using a DS2500 Liquid Analyzer. The lab value was evaluated using gas chromatography (GC).

Figures of Merit	Value
R^2	0.999
Standard Error of Calibration	0.88 vol%
Standard Error of Cross-Validation	0.91 vol%

RESULT BENZENE CONTENT

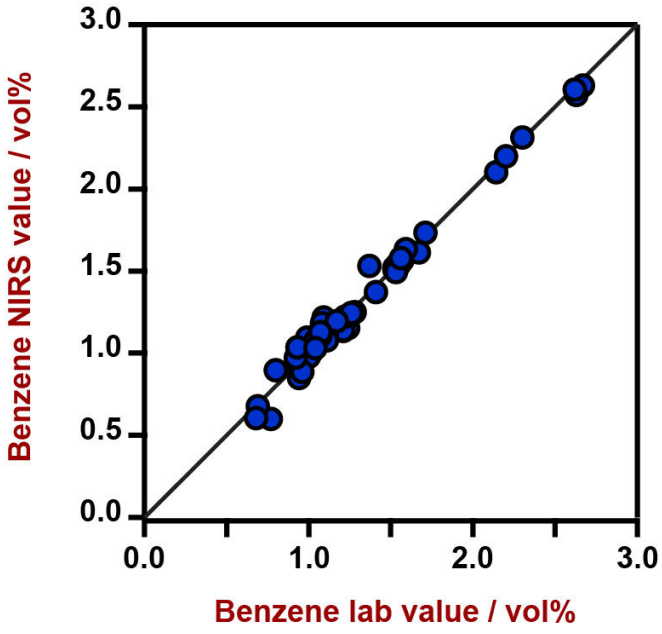

Figure 5. Correlation diagram and the respective figures of merit for the prediction of benzene content using a DS2500 Liquid Analyzer. The lab value was evaluated using gas chromatography (GC).

Figures of Merit	Value
R^2	0.984
Standard Error of Calibration	0.066 vol%
Standard Error of Cross-Validation	0.088 vol%

RESULT OLEFIN CONTENT

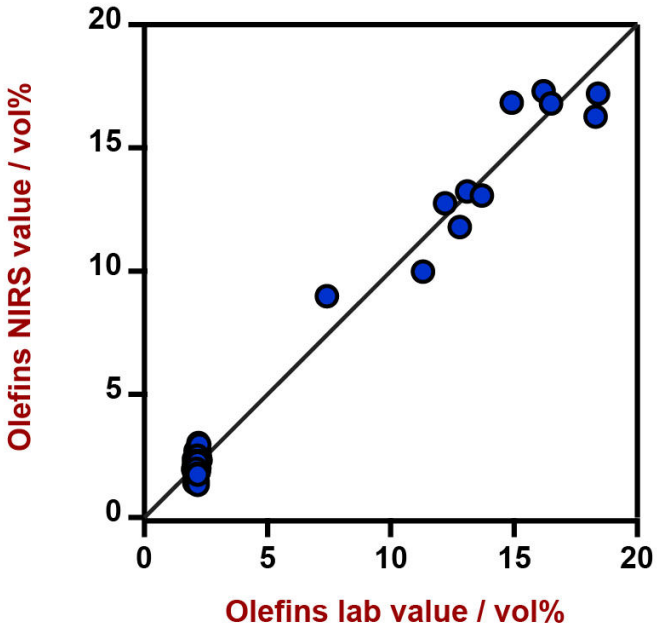

Figure 6. Correlation diagram and the respective figures of merit for the prediction of olefin content using a DS2500 Liquid Analyzer. The lab value was evaluated using gas chromatography (GC).

Figures of Merit	Value
R^2	0.982
Standard Error of Calibration	0.71 vol%
Standard Error of Cross-Validation	0.87 vol%

RESULT DENSITY VALUE

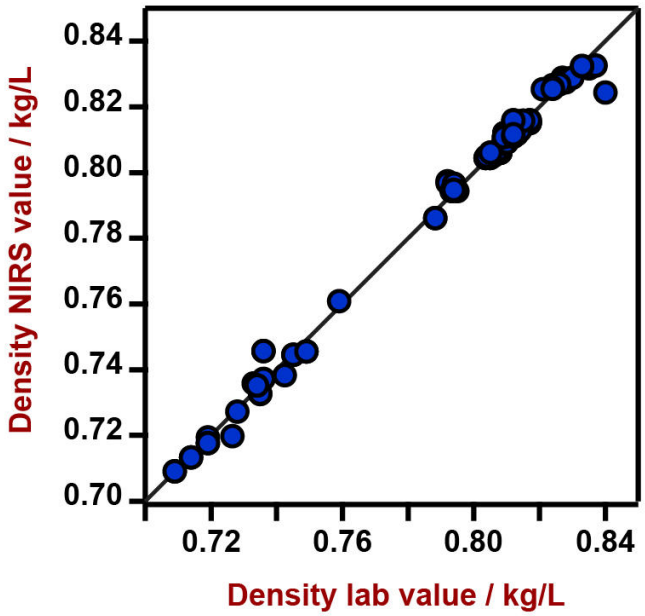

Figure 7. Correlation diagram and the respective figures of merit for the prediction of benzene content using a DS2500 Liquid Analyzer. The lab value was evaluated using a density meter.

Figures of Merit	Value
R^2	0.993
Standard Error of Calibration	0.0029 kg/L
Standard Error of Cross-Validation	0.0034 kg/L

CONCLUSION

This Application Note demonstrates the feasibility of the Metrohm DS2500 Liquid Analyzer for the determination of RON, aromatic content, benzene content, olefin content, and density in reformate samples. Compared to the conventional methods, Vis-NIR spectroscopy enables fast determination (Table 2) without any sample preparation. Significant gains are achieved through time savings as well as the reduction in chemical usage and waste.

Table 2. Time to result overview for the parameters of RON, aromatic content, benzene content, and olefin content by standard methods.

Parameter	Method	Time to result
RON	CFR engine test	30 minutes per sample
Aromatic content	Gas Chromatography	45 minutes per sample
Benzene content	Gas Chromatography	45 minutes per sample
Olefin content	Gas Chromatography	45 minutes per sample

CONTACT

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CONFIGURATION

DS2500 Liquid Analyzer

Robust near-infrared spectroscopy for quality control, not only in laboratories but also in production environments.

The DS2500 Liquid Analyzer is the tried and tested, flexible solution for routine analysis of liquids along the entire production chain. Its robust design makes the DS2500 Liquid Analyzer resistant to dust, moisture and vibrations, which means that it is eminently suited for use in harsh production environments.

The DS2500 Liquid Analyzer covers the full spectral range from 400 to 2500 nm, heats samples up to 80°C and is compatible with various disposable vials and quartz cuvettes. The DS2500 Liquid Analyzer is thus adaptable to your individual sample requirements and helps you obtain accurate and reproducible results in less than one minute. The integrated sample holder detection and the self-explanatory Vision Air Software also ensure simple and safe operation by the user.

In the case of larger-sized sample quantities, productivity can be considerably increased by using a flow-through cell in combination with a Metrohm sample robot.

DS2500 Holder 8 mm vials

Intelligent holder for disposable glass vials with 8 mm diameter

Vision Air 2.0 Complete

Vision Air - Universal spectroscopy software.

Vision Air Complete is a modern and simple-to-operate software solution for use in a regulated environment.

Overview of the advantages of Vision Air:

- Individual software applications with adapted user interfaces ensure intuitive and simple operation
- Simple creation and maintenance of operating procedures
- SQL database for secure and simple data management

The Vision Air Complete version (66072208) includes all applications for quality assurance using Vis-NIR spectroscopy:

- Application for instrument and data management
- Application for method development
- Application for routine analysis

Additional Vision Air Complete solutions:

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