



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

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 reformat 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 reformat.

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).

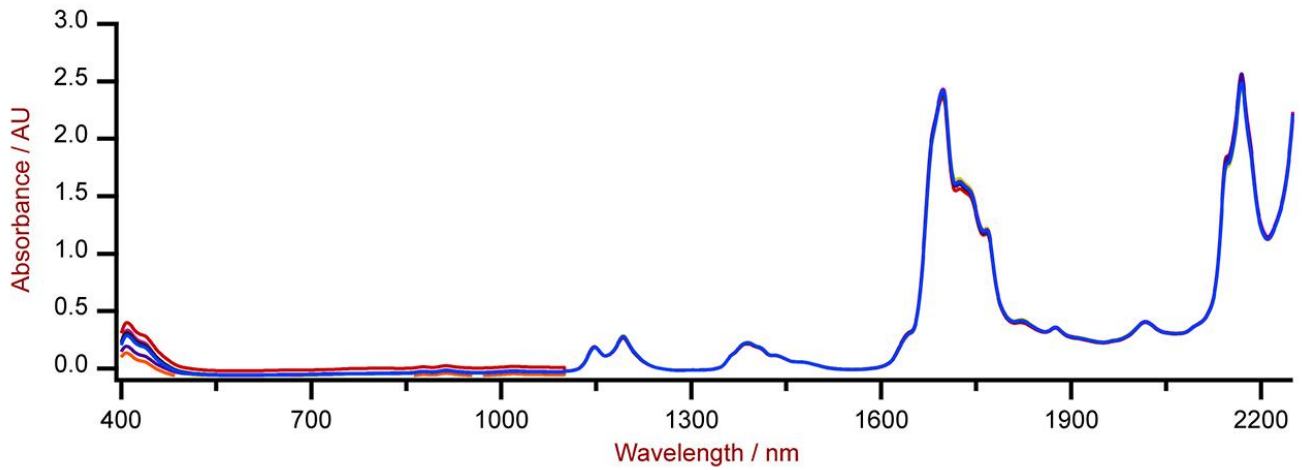


Figure 2. Selection of Vis-NIR spectra of reformate samples analyzed on a Metrohm DS2500 Liquid Analyzer with 8 mm vials.

RESULT RON VALUE

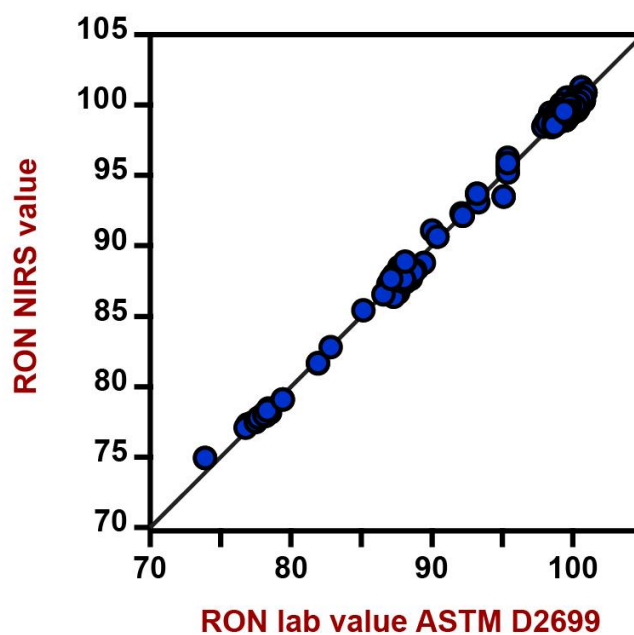


Figure 3. Correlation diagram and the respective figures of merit for the prediction of RON value using a DS2500 Liquid Analyzer. The lab value was evaluated according to ASTM D2699.

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

RESULT AROMATIC CONTENT

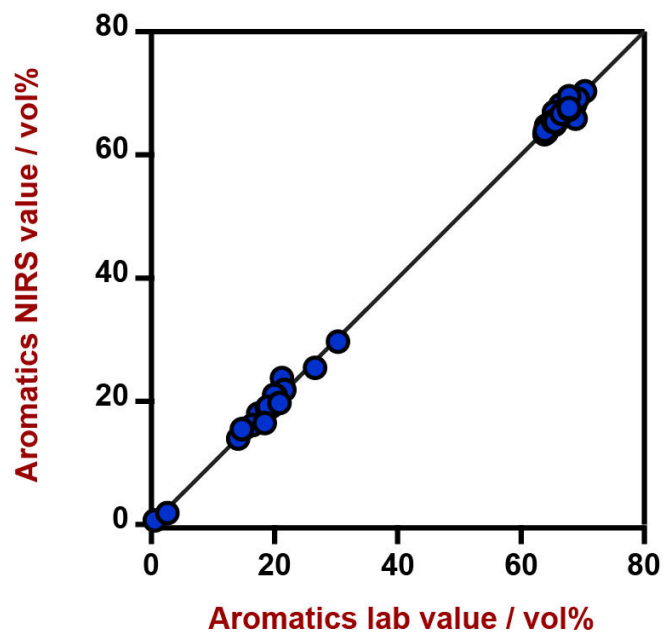


Figure 4. Correlation diagram and the respective figures of merit for the prediction of aromatic content using a DS2500 Liquid Analyzer. The lab value was evaluated using gas chromatography (GC).

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

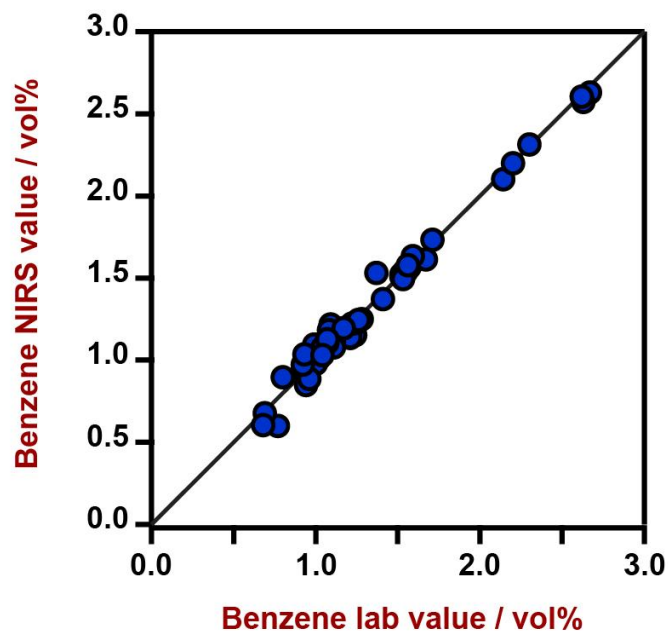


Figure 5. Correlation diagram and the respective figures of merit for the prediction of benzene content using a DS2500 Liquid Analyzer. The lab value was evaluated using gas chromatography (GC).

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

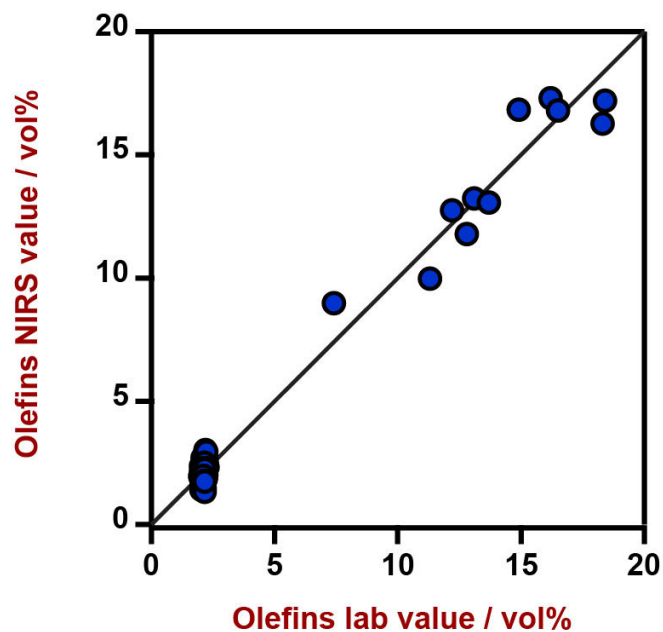


Figure 6. Correlation diagram and the respective figures of merit for the prediction of olefin content using a DS2500 Liquid Analyzer. The lab value was evaluated using gas chromatography (GC).

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

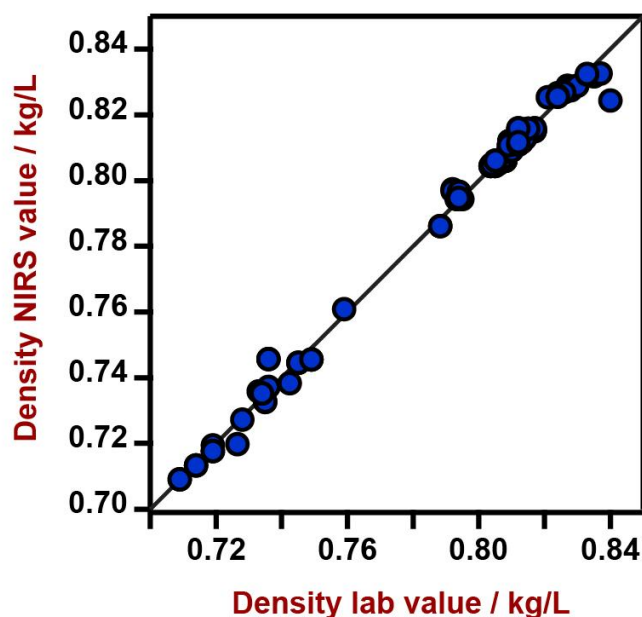


Figure 7. Correlation diagram and the respective figures of merit for the prediction of benzene content using a DS2500 Liquid Analyzer. The lab value was evaluated using a density meter.

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 reformat 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

Spectroscopie proche infrarouge robuste pour le contrôle qualité en laboratoire et en environnement de production.

L'analyseur DS2500 Liquid Analyzer est la solution éprouvée et souple destinée aux analyses de routine d'échantillons liquides, tout au long de la chaîne de fabrication. Sa conception robuste fait du DS2500 Liquid Analyzer un appareil insensible à la poussière, à l'humidité et aux vibrations, et donc particulièrement adapté aux rudes conditions d'un environnement de production.

Le DS2500 Liquid Analyzer couvre l'ensemble de la gamme spectrale de 400 à 2500 nm, chauffe les échantillons jusqu'à 80 °C et est compatible avec divers flacons à usage unique et cuves en quartz. Le DS2500 Liquid Analyzer, lequel s'adapte à vos exigences individuelles en matière d'échantillons, vous permet d'obtenir des résultats précis et reproductibles en moins d'une minute. Avec sa détection du support d'échantillon intégrée et le logiciel Vision Air intuitif, un maniement simple et sûr est également garanti pour l'utilisateur.

En présence de grandes quantités d'échantillons, l'utilisation d'une cellule à flux continu associée à un robot passeur d'échantillons Metrohm peut augmenter considérablement la productivité.

DS2500 - Support pour flacons à usage unique 8 mm

Support intelligent pour flacons en verre à usage unique de 8 mm de diamètre





Vision Air 2.0 Complete

Vision Air - logiciel universel de spectroscopie.

Vision Air Complete est une solution logicielle moderne et simple d'utilisation pour une application dans un environnement réglementé.

Aperçu des avantages de Vision Air :

- Des applications logicielles individuelles avec interface utilisateur adaptée sont le garant d'un maniement intuitif et simple
- Établissement et suivi simples des procédures de travail
- Base de données SQL pour une gestion sûre et simple des données

La version Vision Air Complete (66072208) comprend toutes les applications d'assurance qualité par spectroscopie Vis-NIR :

- Application de gestion des instruments et des données
- Application de développement de méthodes
- Application d'analyse de routine

Autres solutions Vision Air Complete :

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