



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**).

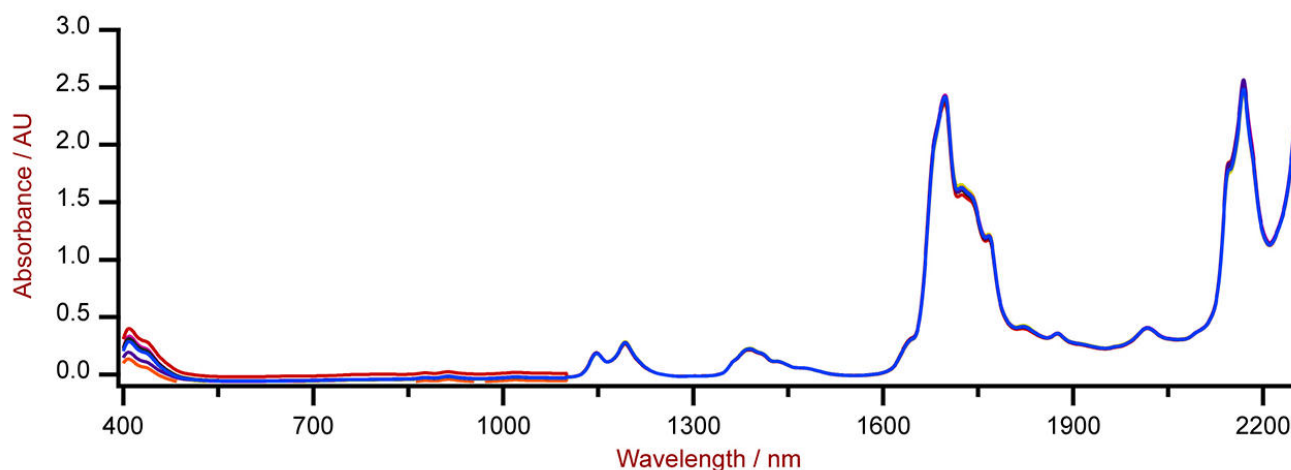


Figure 2. Selection of Vis-NIR spectra of reformat samples analyzed on a Metrohm DS2500 Liquid Analyzer with 8 mm vials.

RESULT RON VALUE

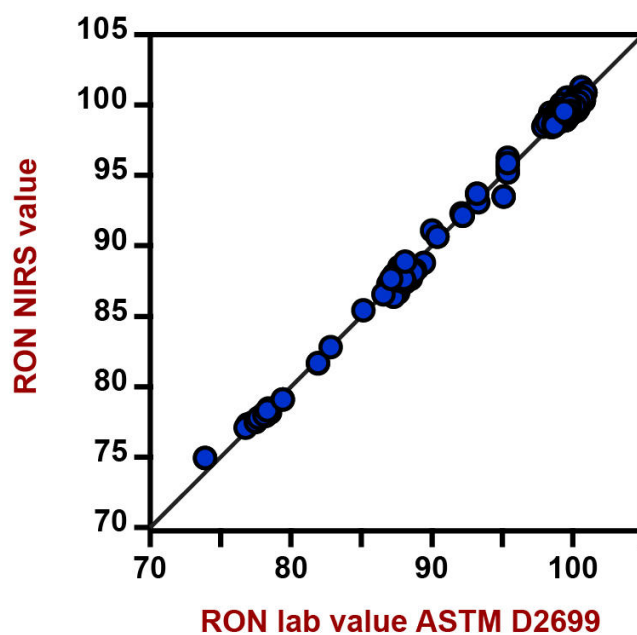


Figure 3. Correlation diagram and the respective figures of merit for the prediction of RON value using a DS2500 Liquid Analyzer. The lab value was evaluated according to ASTM D2699.

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

RESULT AROMATIC CONTENT

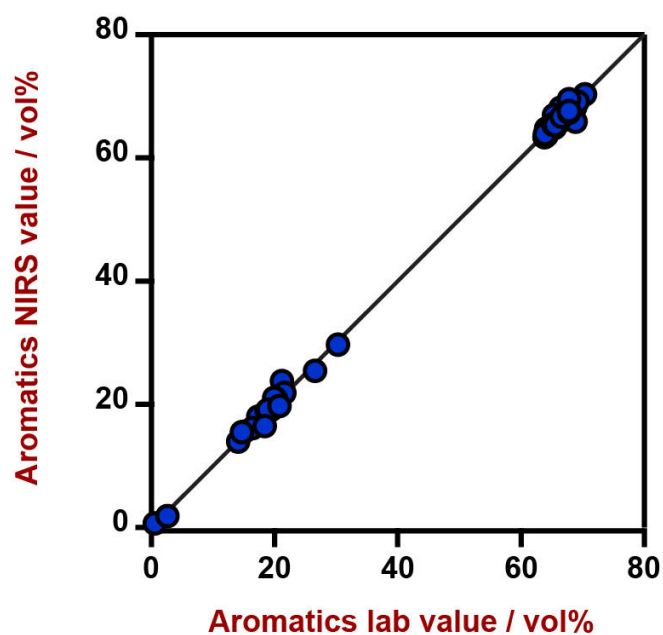


Figure 4. Correlation diagram and the respective figures of merit for the prediction of aromatic content using a DS2500 Liquid Analyzer. The lab value was evaluated using gas chromatography (GC).

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

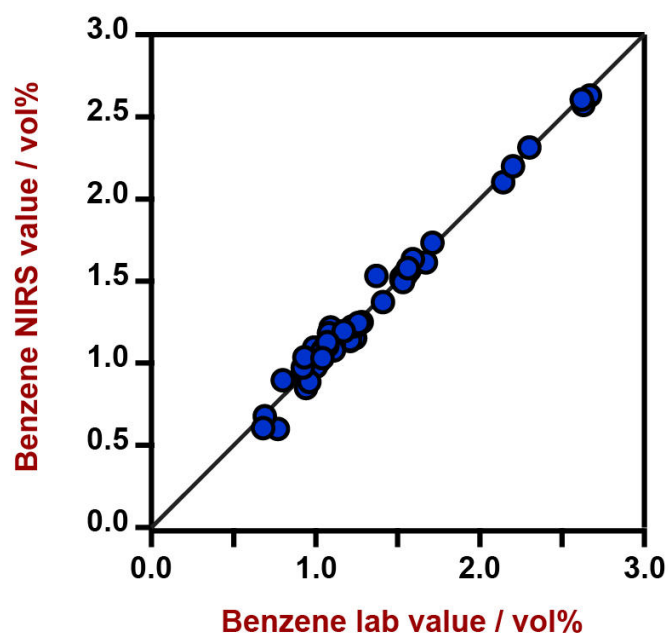


Figure 5. Correlation diagram and the respective figures of merit for the prediction of benzene content using a DS2500 Liquid Analyzer. The lab value was evaluated using gas chromatography (GC).

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

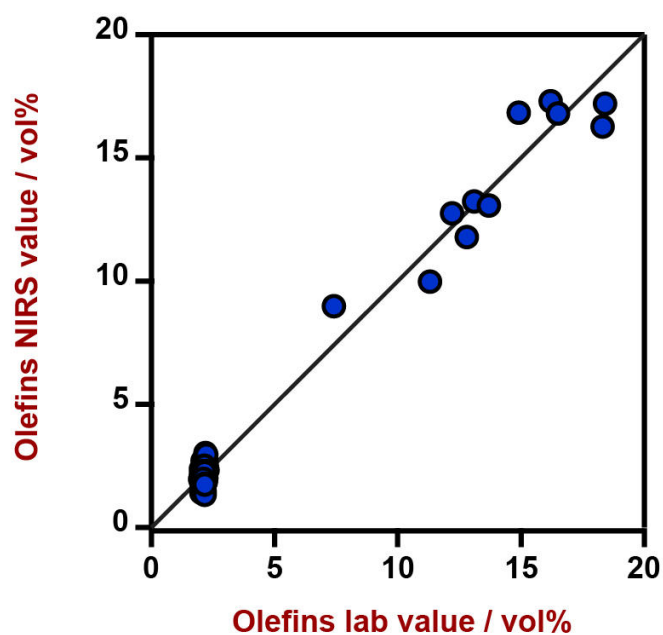


Figure 6. Correlation diagram and the respective figures of merit for the prediction of olefin content using a DS2500 Liquid Analyzer. The lab value was evaluated using gas chromatography (GC).

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

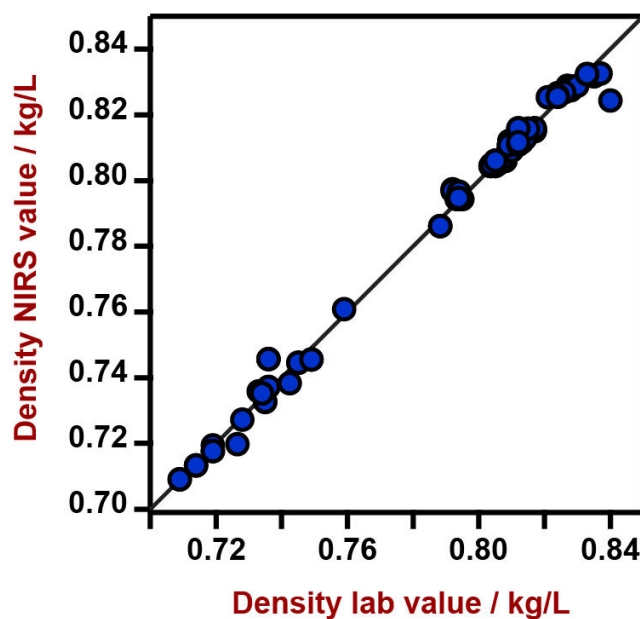


Figure 7. Correlation diagram and the respective figures of merit for the prediction of benzene content using a DS2500 Liquid Analyzer. The lab value was evaluated using a density meter.

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

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CONFIGURATION



DS2500 Liquid Analyzer
固的近外光,用于生境和室中的量。

DS2500 Liquid Analyzer 是一成熟且活的解决方案,其用于在整个生中行液体常分析。其固的使 DS2500 Liquid Analyzer 不受灰、潮湿、振的影,因此非常用于在劣的生境中使用。

DS2500 Liquid Analyzer 覆盖 400 至 2500 nm 的整个光范,将品加至 80° C 高温,并与各不同的一次性小瓶和石英比色皿兼容。因此,DS2500 Liquid Analyzer 可的个性化品要求,助在一分内得精和具有可重性的果。借助集成的品架装置和自的 Vision Air 件,保了用能松和安全地行操作。

如果是大的品量,可通将流通池与一个 Metrohm 机器人自器搭配使用的方法著提高生率。



DS2500 8 mm

直径 8 mm 且更加智能的一次性玻璃小瓶支架



Vision Air 2.0 Complete

Vision Air – 通用的光分析件。

Vision Air Complete 是用于管范境的先易用的件解决方案。

Vision Air 点一:

- 便捷的件用和配的用界面保了直的操作方式
- 操作程的建与方式
- SQL 数据,可安全且地管理数据

Vision Air Complete (66072208) 版本包含所有用于可近外光分析量保程的用:

- 器和数据管理用
- 方法用
- 常分析用

其它 Vision Air Complete 解决方案:

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