



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**).

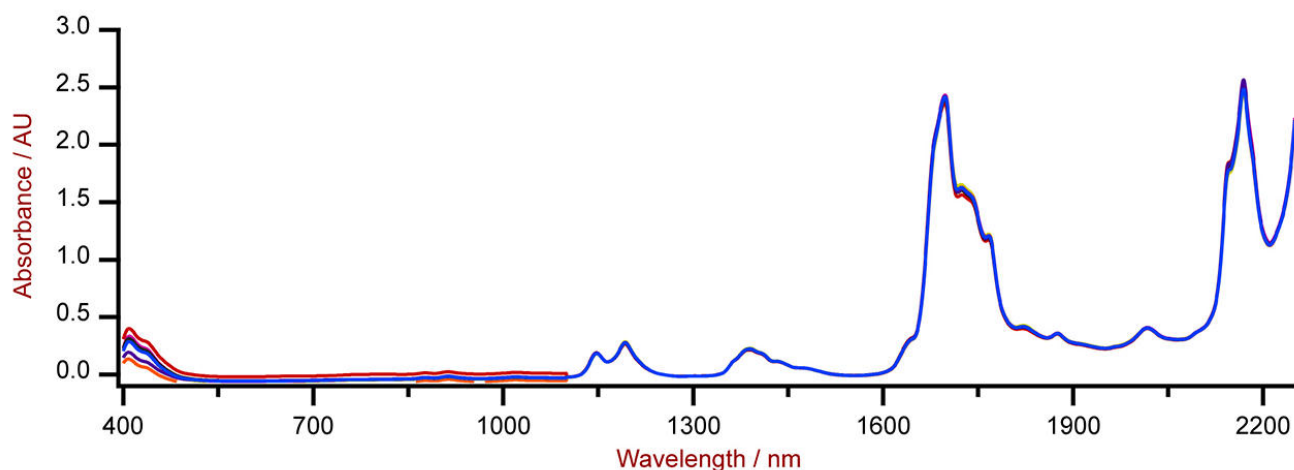


Figure 2. Selection of Vis-NIR spectra of reformat samples analyzed on a Metrohm DS2500 Liquid Analyzer with 8 mm vials.

RESULT RON VALUE

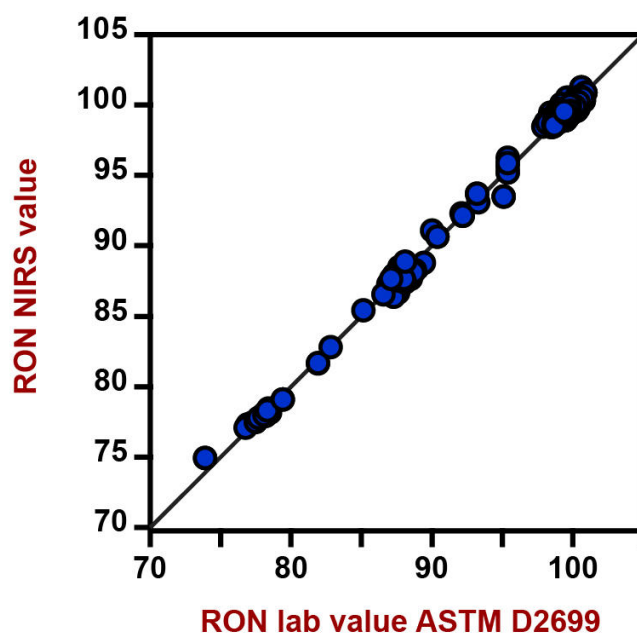


Figure 3. Correlation diagram and the respective figures of merit for the prediction of RON value using a DS2500 Liquid Analyzer. The lab value was evaluated according to ASTM D2699.

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

RESULT AROMATIC CONTENT

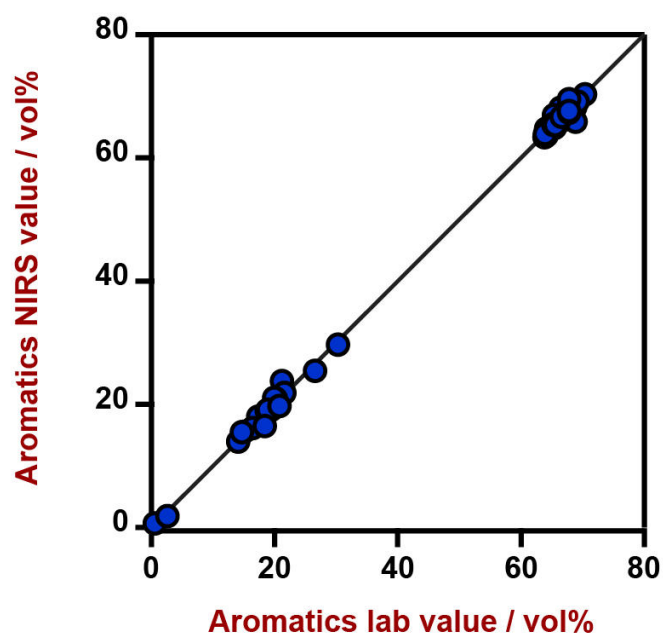


Figure 4. Correlation diagram and the respective figures of merit for the prediction of aromatic content using a DS2500 Liquid Analyzer. The lab value was evaluated using gas chromatography (GC).

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

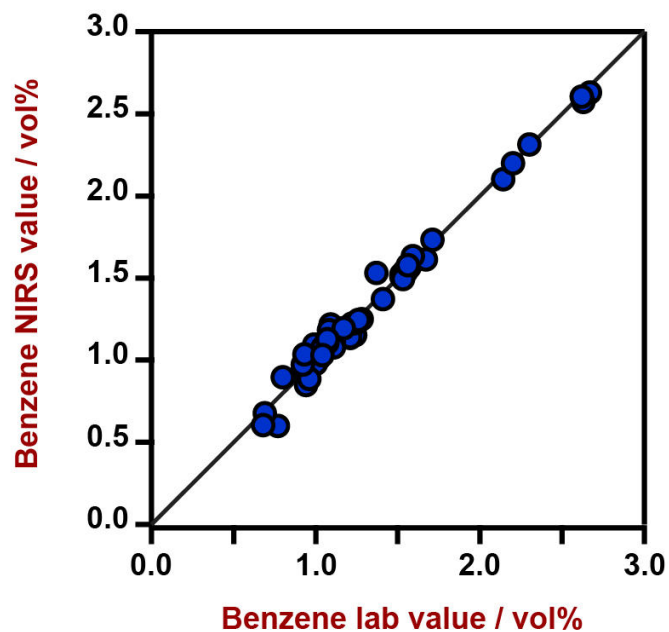


Figure 5. Correlation diagram and the respective figures of merit for the prediction of benzene content using a DS2500 Liquid Analyzer. The lab value was evaluated using gas chromatography (GC).

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

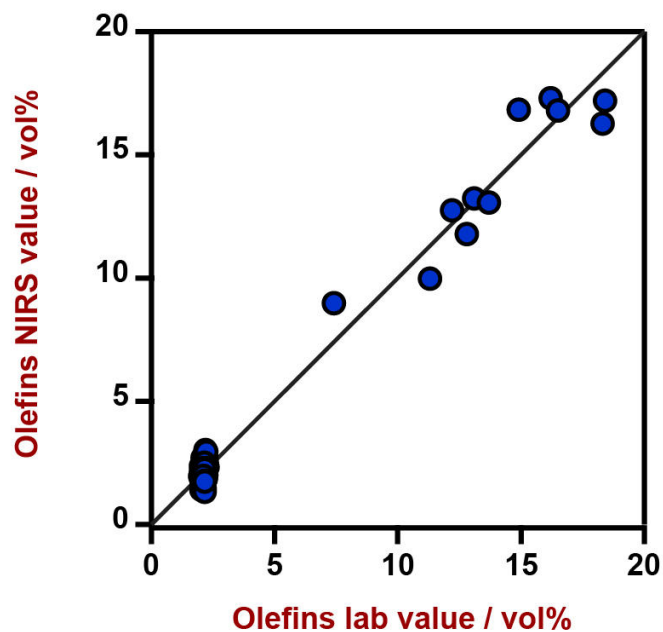


Figure 6. Correlation diagram and the respective figures of merit for the prediction of olefin content using a DS2500 Liquid Analyzer. The lab value was evaluated using gas chromatography (GC).

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

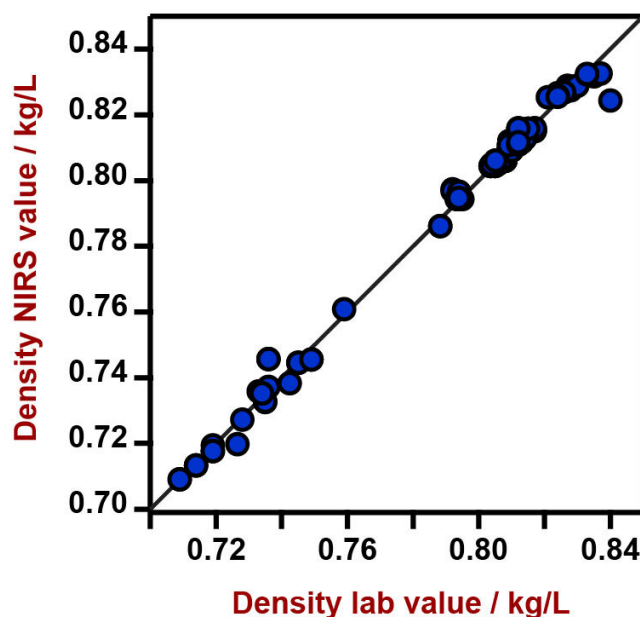


Figure 7. Correlation diagram and the respective figures of merit for the prediction of benzene content using a DS2500 Liquid Analyzer. The lab value was evaluated using a density meter.

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

坚固结实的近红外光谱仪,用于生产环境和试验室中的质量检查。

DS2500 Liquid Analyzer 是一种成熟且灵活的解决方案,其用于在整个生产链中进行液体常规分析。其坚固结实的设计使 DS2500 Liquid Analyzer 不受灰尘、潮湿、振动的影响,因此非常适用于在恶劣的生产环境中使用。

DS2500 Liquid Analyzer 覆盖 400 至 2500 nm 的整个光谱范围,将样品加热至 80° C 高温,并与各种不同的一次性小瓶和石英比色皿兼容。因此,DS2500 Liquid Analyzer 可适应您的个性化样品要求,帮助您在几分钟内获得精确和具有可重现性的结果。借助集成的样品架识别装置和自带的 Vision Air 软件,还保证了用户能轻松和安全地进行操作。

如果是较大的样品量,则可通过将流通池与一个 Metrohm 机器人自动进样器搭配使用的方法显著提高生产率。



DS2500 8 mm

直径为 8 mm 且更加智能的一次性玻璃小瓶支架



Vision Air 2.0 Complete

Vision Air – 通用的光谱分析软件。

Vision Air Complete 是用于监管规范环境的先进易用的软件解决方案。

Vision Air 优点一览:

- 便捷的软件应用和经过适配的用户界面保证了直观简单的操作方式
- 操作过程的创建与维护方式简单
- SQL 数据库,可安全且简单地管理数据

Vision Air Complete (66072208) 版本包含所有用于可见近红外光谱分析质量保证过程的应用:

- 仪器和数据管理应用
- 方法开发应用
- 常规分析应用

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)