



Application Note AN-NIR-113

Research octane number (RON) determination in isomerate

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.

EXPERIMENTAL EQUIPMENT

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).

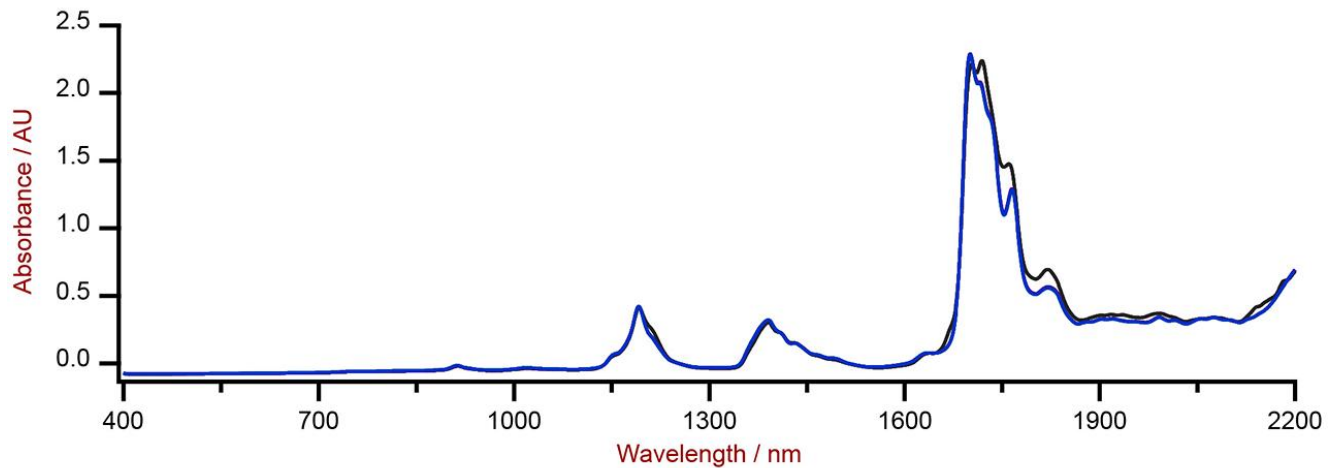


Figure 2. Selection of Vis-NIR spectra of isomerate samples analyzed on a DS2500 Liquid Analyzer with 8 mm vials.

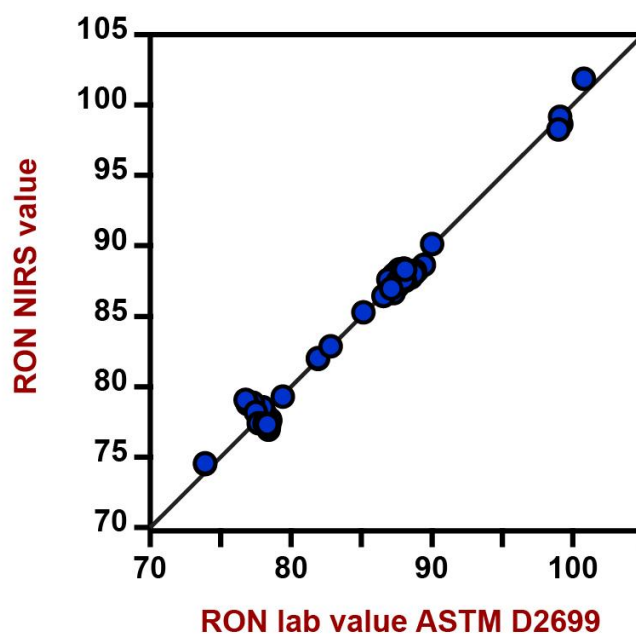


Figure 3. Correlation diagram and the respective figures of merit for the prediction of RON value using a DS2500 Liquid Analyzer. The lab value was evaluated according to ASTM D2699.

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

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CONFIGURATION



DS2500 Liquid Analyzer
固耐用的近外光,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。其固耐用的使 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:

- 独特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)