



Application Note AN-NIR-113

异构体中研究辛烷值(RON)的测定

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 isomerase 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 isomerase 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**).

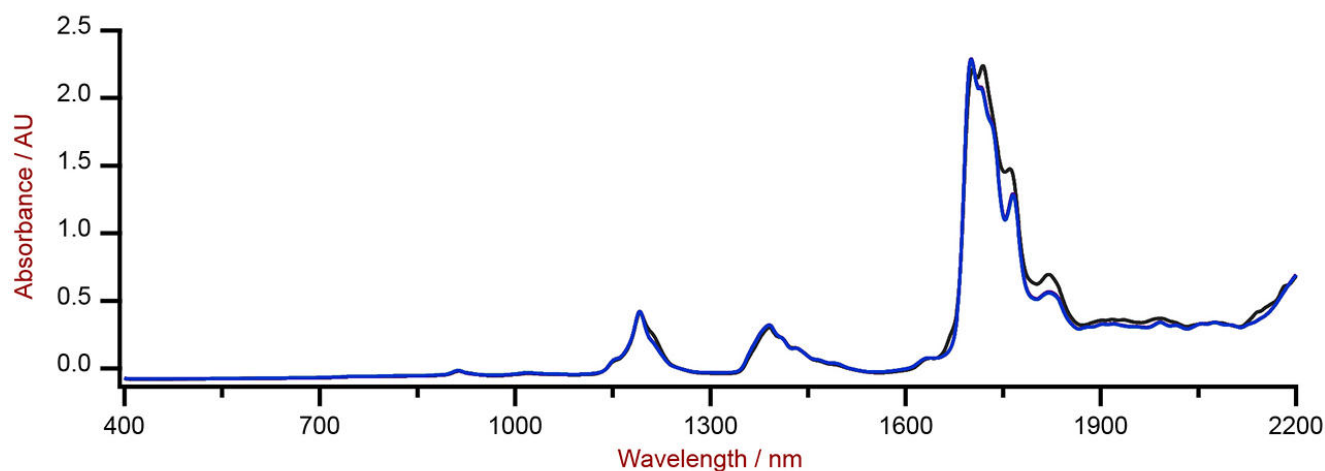


Figure 2. Selection of Vis-NIR spectra of isomerate samples analyzed on a DS2500 Liquid Analyzer with 8 mm vials.

RESULT RON VALUE

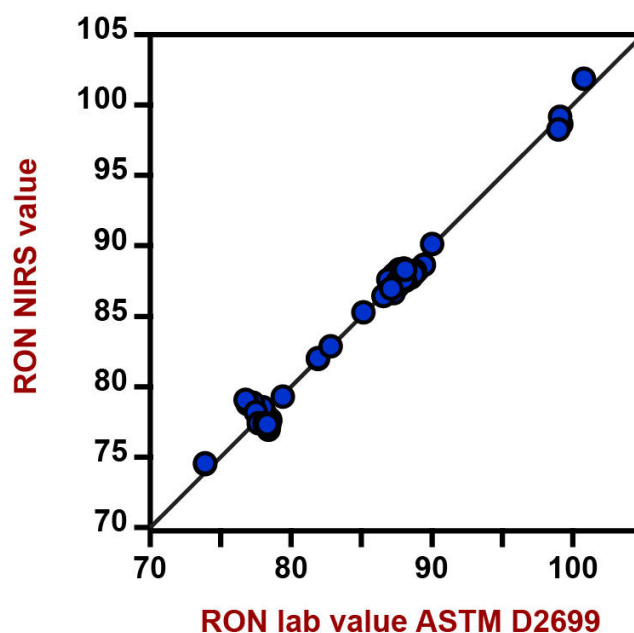


Figure 3. Correlation diagram and the respective figures of merit for the prediction of RON value using a DS2500 Liquid Analyzer. The lab value was evaluated according to ASTM D2699.

Figures of Merit	Value
R^2	0.986
Standard Error of Calibration	0.73
Standard Error of Cross-Validation	0.76

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

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)