



Application Note AN-NIR-080

# Quality Control of Diesel

Fast and straightforward determination of cetane index, flash point, CFPP, D95, and viscosity with NIRS

The cetane index (ASTM D613), flash point (ASTM D56), cold filter plug point (CFPP) (ASTM D6371), D95 (ISO 3405), and viscosity at 40 ° C (ISO 3104) are key parameters to determine for diesel quality. The primary test methods are labor intensive and challenging due to the need to use different analytical methods.

This application note demonstrates that the XDS

RapidLiquid Analyzer, operating in the visible and near-infrared spectral region (Vis-NIR) provides a **cost-efficient and fast** solution for the **simultaneous determination** of these key parameters in diesel. Vis-NIR spectroscopy allows for the analysis of diesel in **less than one minute without sample preparation or using any chemical reagents**.

## EXPERIMENTAL EQUIPMENT

Diesel samples were measured in transmission mode with a XDS RapidLiquid Analyzer (RLA) over the full wavelength range (400–2500 nm). The built-in temperature controlled sample chamber was set to 30 ° C to provide a stable sample environment. For convenience reasons, disposable vials with a path length of 8 mm were used, which made a cleaning procedure obsolete. The Metrohm software package Vision Air Complete was used for data acquisition and prediction model development.



**Figure 1.** XDS RapidLiquid Analyzer with 8 mm disposable vial filled with a diesel sample.

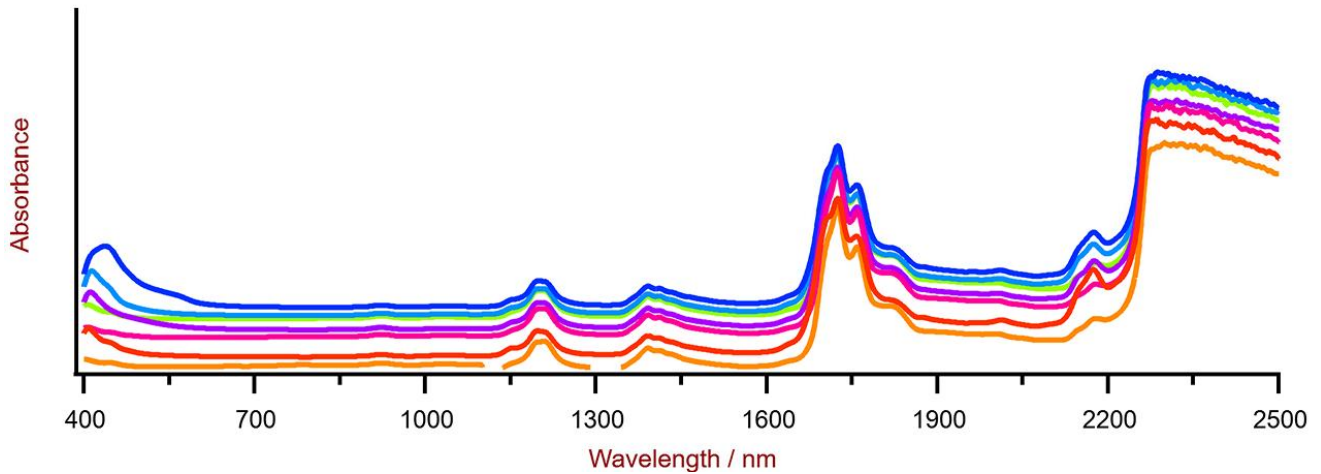
**Table 1.** Hardware and software equipment overview

Equipment	Metrohm number
XDS RapidLiquid Analyzer	2.921.1410
Disposable vials, 8 mm diameter, transmission	6.7402.000
Vision Air 2.0 Complete	6.6072.208

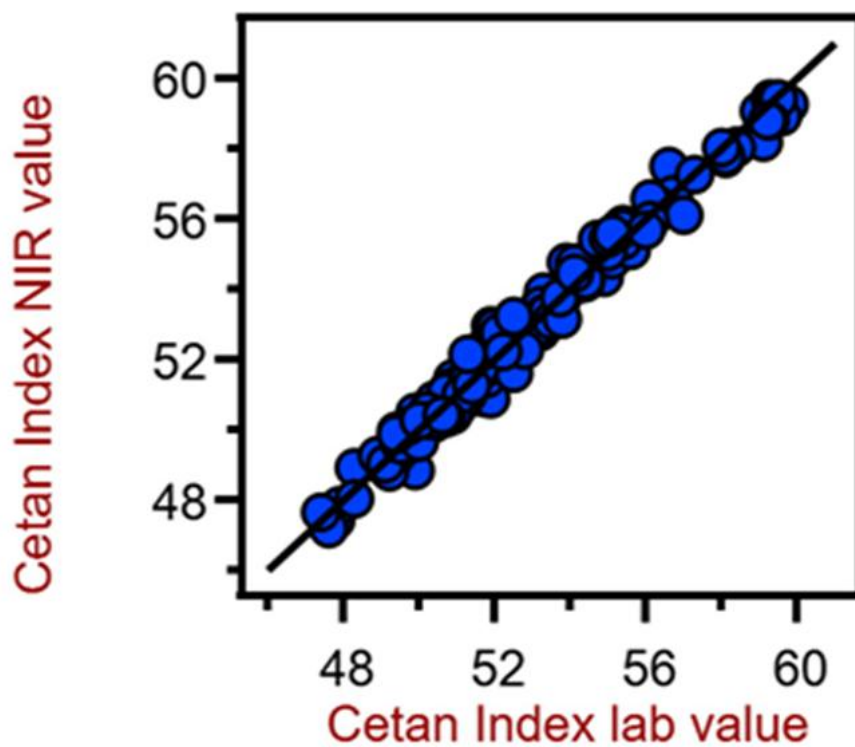
## RESULTS

The obtained Vis-NIR spectra (**Figure 2**) were used to create prediction models for the determination of key diesel parameters. The quality of the prediction models was evaluated using correlation diagrams, which display the

correlation between Vis-NIR prediction and primary method values. The respective figures of merit (FOM) display the expected precision of a prediction during routine analysis.



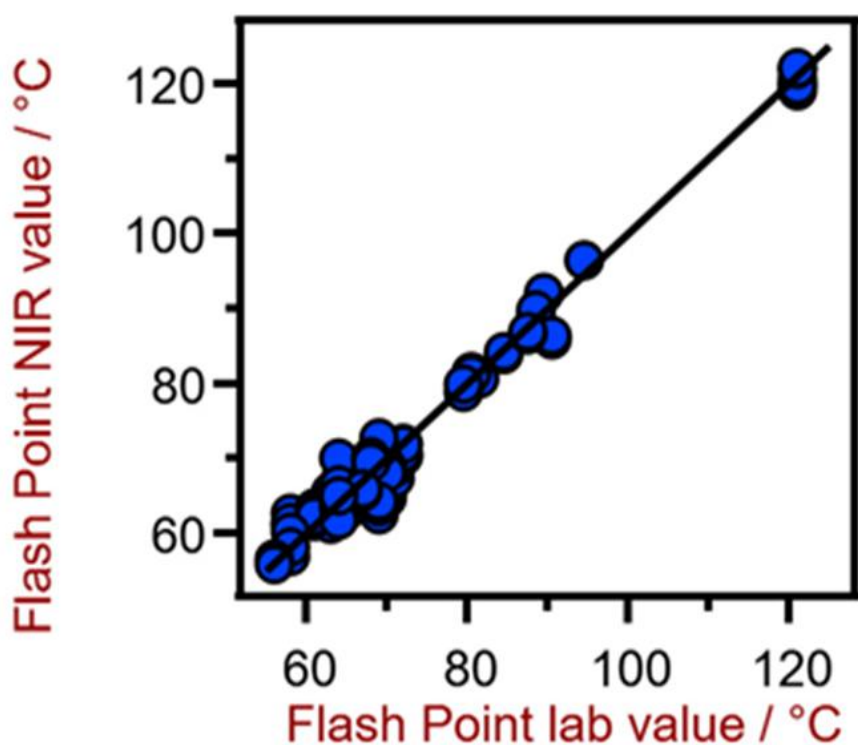
**Figure 2.** Selection of diesel Vis-NIR spectra obtained using a XDS RapidLiquid Analyzer and 8 mm disposable vials. For display reasons a spectra offset was applied.



**Figure 3.** Correlation diagram for the prediction of the cetane index using a XDS RapidLiquid Analyzer. The cetane index lab value was calculated based on the density and distillation range.

**Table 2.** Figures of merit for the prediction of the cetane index using a XDS RapidLiquid Analyzer.

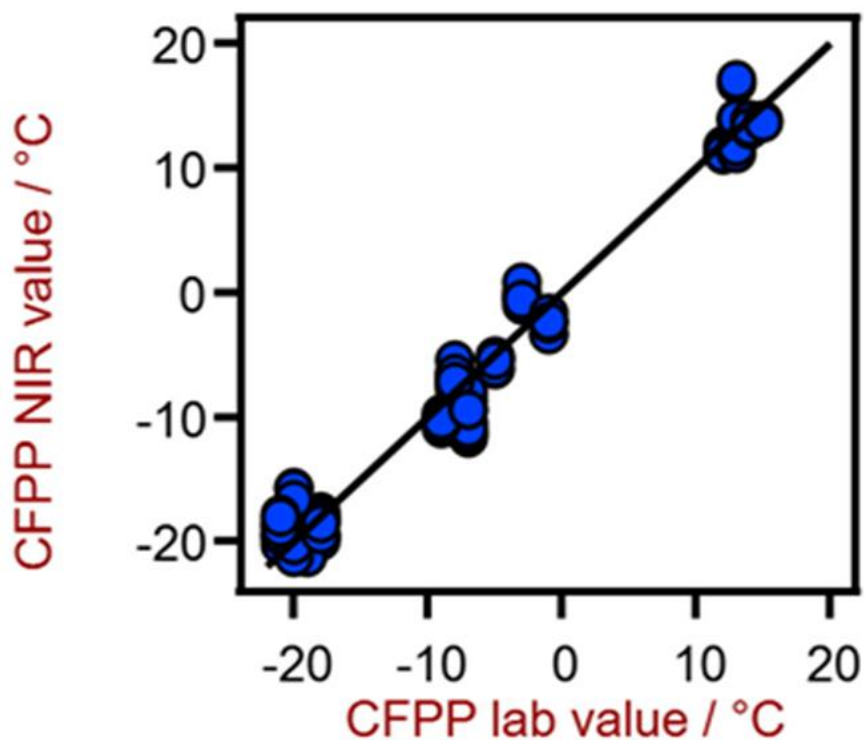
Figures of merit	Value
R <sup>2</sup>	0.991
Standard error of calibration	0.093
Standard error of cross-validation	0.143



**Figure 4.** Correlation diagram for the prediction of the flash point using a XDS RapidLiquid Analyzer. The flash point lab value was evaluated using a dedicated flash point analyzer.

**Table 3.** Figures of merit for the prediction of the flash point using a XDS RapidLiquid Analyzer.

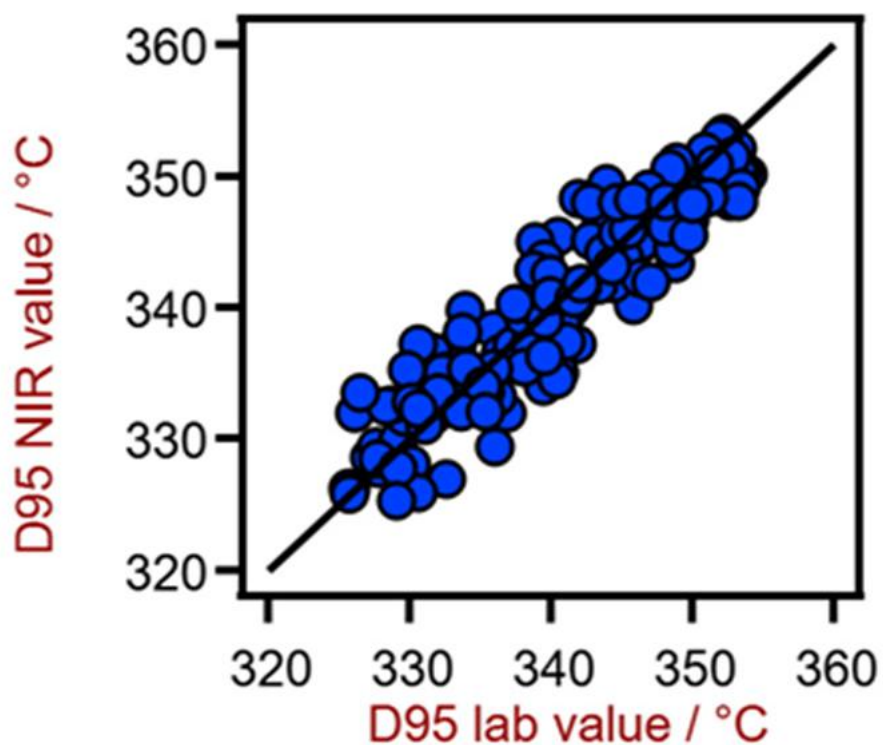
Figures of merit	Value
R <sup>2</sup>	0.977
Standard error of calibration	2.22 ° C
Standard error of cross-validation	2.50 ° C



**Figure 5.** Correlation diagram for the prediction of CFPP using a XDS RapidLiquid Analyzer. The lab value was evaluated using flow meters.

**Table 4.** Figures of merit for the prediction of CFPP using a XDS RapidLiquid Analyzer.

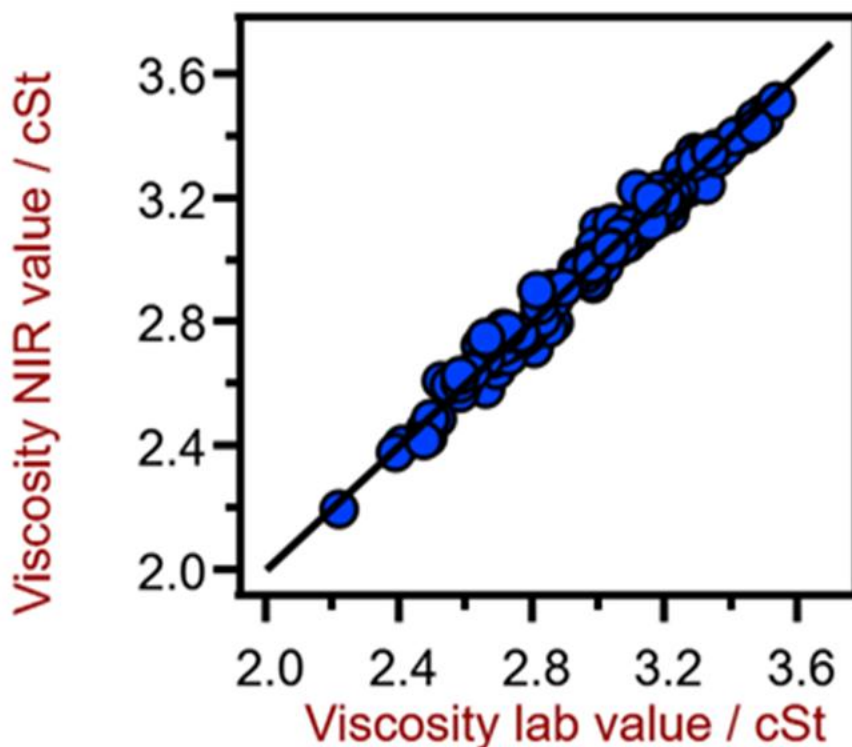
Figures of merit	Value
R <sup>2</sup>	0.973
Standard error of calibration	1.99 ° C
Standard error of cross-validation	2.24 ° C



**Figure 6.** Correlation diagram for the prediction of D95 value using a XDS RapidLiquid Analyzer. The D95 lab value was evaluated using distillation.

**Table 5.** Figures of merit for the prediction of D95 using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R <sup>2</sup>	0.861
Standard error of calibration	3.07 ° C
Standard error of cross-validation	3.47 ° C



**Figure 7.** Correlation diagram for the prediction of the viscosity at 40 ° C using a XDS RapidLiquid Analyzer. The viscosity lab value was evaluated using viscometry.

**Table 6.** Figures of merit for the prediction of the viscosity at 40 ° C using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R <sup>2</sup>	0.983
Standard error of calibration	0.038 cSt
Standard error of cross-validation	0.047 cSt

## CONCLUSION

This study demonstrates the feasibility of NIR spectroscopy for the analysis of the key parameters of diesel samples. In comparison to the standard methods, **no sample preparation is needed**. Samples are analyzed as they are, which allows for simple operation when using NIR

spectroscopy.

To view the information for all key parameters and to get the latest information, please check out our precalibrations:

[Pre-calibrations](#)

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### NIRS XDS RapidLiquid Analyzer

あらゆる種類の液体および懸濁液の迅速で正確な分析。

NIRS XDS RapidLiquid Analyzerは、液体製剤および物質の迅速で正確な分析を可能にします。ボタンを押すだけで正確な測定結果が得られるため、NIRS XDS RapidLiquid Analyzerはラボおよびプロセスにおける品質管理のための信頼性が高くシンプルなソリューションです。サンプルは、再使用可能な石英製キュベットまたは使い捨てガラス製ハイアルに置かれます。温度調整されたサンプルコンパートメントは、再現性のある分析条件、およびそれによる正確な測定結果を保証します。





## Vision Air 2.0 Complete

Vision Air - 汎用性に優れた分光法ソフトウェア。

Vision Air Complete は、規制環境下での使用のための、操作の容易な最新のソフトウェアソリューションです。

Vision Air の利点の概要:

- 調整済みのユーザーインターフェースを伴う個別のソフトウェアアプリケーションにより、直観的かつ容易な操作が保証されます。
- 作業手順の容易な作成およびメンテナンス
- 安全かつ容易なデータ管理のための SQL データベース

バージョン Vision Air Complete (66072208) には、可視近赤外分光法を用いた品質管理のための全てのアプリケーションが含まれています:

- 装置管理およびデータ管理のためのアプリケーション
- メソッド開発のためのアプリケーション
- ルーチン分析のためのアプリケーション

その他の Vision Air Complete ソリューション:

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