



NIR APPLICATION NOTE NIR-080

# Quality Control of Diesel

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

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.

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

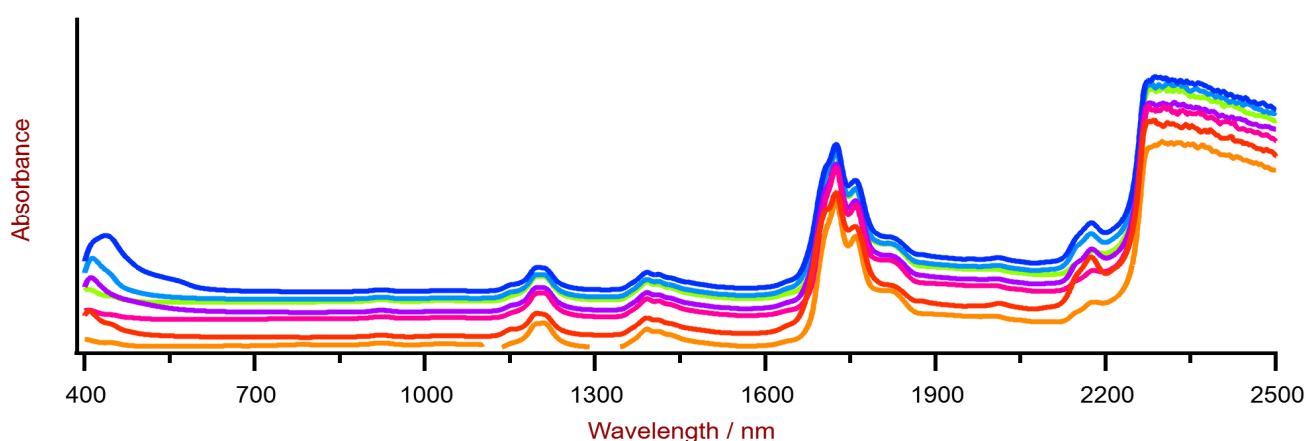
Equipment	Metrohm number
XDS RapidLiquid Analyzer	2.921.1410
Disposable vials, 8 mm diameter, transmission	6.7402.000
Vision Air 2.0 Complete	6.6072.208



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

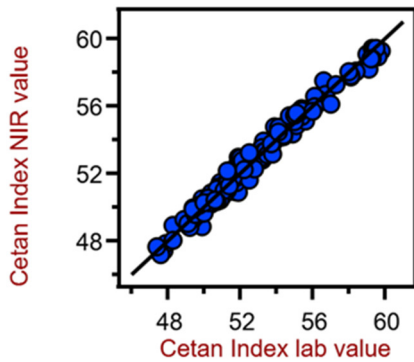
## RESULT

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.

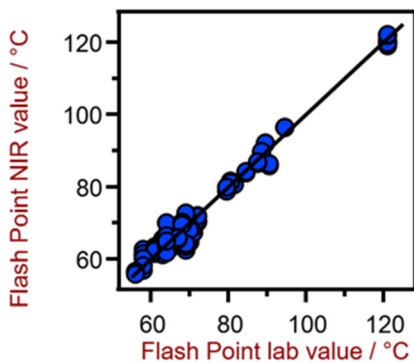
### RESULT CETANE INDEX



Figures of Merit	Value
R <sup>2</sup>	0.991
Standard Error of Calibration	0.093
Standard Error of Cross-Validation	0.143

Figure 3. Correlation diagram and the respective figures of merit 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.

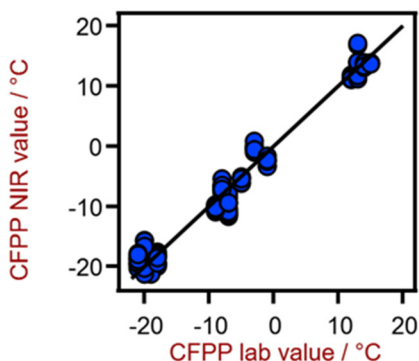
### RESULT FLASH POINT



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 4. Correlation diagram and the respective figures of merit for the prediction of Flash Point using a XDS RapidLiquid Analyzer. The flash point lab value was evaluated using a dedicated flash point analyzer.

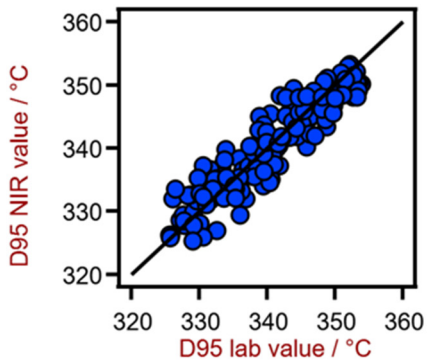
### RESULT CFPP



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 5. Correlation diagram and the respective figures of merit for the prediction of CFPP using a XDS RapidLiquid Analyzer. The lab value was evaluated using flow meters.

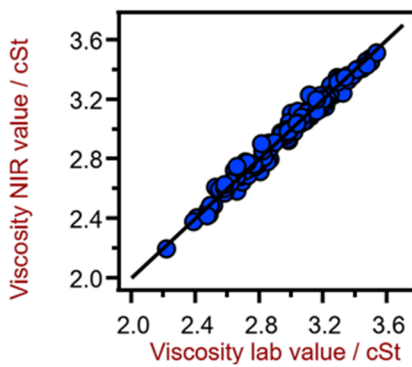
## RESULT D95



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

## RESULT VISCOSITY



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

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

## 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 pre-calibrations:

[www.metrohm.com/pre-calibrations](http://www.metrohm.com/pre-calibrations)

Analytes:	Cetane Index, Flash Point, Viscosity, CFPP, D 95
Matrix:	Diesel
Industry:	Petrochemical Industry
Standards:	ASTM E1655

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