



Application Note AN-NIR-022

Automated quality control of gasoline using NIR spectroscopy

Rapid determination of AKI, RON, MON, density, oxygenates, benzene, olefins, and aromatic content in gasoline

Determining the key quality parameters of gasoline, namely research octane number (RON), motor octane number (MON), anti-knock index (AKI), oxygenates, benzene, olefins, and aromatic content, conventionally requires several laborious analytical methods which need trained personnel. This Application Note demonstrates that the OMNIS NIR Analyzer Liquid, operating in the near-infrared (NIR)

spectral region, provides a cost-efficient, fast solution for the multiparameter analysis of gasoline. Its precise temperature control ensures that all samples are measured in compliance with ASTM D8340, ASTM D8321, and ASTM D6122. The system offers fully automated operation when combined with the OMNIS Sample Robot M – NIR.

EXPERIMENTAL EQUIPMENT

Gasoline fuel samples were measured with an OMNIS NIR Analyzer Liquid (Figure 1) in transmission mode (1000–2250 nm) at 30 °C. The OMNIS Sample Robot M – NIR was used for fully automated sample measurement with disposable vials (8 mm pathlength). The vials are closed, reducing the flammability risk for fuel samples to an absolute minimum. All data acquisition and prediction model development was performed with OMNIS Software.



Figure 1. OMNIS NIR Analyzer Liquid combined with OMNIS Sample Robot M – NIR.

RESULT

The NIR spectra (Figure 2), along with the corresponding reference values, were used to create prediction models for quantification of RON, MON, AKI, density, oxygenates, benzene, olefins, and aromatic content in gasoline samples. The quality of the prediction models was evaluated using correlation diagrams (Figures 3–10). These

diagrams display very high correlations between the NIR predictions and the measured values of different parameters using lengthy conventional methods. Out of the total, 25% of the samples were selected as the validation set and the other 75% as a calibration set. The respective figures of merit (FOM) display the expected precision during routine analysis.

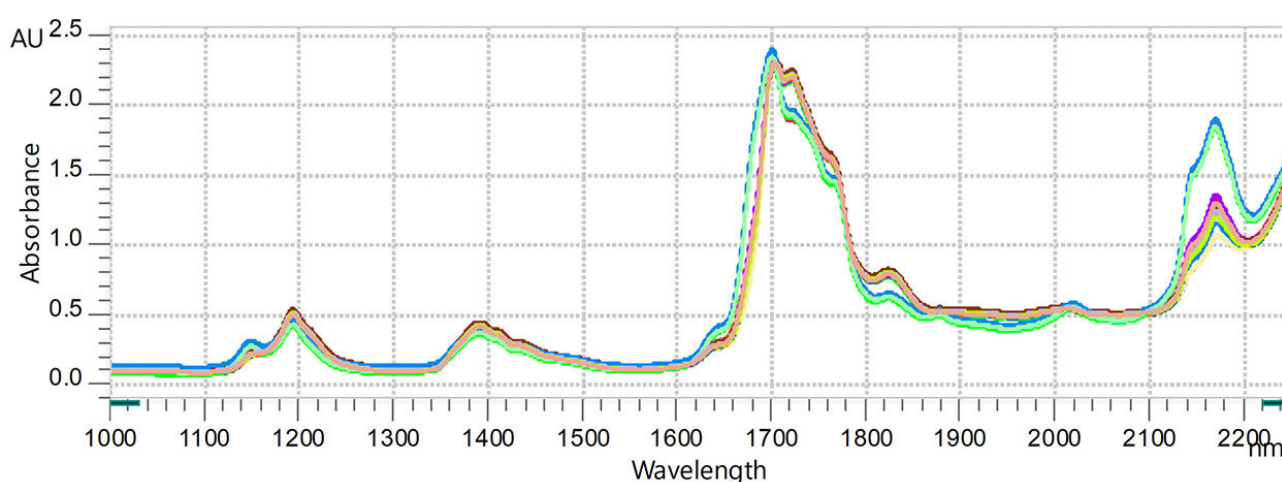


Figure 2. Stacked collection of NIR spectra from gasoline samples analyzed with the OMNIS NIR Analyzer Liquid.

RESULT AKI IN GASOLINE

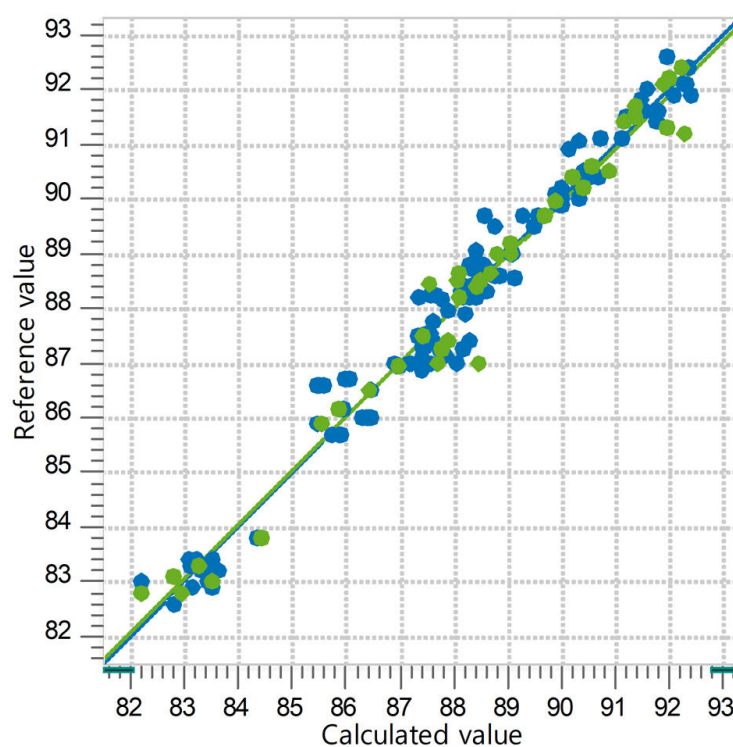


Figure 3. Correlation diagram and the respective figures of merit for the prediction of gasoline AKI using an OMNIS NIR Analyzer Liquid. The reference lab values were determined according to CFR engine tests under controlled conditions. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2_P	SEC	SECV	SEP
0.974	0.41	0.43	0.45

RESULT MON IN GASOLINE

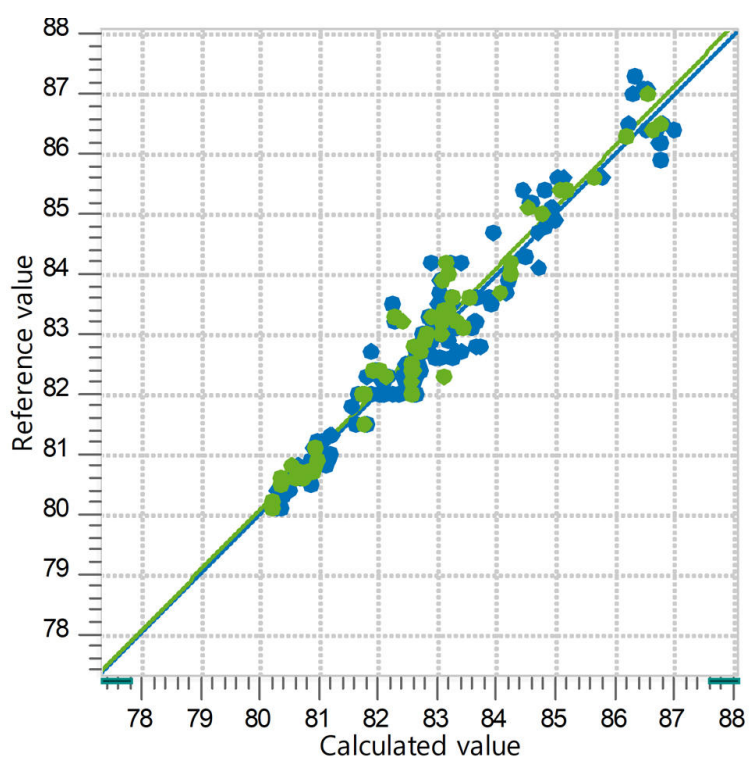


Figure 4. Correlation diagram and the respective figures of merit for the prediction of gasoline MON using an OMNIS NIR Analyzer Liquid. The reference lab values were determined according to CFR engine tests under controlled conditions. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2_P	SEC	SECV	SEP
0.958	0.35	0.39	0.37

RESULT RON IN GASOLINE

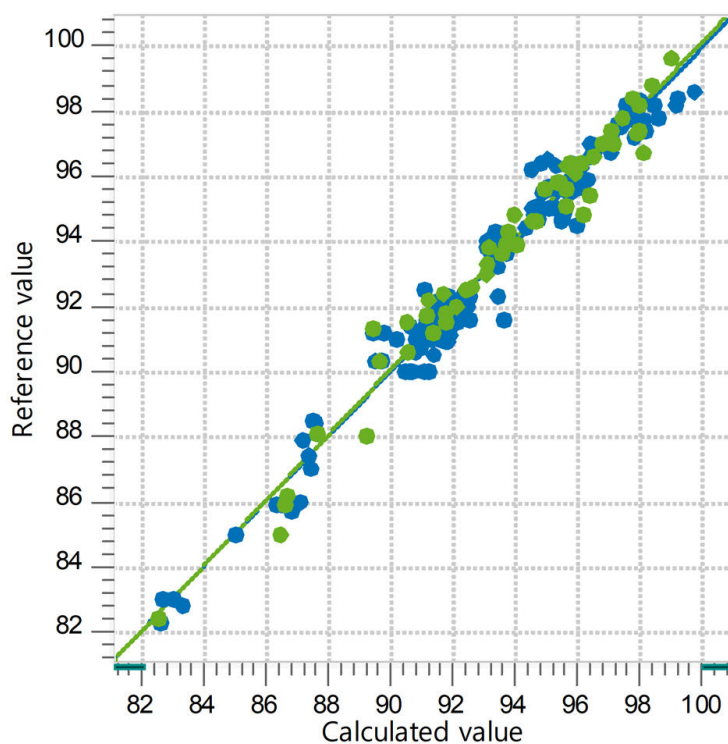


Figure 5. Correlation diagram and the respective figures of merit for the prediction of gasoline RON using an OMNIS NIR Analyzer Liquid. The reference lab values were determined according to CFR engine tests under controlled conditions. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2_P	SEC	SECV	SEP
0.970	0.58	0.64	0.64

RESULT OLEFINS IN GASOLINE

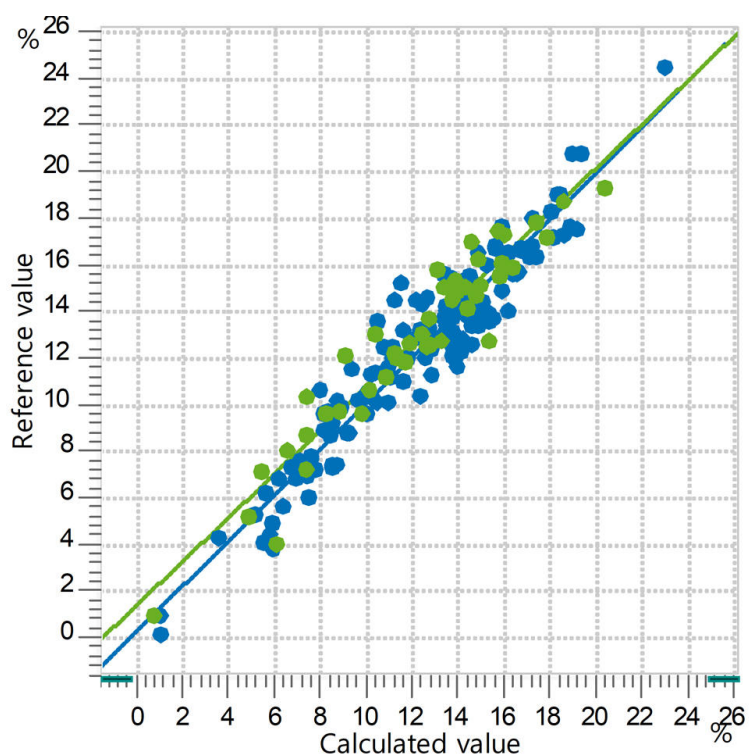


Figure 6. Correlation diagram and the respective figures of merit for the prediction of gasoline olefins using an OMNIS NIR Analyzer Liquid. The reference lab values were determined according to gas chromatography. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2P	SEC (%)	SECV (%)	SEP (%)
0.916	1.12	1.22	1.31

RESULT DENSITY IN GASOLINE

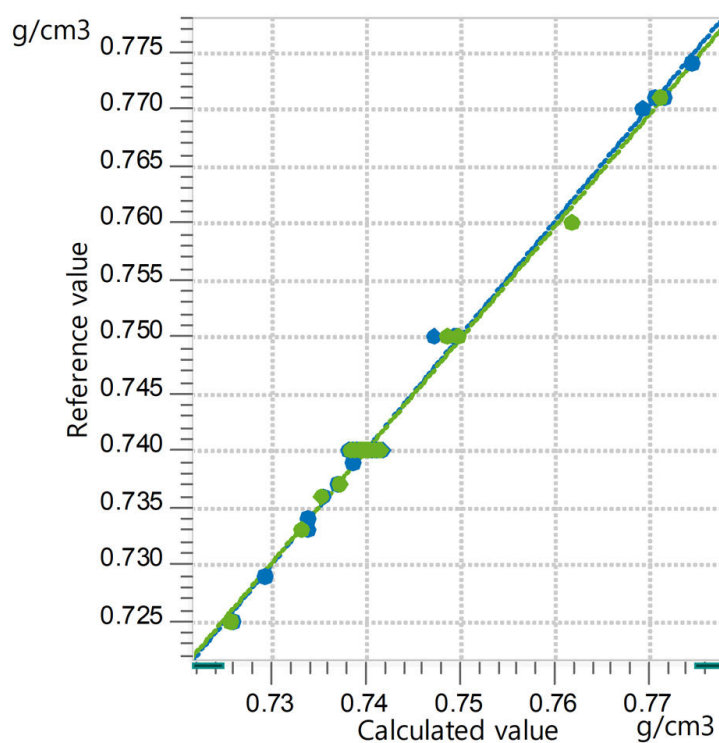


Figure 7. Correlation diagram and the respective figures of merit for the prediction of gasoline density using an OMNIS NIR Analyzer Liquid. The reference lab values were determined using a density meter. The calibration dataset is shown in blue, and the external validation dataset is in green.

R ² P	SEC (g/cm ³)	SECV (g/cm ³)	SEP (g/cm ³)
0.991	0.0007	0.0007	0.0009

RESULT AROMATICS IN GASOLINE

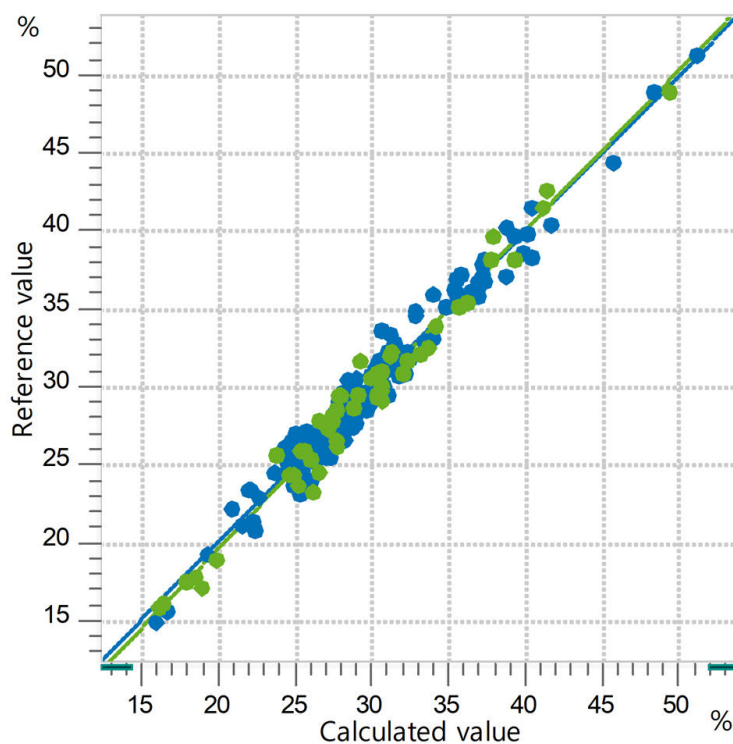


Figure 8. Correlation diagram and the respective figures of merit for the prediction of gasoline aromatic content using an OMNIS NIR Analyzer Liquid. The reference lab values were determined using gas chromatography. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2_P	SEC (%)	SECV (%)	SEP (%)
0.973	0.94	1.09	0.973

RESULT BENZENE IN GASOLINE

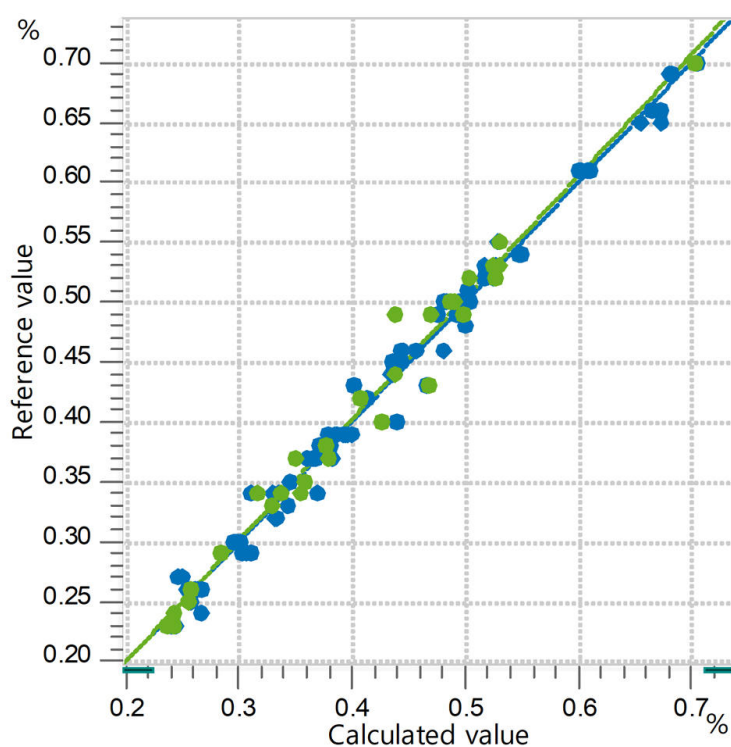


Figure 9. Correlation diagram and the respective figures of merit for the prediction of gasoline benzene content using an OMNIS NIR Analyzer Liquid. The reference lab values were determined using gas chromatography. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2_P	SEC (%)	SECV (%)	SEP (%)
0.979	0.01	0.01	0.02

RESULT OXYGENATES IN GASOLINE

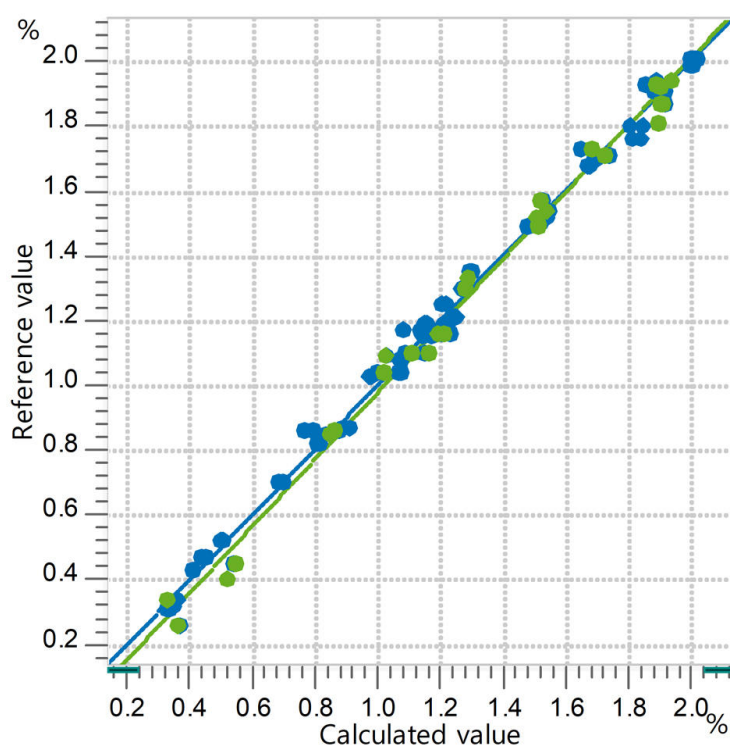


Figure 10. Correlation diagram and the respective figures of merit for the prediction of oxygenates in gasoline using an OMNIS NIR Analyzer Liquid. The reference lab values were determined using gas chromatography. The calibration dataset is shown in blue, and the external validation dataset is in green.

R ² P	SEC (%)	SECV (%)	SEP (%)
0.992	0.0398	0.0435	0.0496

CONCLUSION

This Application Note shows the feasibility of using NIR spectroscopy for gasoline quality testing. Compared to wet chemical methods, the time to result is a major advantage of NIRS. Each measurement is performed in a few seconds, and all parameters are measured simultaneously. The

possibility of fully automated analysis in combination with the OMNIS Sample Robot M – NIR increases throughput, maximizing gasoline quality control efficiency. With the OMNIS gasoline pre-calibration (6.06008.008), users can measure all the mentioned parameters from day one.

CONTACT

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CONFIGURATION



OMNIS NIR Analyzer Liquid

Near-infrared spectrometer for liquid samples.

Developed and produced in accordance with Swiss quality standards, the OMNIS NIR Analyzer is the near-infrared spectroscopy (NIRS) solution for routine analysis along the entire production chain. Its application of the latest technologies and its integration in the modern OMNIS Software are reflected in its speed, operability, and flexible utilization of this NIR spectrometer.

Overview of the advantages of the OMNIS NIR Analyzer Liquid:

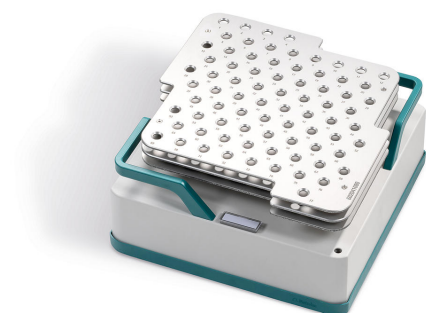
- Measurements of liquid samples in less than 10 seconds
- Temperature control on the sample from 25–80 °C
- Automatic detection of the insertion and removal of the sample vessel
- Simple integration in an automation system or link with additional analysis technologies (titration)
- Supports numerous sample vessels with different path lengths



OMNIS Sample Robot M – NIR

OMNIS Sample Robot M – NIR for the direct transition to fully automated spectroscopy. The system provides space for 3 sample racks for up to 231 vials with diameters of 8–28 mm.

The OMNIS Sample Robot M – NIR supports the analyses of both liquid and solid samples.



OMNIS sample rack 77 x 8 mm

OMNIS sample rack for OMNIS Sample Robot – NIR suitable for 77 disposable vials with an optical path length of 8 mm for measurements in transmission (6.7402.240).



Holder OMNIS NIR, vial, 8 mm

Vial Holder for the OMNIS NIR Analyzer for 8 mm disposable vials (6.7402.240).



Disposable vial, 8 mm, transmission, qty. 100

100 disposable glass vials (borosilicate) with an optical path length of 8 mm for analyses of liquids in transmission. The disposable vials are supplied with the associated stoppers (number of pieces = 100).

Compatible with:

- Holder OMNIS NIR, vial, 8 mm (6.07401.070)
- DS2500 holder for 8 mm disposable vials (6.7492.020)

OMNIS

A WHOLE NEW LEVEL OF PERFORMANCE

OMNIS stand-alone license with 2 instrument licenses

Enables stand-alone operation of the OMNIS Software on a Windows™ computer.

Features:

- The license already includes two OMNIS instrument licenses.
- Must be activated via the Metrohm licensing portal.

OMNIS

A WHOLE NEW LEVEL OF PERFORMANCE

Software license Quant Development

Software license for the creation and editing of quantification models in a stand-alone OMNIS Software installation.