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.

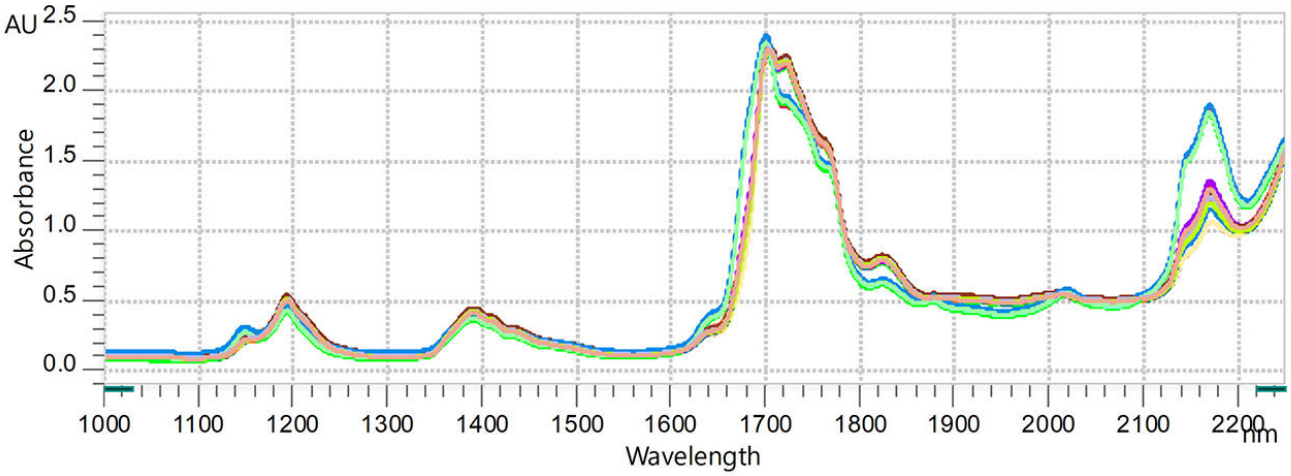

Figure 2. Stacked collection of NIR spectra from gasoline samples analyzed with the OMNIS NIR Analyzer Liquid.

RESULT AKI IN GASOLINE

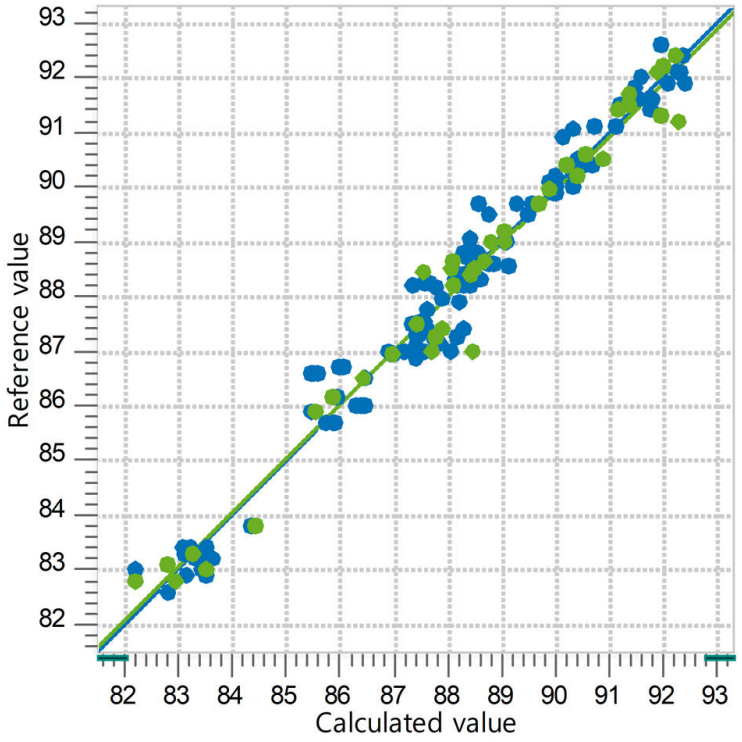

Figure 3. Correlation diagram and the respective figures of merit for the prediction of gasoline AKI using an OMNIS NIR Analyzer Liquid. The reference lab values were determined according to CFR engine tests under controlled conditions. The calibration dataset is shown in blue, and the external validation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

R^2P	SEC	SECV	SEP
0.974	0.41	0.43	0.45

RESULT MON IN GASOLINE

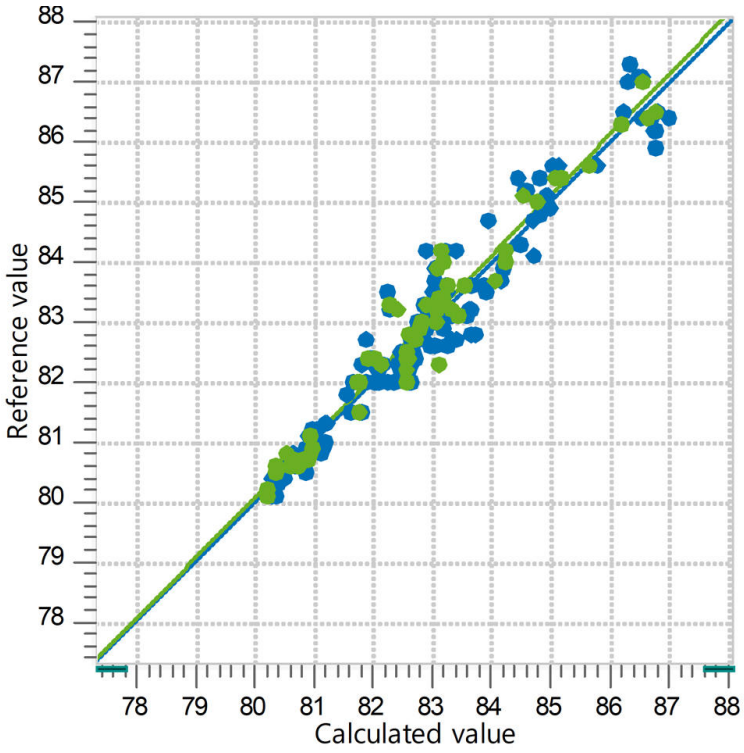

Figure 4. Correlation diagram and the respective figures of merit for the prediction of gasoline MON using an OMNIS NIR Analyzer Liquid. The reference lab values were determined according to CFR engine tests under controlled conditions. The calibration dataset is shown in blue, and the external validation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

R^2P	SEC	SECV	SEP
0.958	0.35	0.39	0.37

RESULT RON IN GASOLINE

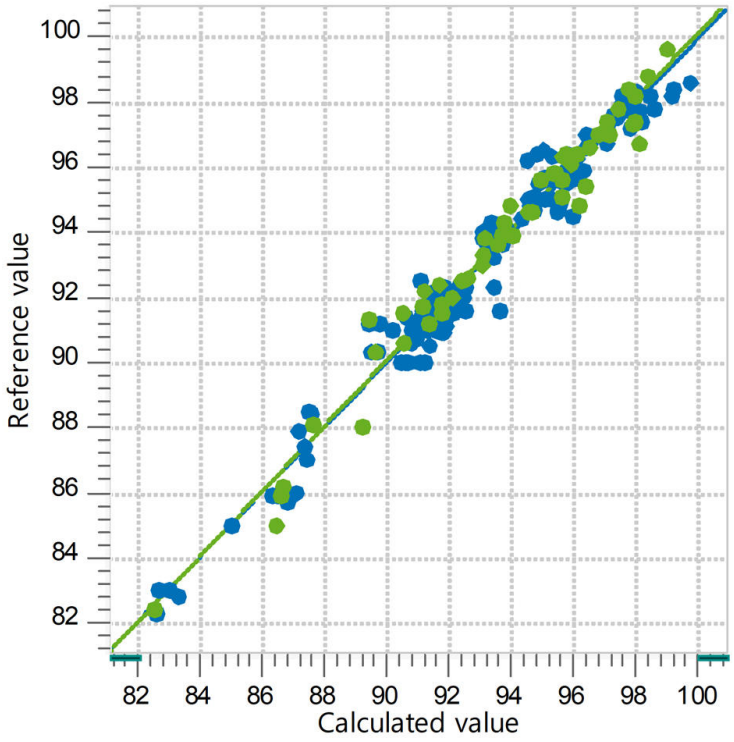

Figure 5. Correlation diagram and the respective figures of merit for the prediction of gasoline RON using an OMNIS NIR Analyzer Liquid. The reference lab values were determined according to CFR engine tests under controlled conditions. The calibration dataset is shown in blue, and the external validation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

R^2P	SEC	SECV	SEP
0.970	0.58	0.64	0.64

RESULT OLEFINS IN GASOLINE

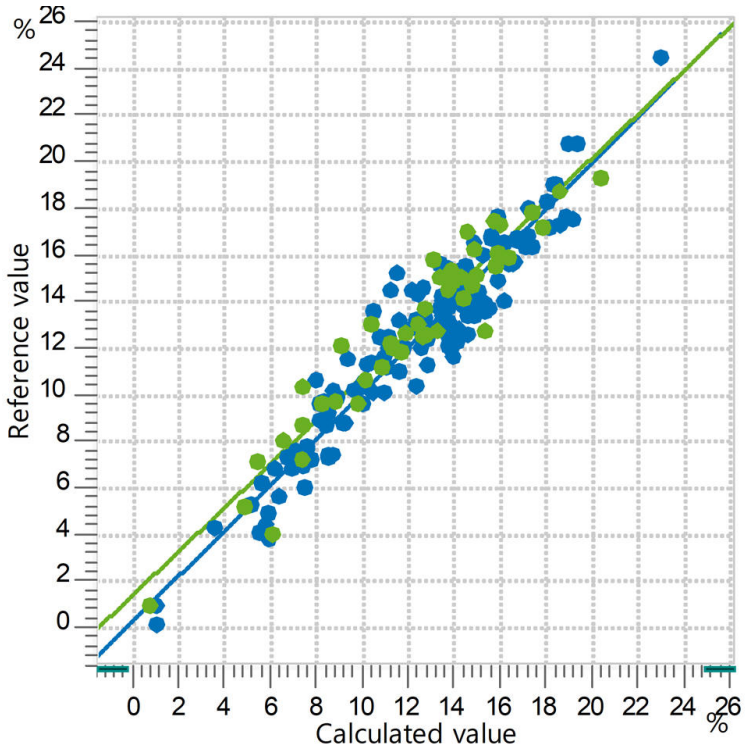

Figure 6. Correlation diagram and the respective figures of merit for the prediction of gasoline olefins using an OMNIS NIR Analyzer Liquid. The reference lab values were determined according to gas chromatography. The calibration dataset is shown in blue, and the external validation dataset is in green.

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

RESULT DENSITY IN GASOLINE

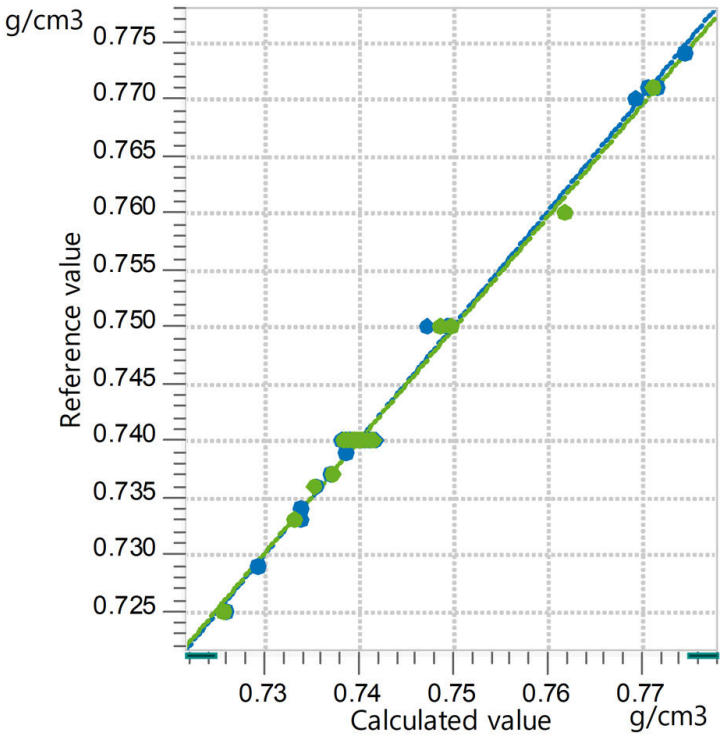

Figure 7. Correlation diagram and the respective figures of merit for the prediction of gasoline density using an OMNIS NIR Analyzer Liquid. The reference lab values were determined using a density meter. The calibration dataset is shown in blue, and the external validation dataset is in green.

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

RESULT AROMATICS IN GASOLINE

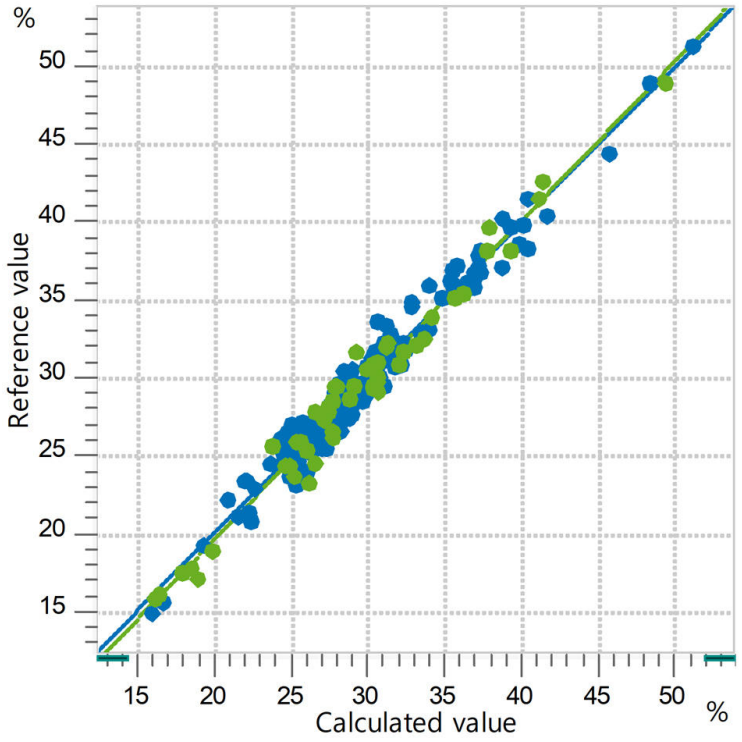

Figure 8. Correlation diagram and the respective figures of merit for the prediction of gasoline aromatic content using an OMNIS NIR Analyzer Liquid. The reference lab values were determined using gas chromatography. The calibration dataset is shown in blue, and the external validation dataset is in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

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

RESULT BENZENE IN GASOLINE

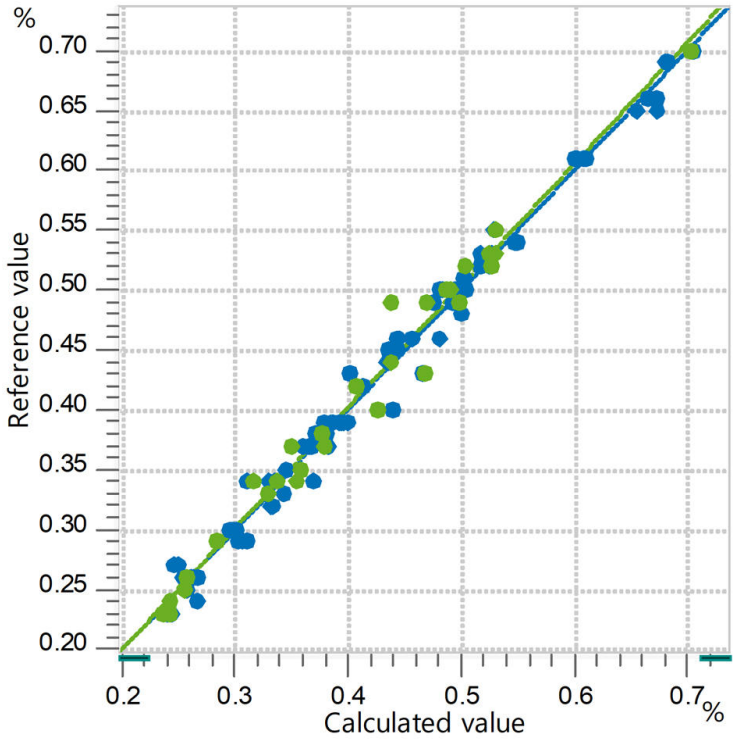

Figure 9. Correlation diagram and the respective figures of merit for the prediction of gasoline benzene content using an OMNIS NIR Analyzer Liquid. The reference lab values were determined using gas chromatography. The calibration dataset is shown in blue, and the external validation dataset is in green.

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

RESULT OXYGENATES IN GASOLINE

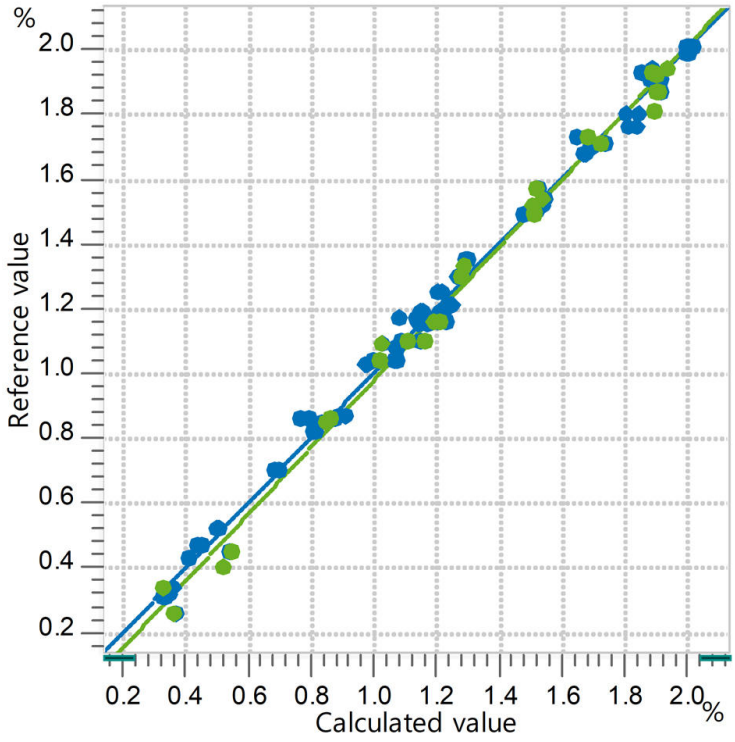

Figure 10. Correlation diagram and the respective figures of merit for the prediction of oxygenates in gasoline using an OMNIS NIR Analyzer Liquid. The reference lab values were determined using gas chromatography. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2P	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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info@metrohm.fr

CONFIGURATION

OMNIS NIR Analyzer Liquid

Spectromètre proche infrarouge pour échantillons liquides.

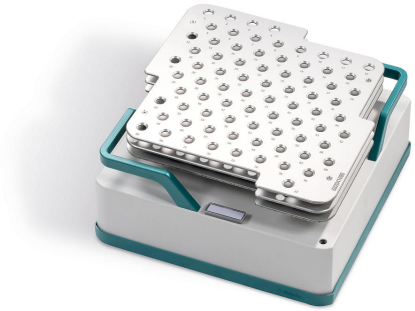
L'OMNIS NIR Analyzer est la solution de spectroscopie proche infrarouge (NIRS) développée et produite selon les normes de qualité suisses pour les analyses de routine tout au long de la chaine de fabrication. L'application des technologies les plus récentes et l'intégration dans le logiciel OMNIS moderne se reflètent dans la vitesse, le maniement et la flexibilité d'utilisation de ce spectromètre NIR.

Apercu des avantages de l'OMNIS NIR Analyzer Liquid :

- Mesures d'échantillons liquides en moins de 10 secondes
- Régulation de température sur l'échantillon de 25 à 80 °C
- Détection automatique de l'insertion et du retrait d'échantillons du récipient d'échantillon
- Intégration simple dans un système d'automatisation ou liaison avec d'autres technologies d'analyse (titrage)
- Prise en charge de nombreux récipients d'échantillon de différentes longueurs de chemin

OMNIS Sample Robot M – NIR

OMNIS Sample Robot M – NIR permet de passer directement à la spectroscopie entièrement automatisée. Ce système prévoit trois emplacements de rack d'échantillons pour maximum 231 flacons d'un diamètre de 8 à 28 mm.
L'OMNIS Sample Robot M – NIR permet d'analyser aussi bien des échantillons liquides que solides.



Rack d'échantillons OMNIS 77 x 8 mm

Rack d'échantillons OMNIS pour OMNIS Sample Robot – NIR, pouvant accueillir 77 flacons à usage unique avec une longueur de chemin optique de 8 mm pour des mesures en transmission (6.7402.240).

Support OMNIS NIR, flacon, 8 mm

Support de flacon pour l'OMNIS NIR Analyzer pour flacons à usage unique de 8 mm (6.7402.240).

Flacon à usage unique, 8 mm, transmission, Qté 100

100 flacons en verre (borosilicate) à usage unique avec une longueur de chemin de 8 mm pour des analyses de liquides lors d'une transmission. Les flacons à usage unique sont fournis avec les bouchons de fermeture correspondants (quantité = 100).
Compatible avec :

- Support OMNIS NIR, flacon, 8 mm (**6.07401.070**)
- Support DS2500 pour flacons à usage unique 8 mm (**6.7492.020**)

OMNIS
A WHOLE NEW LEVEL OF PERFORMANCE

Licence OMNIS autonome avec 2 licences appareil

Elle permet l'utilisation du mode autonome du logiciel OMNIS sur un ordinateur WindowsTM.
Caractéristiques :

- La licence comprend déjà deux licences pour appareils OMNIS.
- Elle doit être activée via le portail d'octroi de licences Metrohm.

OMNIS
A WHOLE NEW LEVEL OF PERFORMANCE

Licence logicielle Quant Development

Licence logicielle pour la création et l'édition de modèles de quantification dans une installation du logiciel OMNIS Stand-Alone.