



Application Note AN-NIR-068

# Quality Control of Isocyanates

## Chemical-free and fast determination of isocyanate content with NIRS

Determination of isocyanates (ASTM D7252) is a challenging procedure due to the reactivity of these organic species with atmospheric moisture, as well as their toxicity. Furthermore, HPLC analysis typically used for this kind of analysis involves sample preparation steps and chemicals, with each measurement taking up to 20 minutes to complete.

This application note demonstrates that the XDS RapidLiquid Analyzer operating in the visible and near infrared spectral region (Vis-NIR) provides a **chemical-free and fast solution** for determination of isocyanate content. With **no sample preparation needed**, Vis-NIR spectroscopy allows the analysis of isocyanates in **less than a minute**.

## EXPERIMENTAL EQUIPMENT

Isocyanate samples were measured with a XDS RapidLiquid Analyzer in transmission mode over the full wavelength range (400–2500 nm). Reproducible spectrum acquisition was achieved using the built-in temperature control (at 30 °C) of the XDS RapidLiquid Analyzer. For convenience, disposable vials with a path length of 8 mm were used, which made cleaning of the sample vessels unnecessary. The Metrohm software package Vision Air Complete was used for all data acquisition and prediction model development.



**Figure 1.** XDS RapidLiquid Analyzer and an isocyanate sample present in the 8 mm Disposable Vial.

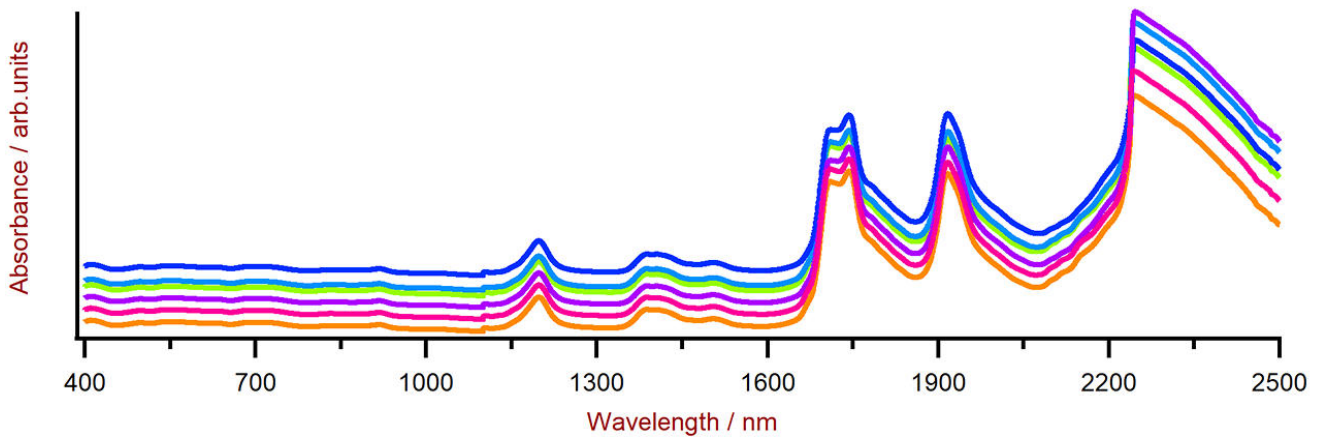
**Table 1.** Hardware and software equipment overview.

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

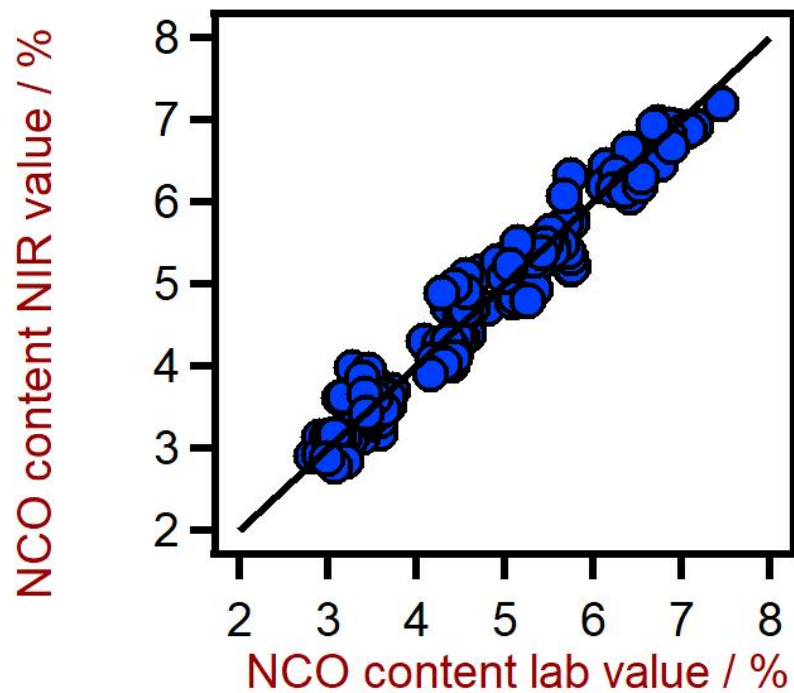
## RESULT

The obtained Vis-NIR spectra (**Figure 2**) were used to create prediction models for quantification of the isocyanate content. The quality of the prediction models was evaluated using correlation diagrams,

which display the relationship 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 Isocyanate 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 isocyanate (NCO) content using a XDS RapidLiquid Analyzer. The isocyanate content lab value was evaluated using titration.

**Table 2.** Figures of merit for the prediction of the isocyanate (NCO) content using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R <sup>2</sup>	0.968
Standard error of calibration	0.24
Standard error of cross-validation	0.26

## CONCLUSION

This study demonstrates the feasibility of NIR spectroscopy for the analysis of isocyanates. In comparison to wet chemical methods (Table 3), the time to result is a major advantage of NIR

spectroscopy, since the isocyanate content is determined **with no sample preparation needed in less than a minute.**

**Table 3.** Time to result overview for the different parameters

Parameter	Method	Time to result
Isocyanate	HPLC	20 min (preparation) + 20 min (HPLC)

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### NIRS XDS RapidLiquid Analyzer

Des analyses rapides et précises de liquides et suspensions de toutes sortes.

L'analyseur NIRS XDS RapidLiquid Analyzer permet des analyses rapides et précises de formules et substances liquides. Des résultats de mesure précis obtenus par simple pression d'une touche font du NIRS XDS RapidLiquid Analyzer une solution aussi fiable que simple pour le contrôle qualité en laboratoire et en production. Les échantillons sont présentés dans des cuvettes en quartz réutilisables ou des flacons en verre à usage unique ; une chambre à échantillons tempérée assure la reproductibilité des conditions d'analyse et, par conséquent, l'exactitude des résultats de mesure.



### Vision Air 2.0 Complete

**Vision Air - logiciel universel de spectroscopie.**

Vision Air Complete est une solution logicielle moderne et simple d'utilisation pour une application dans un environnement réglementé.

Aperçu des avantages de Vision Air :

- Des applications logicielles individuelles avec interface utilisateur adaptée sont le garant d'un maniement intuitif et simple
- Établissement et suivi simples des procédures de travail
- Base de données SQL pour une gestion sûre et simple des données

La version Vision Air Complete (66072208) comprend toutes les applications d'assurance qualité par spectroscopie Vis-NIR :

- Application de gestion des instruments et des données
- Application de développement de méthodes
- Application d'analyse de routine

Autres solutions Vision Air Complete :

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