



Application Note AN-NIR-095

Quality Control of Hand Sanitizers

Multiparameter determination within one minute

The most effective hand sanitizers contain between 62–95% alcohol. Alcohols are effective against most vegetative forms of bacteria, fungi, and enveloped viruses, but are ineffective against bacterial spores. The addition of hydrogen peroxide (3%) to the product may solve this, but due to its corrosive nature it must be handled with caution during production. Additionally, water and small amounts of emollient (e.g. glycerol) are added to protect the skin. Depending on the exact percentage of these constituents, hand sanitizer is either found

in a liquid or gel form. Determination of the concentrations of these reagents is typically performed with gas chromatography (for glycerol and ethanol), Karl Fischer titration (for water), and redox titration (for H_2O_2). The disadvantage is that two different methods are needed which are time-consuming and require chemical reagents. Near-infrared spectroscopy (NIRS) on the other hand allows for the **rapid and reliable simultaneous quantification** of ethanol, glycerol, hydrogen peroxide, and water content in hand sanitizer formulations.

EXPERIMENTAL EQUIPMENT

A total of 98 samples of hand sanitizer gel with different concentrations of glycerol (0.5–3 w/w %), ethanol (70–85 w/w %), and water (20–22 w/w %) were collected to create a prediction model for quantification. A total of 91 samples of liquid hand sanitizer used for sanitizing wipes were measured with different concentrations of ethanol (70–95 w/w %), water (2–40 w/w %), and hydrogen peroxide (0–4 w/w %). All samples were measured with a DS2500 Liquid Analyzer in transmission mode (400–2500 nm). Reproducible spectrum acquisition was achieved using the built-in temperature control at 40 ° C: For convenience, disposable vials with a pathlength 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. DS2500 Liquid Analyzer and a sample filled in a disposable vial.

Table 1. Hardware and software equipment overview

Equipment	Metrohm number
DS2500 Liquid Analyzer	2.929.0010
DS2500 Holder 8 mm vials	6.7492.020
Disposable vials, 8 mm	6.7402.000
Vision Air 2.0 Complete	6.6072.208

RESULTS

All measured Vis-NIR spectra (**Figure 2**) were used to create a prediction model for quantification of the key quality parameters of gel and liquid sanitizer formulations. The quality of the prediction model was evaluated using

correlation diagrams, which display a very high correlation between the Vis-NIR prediction and the reference values. The respective figures of merit (FOM) display the expected precision of a prediction during routine analysis.

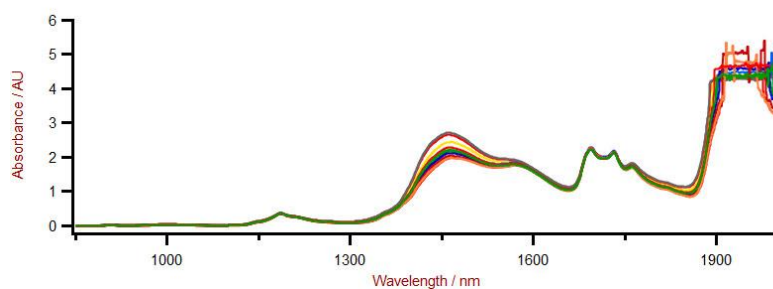


Figure 2. Vis-NIR spectra hand sanitizer gel samples analyzed on a DS2500 Liquid Analyzer.

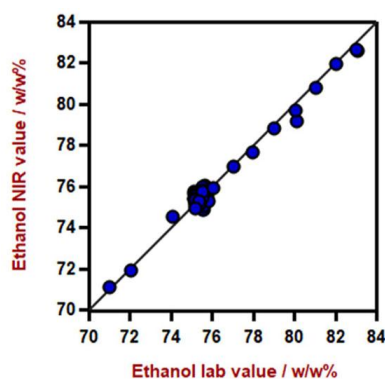


Figure 3. Correlation diagram for the prediction of ethanol content in hand sanitizer gel using a DS2500 Liquid Analyzer. The lab value was evaluated using gas chromatography.

Table 2. Figures of merit for the prediction of ethanol content in hand sanitizer gel using a DS2500 Liquid Analyzer.

Figures of Merit	Value
R^2	0.9832
Standard Error of Calibration	0.33 w/w%
Standard Error of Cross-Validation	0.37 w/w%

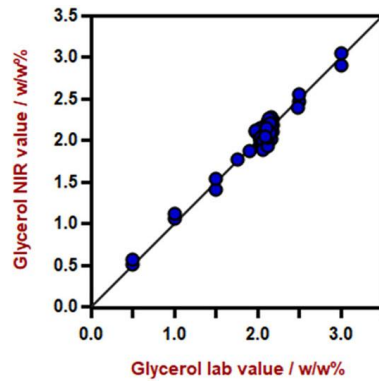


Figure 4. Correlation diagram for the prediction of glycerol content in hand sanitizer gel using a DS2500 Liquid Analyzer. The lab value was evaluated by gas chromatography.

Table 3. Figures of merit for the prediction of glycerol content in hand sanitizer gel using a DS2500 Liquid Analyzer.

Figures of Merit	Value
R ²	0.9632
Standard Error of Calibration	0.08 w/w%
Standard Error of Cross-Validation	0.11 w/w%

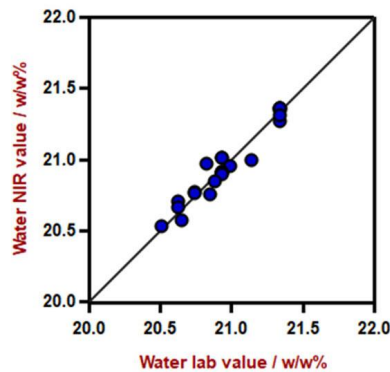


Figure 5. Correlation diagram for the prediction of water content in hand sanitizer gel using a DS2500 Liquid Analyzer. The lab value was evaluated by Karl Fischer titration.

Table 4. Figures of merit for the prediction of water content in hand sanitizer gel using a DS2500 Liquid Analyzer.

Figures of Merit	Value
R ²	0.941
Standard Error of Calibration	0.07 w/w%
Standard Error of Cross-Validation	0.09 w/w%

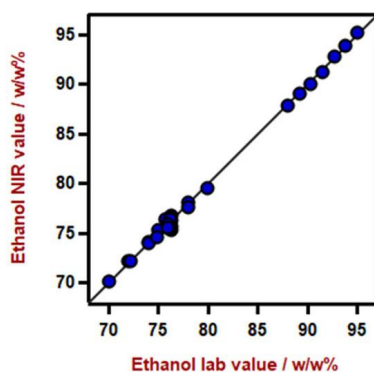


Figure 6. Correlation diagram for the prediction of ethanol content in hand sanitizer wipes using a DS2500 Liquid Analyzer. The lab value was evaluated by gas chromatography.

Table 5. Figures of merit for the prediction of ethanol content in hand sanitizer wipes using a DS2500 Liquid Analyzer.

Figures of Merit	Value
R ²	0.9964
Standard Error of Calibration	0.36 w/w%
Standard Error of Cross-Validation	0.36 w/w%

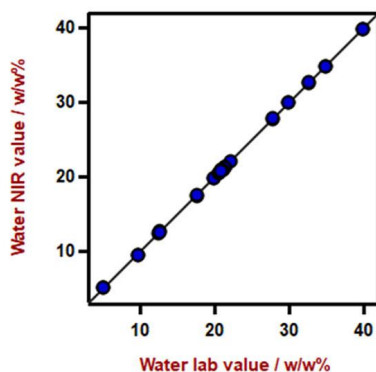


Figure 7. Correlation diagram for the prediction of water content in hand sanitizer wipes using a DS2500 Liquid Analyzer. The lab value was evaluated by Karl Fischer titration.

Table 6. Figures of merit for the prediction of water content in hand sanitizer wipes using a DS2500 Liquid Analyzer.

Figures of Merit	Value
R^2	0.9999
Standard Error of Calibration	0.12 w/w%
Standard Error of Cross-Validation	0.18 w/w%

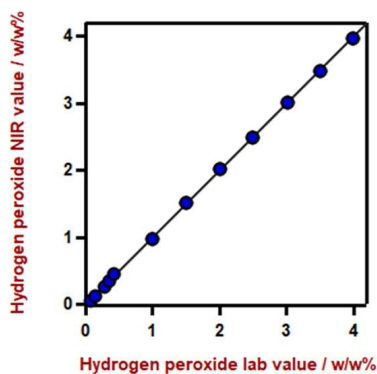


Figure 8. Correlation diagram for the prediction of hydrogen peroxide content in hand sanitizer wipes using a DS2500 Liquid Analyzer. The lab value was evaluated by permanganate titration.

Table 7. Figures of merit for the prediction of hydrogen peroxide content in hand sanitizer wipes using a DS2500 Liquid Analyzer.

Figures of Merit	Value
R ²	0.9986
Standard Error of Calibration	0.05 w/w%
Standard Error of Cross-Validation	0.06 w/w%

CONCLUSION

This application note demonstrates the feasibility to determine multiple key parameters of the quality control of liquid and gel-type hand sanitizer products with NIR spectroscopy. Vis-NIR

spectroscopy enables a fast alternative to primary methods with high accuracy, and therefore represents a suitable alternative to the standard determination methods.

Table 8. Time to result overview for the different parameters

Parameter	Metod	Time to result
Ethanol	GC	~5 minutes (preparation) + ~5 minutes (GC)
Glycerol	GC	~5 minutes (preparation) + ~5 minutes (GC)
Water	Karl Fischer titration	~ 5 minutes
Hydrogen peroxide	Permanganate titration	~5 minutes

CONTACT

メトロームジャパン株式会社
 143-0006 東京都大田区平
 和島6-1-1
 null 東京流通センター アネ
 ックス9階

metrohm.jp@metrohm.jp



DS2500 Liquid Analyzer

ラボおよび生産環境における品質管理用の堅牢な近赤外分光法。

NIRS DS2500 Liquid Analyzerは、生産チェーン全体に沿った液体のルーチン分析に実績のあるフレキシブルなソリューションです。頑丈な仕様により、NIRS DS2500 Liquid Analyzerは粉塵、湿気、および振動に強い為、過酷な生産環境での使用に理想的です。

DS2500 Liquid Analyzer は400~2500 nmのスペクトル範囲全体をカバーし、サンプルを80° Cまで加熱し、様々な使い捨てハイアルやクォーツキュベットとの互換性を有します。このようにして個々のサンプル要件に対応し得るDS2500 Liquid Analyzerは、1分未満で正確かつ再現性ある結果を得られるようサポートします。さらに一体型のサンプルホルダ検出、および説明不要のVision Airソフトウェアを用いることで、ユーザーが簡単かつ安全に操作できることが保証されます。

サンプル量が多い場合、Metrohmサンプルロケットと組み合わされたフローセルの導入によって、生産性を著しく向上させることができます。



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)



8mmDS2500

直径8 mmのガラス製使い捨てハイアル用インテリジェントホルター