



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  $\text{H}_2\text{O}_2$ ). 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.

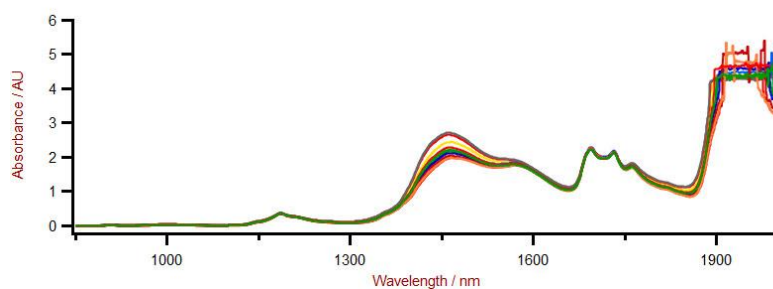
**Table 1.** Hardware and software equipment overview

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

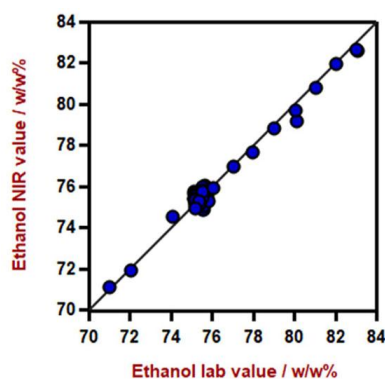
## RESULTS

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.



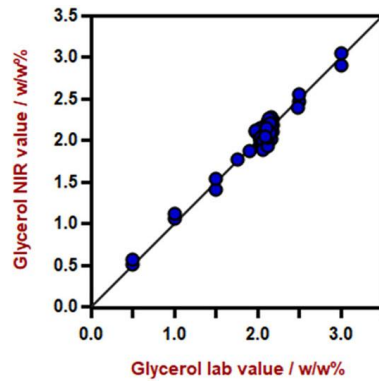
**Figure 2.** Vis-NIR spectra hand sanitizer gel samples analyzed on a DS2500 Liquid Analyzer.



**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.

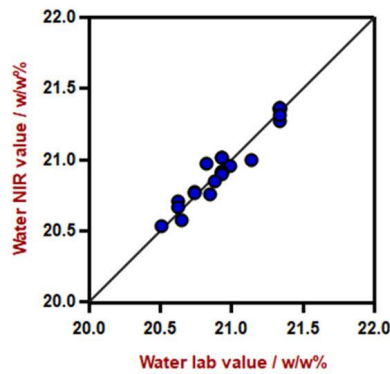
Figures of Merit	Value
$R^2$	0.9832
Standard Error of Calibration	0.33 w/w%
Standard Error of Cross-Validation	0.37 w/w%



**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.

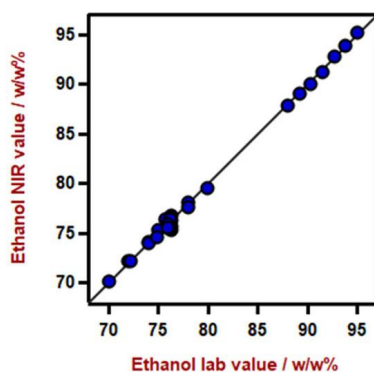
Figures of Merit	Value
$R^2$	0.9632
Standard Error of Calibration	0.08 w/w%
Standard Error of Cross-Validation	0.11 w/w%



**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.

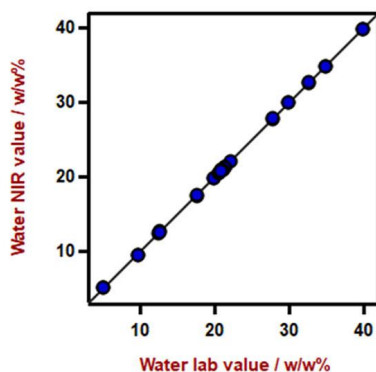
Figures of Merit	Value
R <sup>2</sup>	0.941
Standard Error of Calibration	0.07 w/w%
Standard Error of Cross-Validation	0.09 w/w%



**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.

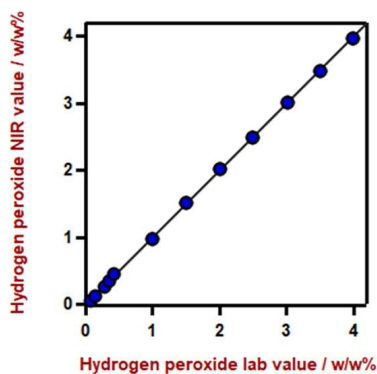
Figures of Merit	Value
R <sup>2</sup>	0.9964
Standard Error of Calibration	0.36 w/w%
Standard Error of Cross-Validation	0.36 w/w%



**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 <sup>2</sup>	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

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## DS2500 Liquid Analyzer 固耐用的近外光,用于生境和室中的量。

DS2500 Liquid Analyzer 是一成熟且活的解决方案,其用于在整个生中行液体常分析。其固耐用的使 DS2500 Liquid Analyzer 不受灰、潮湿、振的影,因此非常用于在劣的生境中使用。

DS2500 Liquid Analyzer 覆盖 400 至 2500 nm 的整个光范,将品加至 80° C 高温,并与各不同的一次性小瓶和石英比色皿兼容。因此,DS2500 Liquid Analyzer 可的个性化品要求,助在一分内得精和具有可重性的果。借助集成的品架装置和自的 Vision Air 件,保了用能松和安全地行操作。

如果是大的品量,可通将流通池与一个 Metrohm 机器人自器搭配使用的方法著提高生率。



## Vision Air 2.0 Complete Vision Air – 通用的光分析件。

Vision Air Complete 是用于管范境的先易用的件解决方案。

Vision Air 点一:

- 独特的件用和配的用界面保了直的操作方式
- 操作程的建与方式
- SQL 数据,可安全且地管理数据

Vision Air Complete (66072208) 版本包含所有用于可近外光分析量保程的用:

- 器和数据管理用
- 方法用
- 常分析用

其它 Vision Air Complete 解决方案:

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





DS2500 8 mm

直径 8 mm 且更加智能的一次性玻璃小瓶支架