



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.

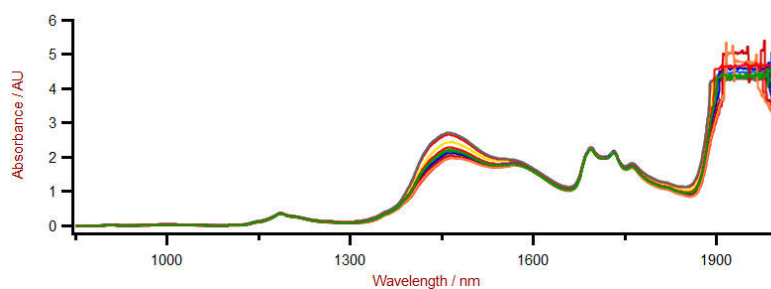


Figure 2. Vis-NIR spectra hand sanitizer gel samples analyzed on a DS2500 Liquid Analyzer.

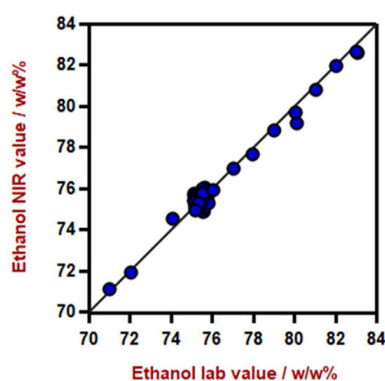


Figure 3. Correlation diagram for the prediction of ethanol content in hand sanitizer gel using a DS2500 Liquid Analyzer. The lab value was evaluated using gas chromatography.

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%

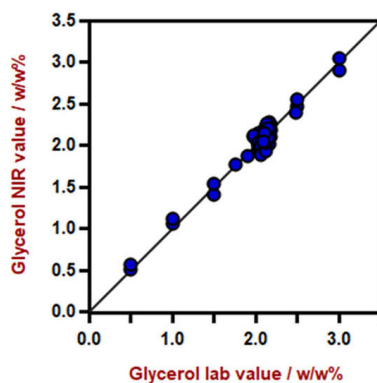


Figure 4. Correlation diagram for the prediction of glycerol content in hand sanitizer gel using a DS2500 Liquid Analyzer. The lab value was evaluated by gas chromatography.

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%

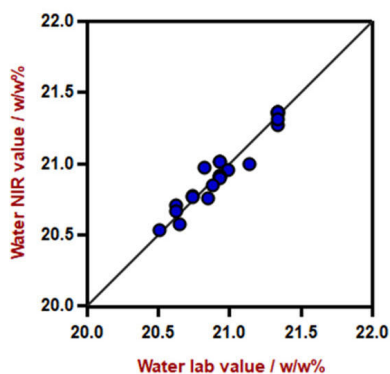


Figure 5. Correlation diagram for the prediction of water content in hand sanitizer gel using a DS2500 Liquid Analyzer. The lab value was evaluated by Karl Fischer titration.

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%

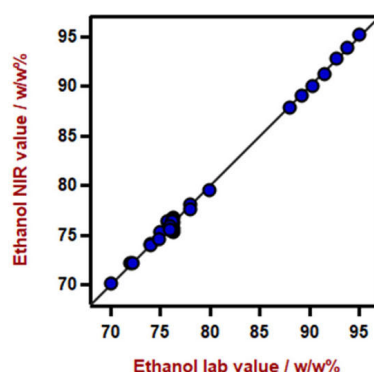


Figure 6. Correlation diagram for the prediction of ethanol content in hand sanitizer wipes using a DS2500 Liquid Analyzer. The lab value was evaluated by gas chromatography.

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%

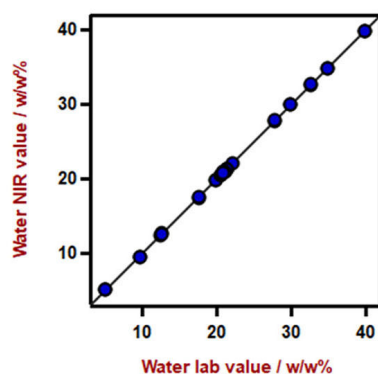


Figure 7. Correlation diagram for the prediction of water content in hand sanitizer wipes using a DS2500 Liquid Analyzer. The lab value was evaluated by Karl Fischer titration.

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%

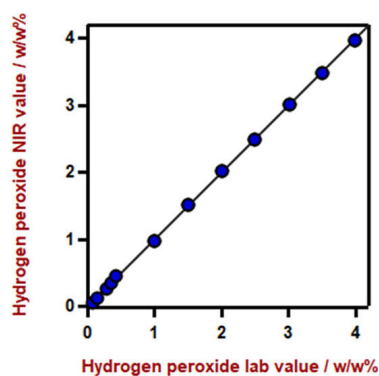


Figure 8. Correlation diagram for the prediction of hydrogen peroxide content in hand sanitizer wipes using a DS2500 Liquid Analyzer. The lab value was evaluated by permanganate titration.

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

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DS2500 Liquid Analyzer

坚固结实的近红外光谱仪,用于生产环境和试验室中的质量检查。

DS2500 Liquid Analyzer 是一种成熟且灵活的解决方案,其用于在整个生产链中进行液体常规分析。其坚固结实的设计使 DS2500 Liquid Analyzer 不受灰尘、潮湿、振动的影响,因此非常适用于在恶劣的生产环境中使用。

DS2500 Liquid Analyzer 覆盖 400 至 2500 nm 的整个光谱范围,将样品加热至 80° C 高温,并与各种不同的一次性小瓶和石英比色皿兼容。因此,DS2500 Liquid Analyzer 可适应您的个性化样品要求,帮助您在几分钟内获得精确和具有可重现性的结果。借助集成的样品架识别装置和自带的 Vision Air 软件,还保证了用户能轻松和安全地进行操作。

如果是较大的样品量,则可通过将流通池与一个 Metrohm 机器人自动进样器搭配使用的方法显著提高生产率。



Vision Air 2.0 Complete

Vision Air – 通用的光谱分析软件。

Vision Air Complete 是用于监管规范环境的先进易用的软件解决方案。

Vision Air 优点一览:

- 便捷的软件应用和经过适配的用户界面保证了直观简单的操作方式
- 操作过程的创建与维护方式简单
- SQL 数据库,可安全且简单地管理数据

Vision Air Complete (66072208) 版本包含所有用于可见近红外光谱分析质量保证过程的应用:

- 仪器和数据管理应用
- 方法开发应用
- 常规分析应用

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

直径为 8 mm 且更加智能的一次性玻璃小瓶支架