



Application Note AN-NIR-087

洗手液中的乙醇含量

Fast and reagent-free ethanol content determination

In 2020, the demand for hand sanitizer skyrocketed due to the COVID-19 pandemic. Many companies shifted gears, streamlining their operations to produce hand sanitizer in large volumes. As in any product manufacturing process, accurate formulation enables good quality and minimizes waste. The alcohol content in hand sanitizers must be greater than 60% (v/v) to be an effective antiseptic. Reagents commonly used in these solutions are water,

alcohol (commonly ethanol or isopropanol), small amounts of emollient (skin softener, e.g. glycerol), and an oxidizing agent (e.g. hydrogen peroxide) to minimize microbial contamination. A safe and fast way to monitor ethanol content in these sanitizing solutions is with **reagent-free** near-infrared spectroscopy, which provides reliable **results in a few seconds**, quickly indicating when adjustments in formulation are necessary.

EXPERIMENTAL EQUIPMENT

Mixtures of ethanol/water standards with a range of ethanol content from 58% to 82% (v/v) were measured in transmission mode with a DS2500 Liquid Analyzer over the full wavelength range (400–2500 nm). Reproducible spectrum acquisition was achieved using the built-in temperature control at 40 ° C. 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. 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 13 measured Vis-NIR spectra (**Figure 2**) were used to create a prediction model for quantification of the ethanol content. The quality of the prediction models was evaluated using correlation diagrams, which display a very

high correlation between VisNIR prediction and primary method values. The respective figures of merit (FOM) display the expected precision of a prediction during routine analysis.



Figure 2. Vis-NIR spectra of hand sanitizers with varying ethanol content measured on a DS2500 Liquid Analyzer.

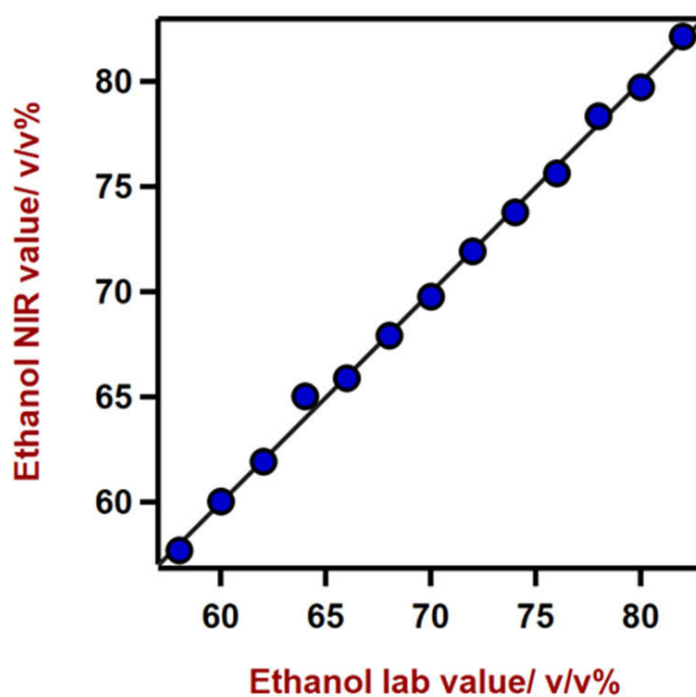


Figure 3. Correlation diagram and the respective figures of merit for the prediction of ethanol content in hand sanitizers using a DS2500 Liquid Analyzer.

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

Figures of merit	Value
R^2	0.9977
Standard error of calibration	0.41 v/v%
Standard error of cross-validation	0.56 v/v%

CONCLUSION

This application note demonstrates the feasibility of the DS2500 Liquid Analyzer for the determination of ethanol in hand sanitizer products. Vis-NIR

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

Table 3. Time to result for the ethanol content determination in hand sanitizers using gas chromatography

Parameter	Method	Time to result and workflow
Ethanol content	GC	5 min (preparation) + 5 min (GC)

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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