



Application Note AN-NIR-087

洗手液中的乙醇含量

Fast and reagent-free ethanol content determination

摘要

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.

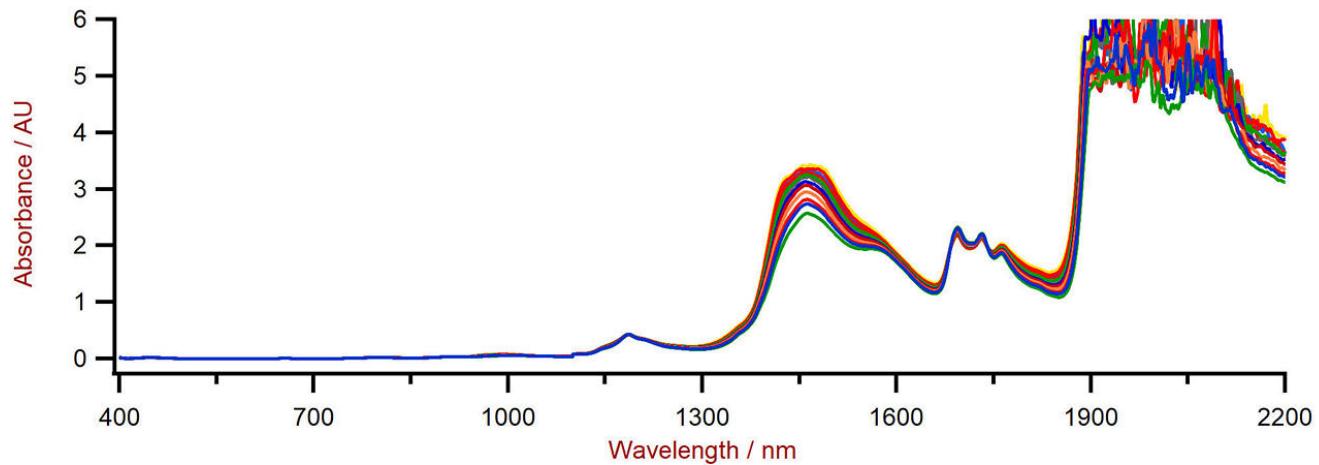


Figure 2. Vis-NIR spectra of hand sanitizers with varying ethanol content measured on a DS2500 Liquid Analyzer.

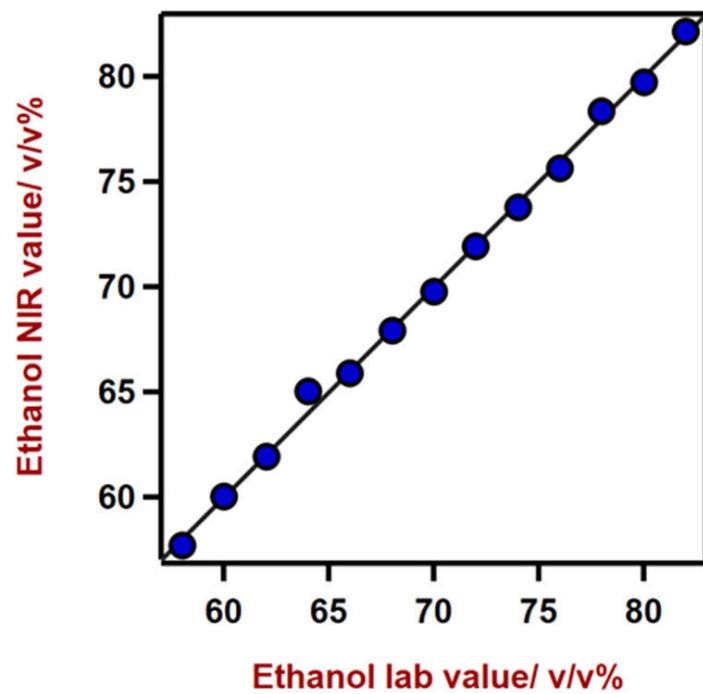


Figure 3. Correlation diagram and the respective figures of merit for the prediction of ethanol content in hand sanitizers using a DS2500 Liquid Analyzer.

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%

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

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DS2500 Liquid Analyzer , DS2500 Liquid Analyzer ,

DS2500 Liquid Analyzer 400 2500 nm , 80°C ,
,DS2500 Liquid Analyzer , Vision Air ,

, Metrohm



Vision Air 2.0 Complete

Vision Air -

Vision Air Complete

Vision Air :

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- SQL ,

Vision Air Complete (66072208) :

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Vision Air Complete :

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



DS2500 8 mm

8 mm