APPLICATION BRIEF

Infrared Spectroscopy

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# Quantification of Ethanol and Isopropanol in Alcohol-Based Hand Sanitizers

## Introduction

In the midst of the COVID-19 outbreak, key hygiene supplies have become in high demand so much so that there are now critical supply shortfalls. One of the most important of these is alcohol-based hand sanitizer. To cope with this shortfall, the food and drug administration (FDA) has produced a guidance document for the compounding of certain alcohol-based hand sanitizer products during this pandemic.[1]

There are two formulations that have been approved for compounding by facilities with the ability to produce hand sanitizer. These are based on formulations recommended by the World Health Organisation (WHO) which is as follows:[2]

- Ethyl alcohol (80 % v/v) OR Isopropyl alcohol (75 % v/v)
- Glycerol (1.45 % v/v)
- Hydrogen Peroxide (0.125 % v/v)
- Sterile or distilled water (Remainder of volume)

The most important parameters to consider in compounding is the type and content of alcohol. It has been established that the aforementioned concentrations used in such formulations are the most effective. Additionally, it has also been determined that hand sanitizer with alcohol concentration below 60% (v/v) is not effective and could leave the user at higher risk of infection.[3]

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It should be noted however that the alcohol type should also be safe for humans, considering exposure to the body. While Isopropyl Alcohol (IPA) or Ethanol are fine, Methanol/Wood Alcohol is harmful and should not be used. There have been instances of hand sanitizers having partial or complete methanol content which would be harmful to users. The PerkinElmer Hand Sanitizer Analyzer can also detect the presence of methanol or other threats before verifying the composition.

## Experimental

Stock solutions of ethanol and isopropanol (Sigma-Aldrich) were used to prepare calibration and validation standards. Calibration standards from 0-90 % (v/v) ethanol and isopropanol were prepared, by volume. Each standard was made up such that all contained the same quantity of glycerol and hydrogen peroxide (1.45 and 0.125 % v/v respectively) and the correct proportion of the alcohol. Solutions were made up to 50 mL using deionised water. All samples were measured using the PerkinElmer Spectrum Two+ FT-IR spectrometer (Figure 1) with attenuated total reflectance accessory using the parameters shown in Table 1.

*Figure 1.* PerkinElmer Spectrum Two+ FT-IR spectrometer with ATR accessory.

*Table 1.* Parameters used for the measurement of hand sanitizer samples.

| Parameter | Value |
|---|---|
| Range | 4000 – 550 $cm^{-1}$ |
| Resolution | 4 $cm^{-1}$ |
| Number of Scans | 4 |
| Corrections | Atmospheric Compensation |

## Results and Discussion

The Beer-Lambert law was used to generate starter calibrations for the two different hand sanitizer models. The ethanol-based hand sanitizer model was created based on the standard curve derived from the area of a peak at 1045 $cm^{-1}$ which corresponds to the C-O stretch in a primary alcohol. The isopropanol-based hand sanitizer model was similarly created based on the area of a peak at 1131 $cm^{-1}$, corresponding to the C-O stretch in a secondary alcohol. As a representative example, FT-IR spectra containing 80% of the active alcohol ingredient in both types of hand sanitizer are shown in Figure 2.

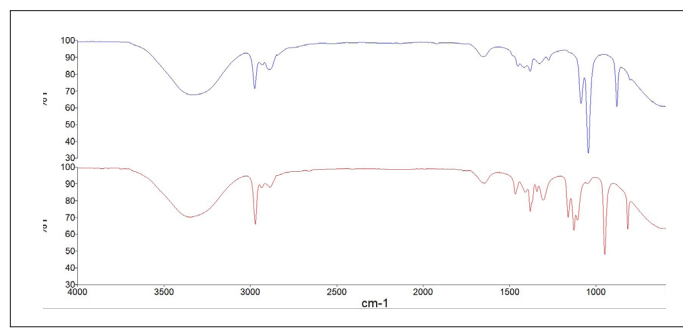


*Figure 2.* FT-IR spectra of hand sanitizer calibration solutions containing 80% v/v Ethanol (blue) and 80% v/v Isopropanol (red).

The calibration curves created using the aforementioned peaks for both ethanol and isopropanol are shown in Figure 3. These have been fit to a linear regression curve.

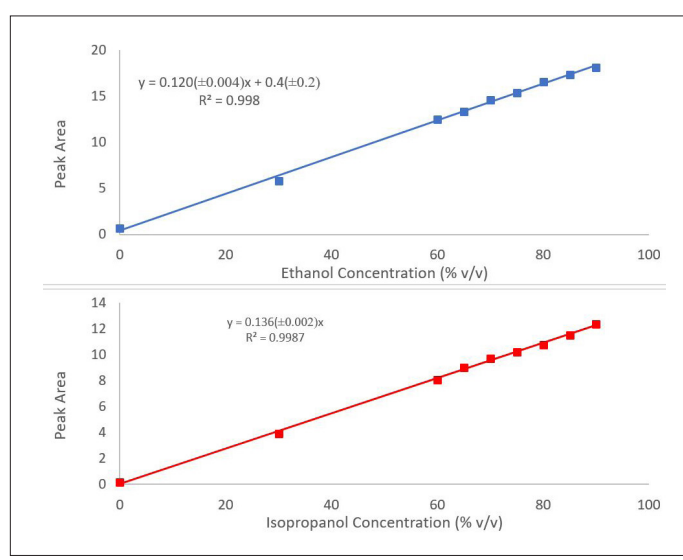


*Figure 3.* Calibration curves for ethanol (top) and isopropanol (bottom) in hand sanitizer.

Using PerkinElmer's Spectrum Two+ FT-IR hand sanitizer analyzer, the calibration models may be implemented in one of three possible ways:

- Using the Predict function in Spectrum Quant™
- Using the Quant function in Spectrum 10™
- Implementing a Touch method

In order to demonstrate the prediction accuracy of the starter calibrations, two samples were used to validate each model. This step involved testing known concentrations of each sample type against the standard curve. The results from the validation are shown in Table 2.

*Table 2.* Validation results for ethanol and isopropanol-based hand sanitizer models.

| Model | Concentration (%) | Predicted Concentration (%) |
|---|---|---|
| Ethanol | 43 | 41 % |
| | 73 | 73 % |
| Isopropanol | 43 | 41 % |
| | 73 | 72 % |

The flexibility of the hand sanitizer analyzer enables analysts to quickly and accurately generate calibrations for their own formulations.

## Detection of Methanol in Hand Sanitizer

During the COVID-19 outbreak, an increasingly pressing issue has been the discovery of methanol in some hand sanitizer. In the month from July to August 2020, the FDA issued warnings against using 130 different brands of hand sanitizer due to methanol contamination.

IR spectroscopy, in conjunction with PerkinElmer's Adulterant Screen™ algorithm, may be use as a screening tool for the detection of methanol in hand sanitizer. It is able to detect methanol contamination down to 300 ppm (0.03 %), far exceeding the limits required by FDA regulation (630 ppm).

Spectrum Touch allows this analytical step to be included into a one-click solution for determination of both alcohol concentration and presence of methanol. An example of the results page from a sample found to contain methanol is shown in Figure 4.

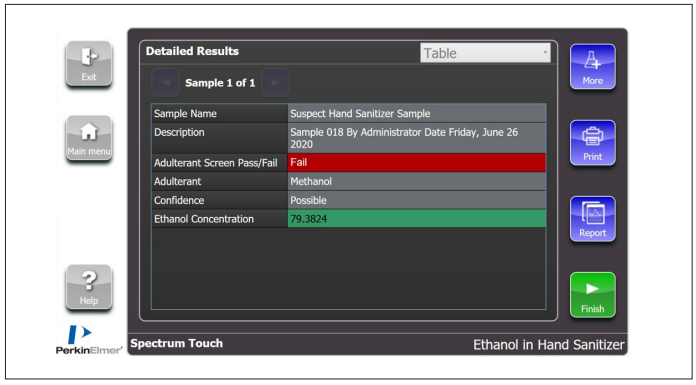


*Figure 4.* Example results page from a sample containing approximately 80% ethanol which has been contaminated with methanol.

## Conclusion

The PerkinElmer Spectrum Two+ FT-IR spectrometer provides a fast and reliable method to determine the ethanol and isopropanol content of hand sanitizers compounded according to WHO and FDA-approved formulations. The quantitative models included demonstrate strong correlation with $R^2$ values of 0.998 and 0.999 for ethanol and isopropanol concentration respectively. In addition, the optional adulterant screen allows users to detect methanol down to 300 ppm, easily fulfilling FDA requirements and ensuring sample safety. The complete analyzer comes with Spectrum Touch software, which allows the user to work with workflow orientated methods, and a starter calibration for hand sanitizer ethanol and isopropanol content. It is also possible to add the methanol adulterant screen to the touch macro providing a fast and simple way to screen for this potential contaminant. This allows analysts to obtain critical information about sample formulations quickly and at the compounding site.

## References


1. https://www.fda.gov/regulatory-information/search-fda-guidance-documents/policy-temporary-compounding-certain-alcohol-based-hand-sanitizer-products-during-public-health (Accessed 19/03/2020)
2. WHO Guidelines on Hand Hygiene in Health Care, Part I, Chapter 12, Page 49
3. WHO Guidelines on Hand Hygiene in Health Care, Part I, Chapter 10, Page 28



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