Technical Overview

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Transitioning from the Agilent Cary 630 FTIR to the Agilent Cary 635 FTIR Spectrometer

Demonstrating methodology equivalence for pharmaceutical applications

Introduction

Fourier transform infrared (FTIR) spectroscopy is a powerful analytical tool used to analyze a wide variety of materials by interpreting their infrared (IR) wavenumber absorptions. Within pharmaceutical and biopharmaceutical industries, FTIR analysis is integral for material identification and quality assurance of pharmaceutical substances.

In the pharmaceutical industry, the Agilent Cary 630 FTIR is used for the identification of drug products, incoming goods, and packaging materials, as specified in global pharmacopoeias, and provides quantitative information such as the concentration of components within pharmaceutical formulations.

Agilent now presents the Cary 635 FTIR spectrometer—an ultracompact, easy-to-use, high-performing, portable FTIR system. With greater IR power, the Cary 635 FTIR features greater detection sensitivity and faster scanning times. With its predecessor's modular design, the Cary 635 FTIR can analyze the same samples with a newly enhanced performance quality and efficiency.

For users in the pharmaceutical industry who have experience with the Cary 630 FTIR, this technical overview demonstrates the common methodologies and workflows between the Cary 635 FTIR and Cary 630 FTIR spectrometers for pharmaceutical purposes. It will compare the ability of the two instruments to measure and label IR spectra, identify relevant compounds such as active pharmaceutical ingredients (APIs), and quantify substances within commercial formulations.

Instrumentation and software

For comparison, all three application tests were conducted using the Cary 630 FTIR and Cary 635 FTIR spectrometers with ZnSe optics and equipped with a single-reflection diamond attenuated total reflectance (ATR) accessory. The specific method parameters are outlined within each corresponding application.

Both the Cary 635 FTIR and Cary 630 FTIR use Agilent MicroLab software, which provides step-by-step instructions with supporting images to guide users through the entire analytical workflow. Both spectrometers follow the same methods and operational procedures from sample loading to data processing (Figure 1). Results are presented in an easy-to-understand, color-coded format with customizable limits, ensuring a rapid and intuitive data review (Figure 2).

Figure 1. The Agilent Cary 635 FTIR spectrometer features the same Agilent MicroLab software methods and measurement capabilities as the Agilent Cary 630 FTIR spectrometer.

Figure 2. Agilent MicroLab software simplifies using the Agilent Cary 630 and 635 FTIR spectrometers. The picture-driven software also reduces training needs and minimizes the risk of user-based errors.

Spectrum collection and labeling

The two spectrometers were compared using the transmission spectra of citric acid and salicylic acid—common excipients used within pharmaceuticals and skincare products (Figures 3 and 4). Table 1 outlines the method parameters used for the spectra collection with both the Cary 630 FTIR and the Cary 635 FTIR.

Table 1. Experimental parameters for spectrum collection using the Agilent Cary 630 and Cary 635 FTIR-ATR.

Parameter	Value
Method	Data collect only
Mode	Transmittance
Spectral Range	650–4,000 cm^{-1}
Number of Background/Sample Scans	32
Spectral Resolution	4 cm^{-1}

Within spectral analysis, the shape of the overall spectrum and the specific wavenumbers of the peaks are necessary to extrapolate information about a substance's identity and molecular structure. The spectra within Figures 3 and 4 depict homologous transmission curves produced by both spectrometers. Partial differences in transmission intensities are expected due to minor crystallinity and pressure variations between measurements.

Furthermore, as demonstrated by Tables 2 and 3, both the Cary 635 FTIR and Cary 630 FTIR produce peaks at identical wavenumbers across the entire spectra. Thus, routine spectrum collection and subsequent interpretation of molecular structure based on peak analysis remains consistent between the two spectrometers. Additionally, due to the shared utilization of MicroLab software, the post-collection processing, including peak labeling and adjustment, is the same between the two instruments, as shown in Figure 5.

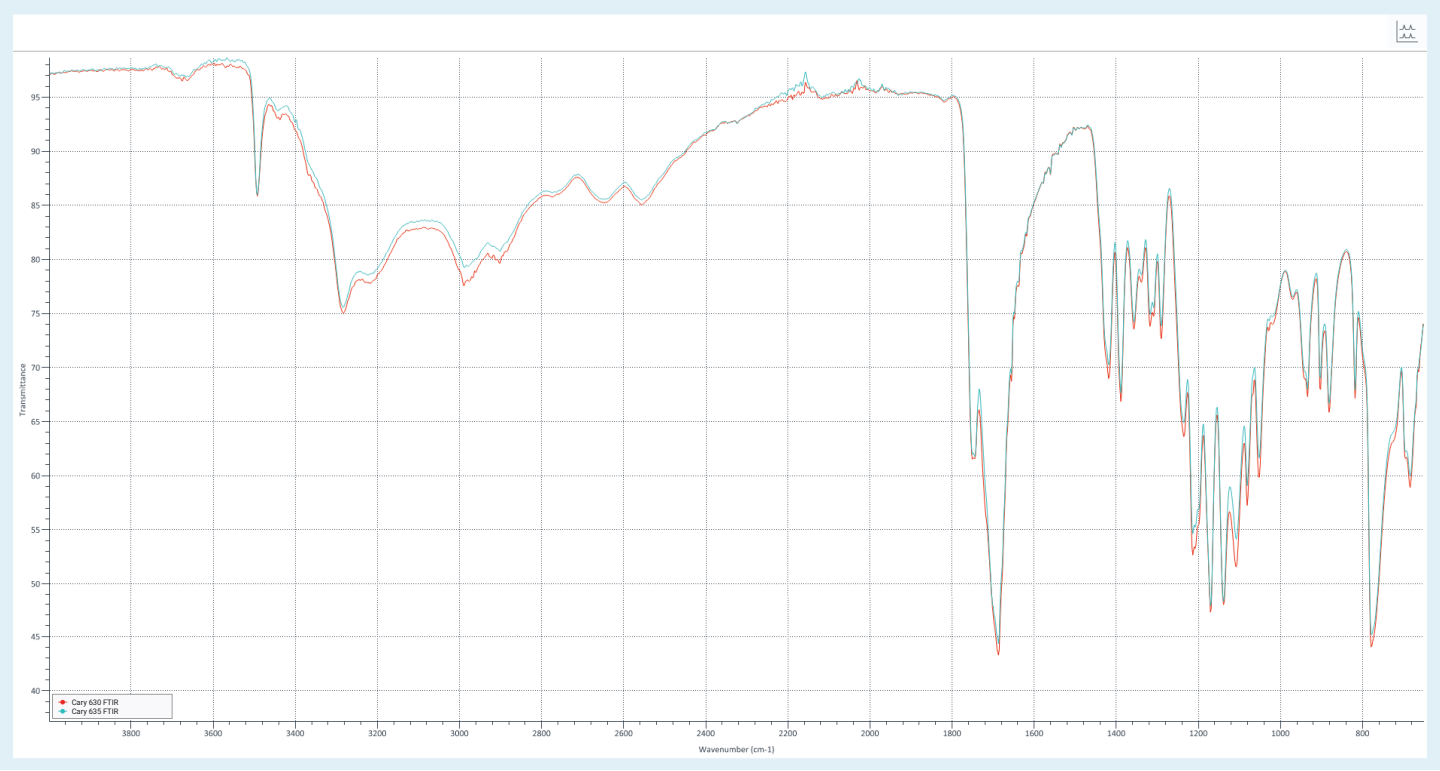

Figure 3. Overlapping IR transmittance spectra of citric acid from the Agilent Cary 635 FTIR (blue) and Cary 630 FTIR (red) spectrometers across 640 to 4,000 cm^{-1}. The citric acid was ground into a powder, and both spectra were collected with the ATR module.

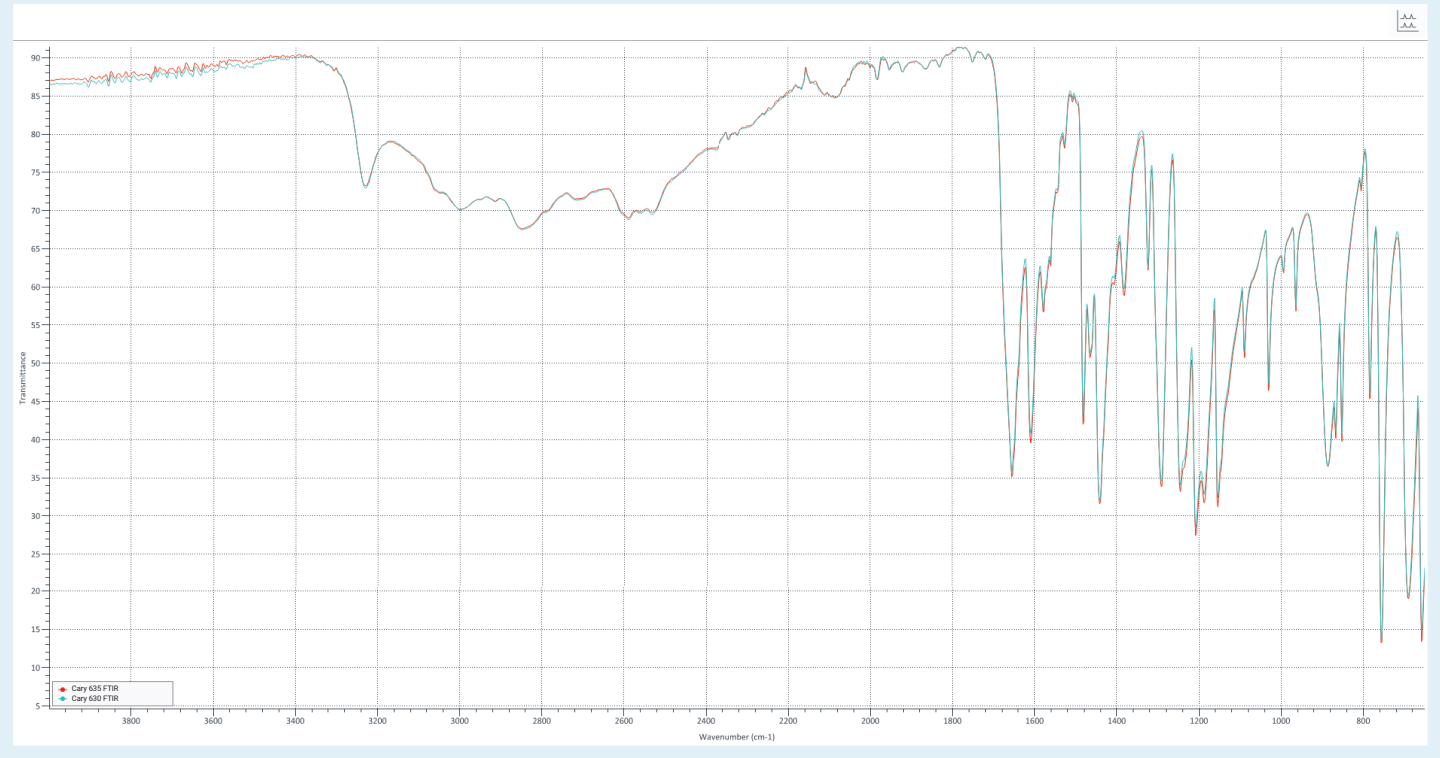

Figure 4. Overlapping IR transmittance spectra of salicylic acid from the Agilent Cary 635 FTIR (red) and Cary 630 FTIR (blue) spectrometers across 640 to 4,000 cm^{-1}. The salicylic acid was ground into a powder, and both spectra were collected with the ATR module.

Table 2. Transmission peak wave numbers of the citric acid spectra measured using the Agilent Cary 635 FTIR and Cary 630 FTIR spectrometers from 640 to 4,000 cm^{-1} (Figure 3).

Cary 635 FTIR	Cary 630 FTIR	Cary 635 FTIR	Cary 630 FTIR
684.0	684.0	1308.3	1308.3
697.0	697.0	1317.6	1317.6
779.0	779.0	1338.1	1338.1
818.2	818.2	1356.8	1356.8
881.5	881.5	1388.4	1388.4
903.9	903.9	1418.3	1418.3
933.7	933.7	1686.6	1686.6
971.0	971.0	1744.4	1744.4
1053.0	1053.0	1818.9	1818.9
1080.9	1080.9	2558.8	2558.8
1108.9	1108.9	2650.1	2650.1
1138.7	1138.7	2901.7	2901.7
1170.4	1170.4	2987.5	2987.5
1213.2	1213.2	3224.1	3224.1
1235.6	1235.6	3283.8	3283.8
1291.5	1291.5	3492.5	3492.5

Table 3. Transmission peak wave numbers of the salicylic acid spectra measured using the Agilent Cary 635 FTIR and Cary 630 FTIR spectrometers from 640 to 4,000 cm^{-1} (Figure 4).

Cary 635 FTIR	Cary 630 FTIR	Cary 635 FTIR	Cary 630 FTIR
657.9	657.9	1381.0	1381.0
691.4	691.4	1440.6	1440.6
756.6	756.6	1464.8	1464.8
784.6	784.6	1481.6	1481.6
851.7	851.7	1526.3	1526.3
866.6	866.6	1578.5	1578.5
885.2	887.1	1608.3	1608.3
963.5	963.5	1654.9	1654.9
993.3	993.3	2085.4	2085.4
1030.6	1030.6	2344.5	2344.5
1090.2	1090.2	2532.7	2532.7
1153.6	1153.6	2592.4	2592.4
1187.2	1187.2	2719.1	2719.1
1207.7	1207.7	2849.6	2849.6
1244.9	1244.9	3002.4	3002.4
1291.5	1291.5	3229.7	3231.6
1323.2	1323.2		

Figure 5. IR transmittance spectra of salicylic acid from the Agilent Cary 635 FTIR (A) and Cary 630 FTIR (B) spectrometers across 640 to 4,000 cm^{-1}. Peaks from the spectra were labeled using Agilent MicroLab software. The salicylic acid sample was ground into a powder, and both spectra were collected with the ATR module.

While the spectra measured by the Cary 635 FTIR are evidently consistent with those produced by the Cary 630 FITR, the increased IR light intensity within the Cary 635 FTIR also improves the signal-to-noise ratio, which is most apparent within Figure 3 from 3,600 to 2,400 cm^{-1}. The smoothness of the spectrum allows both efficiency and accuracy within MicroLab's peak-peaking processes, leading to an overall shorter acquisition time to obtain the same high-quality spectrum.

Compound identification

The two spectrometers were compared based on their ability to correctly identify ibuprofen and acetaminophen, which are both APIs found in common over-the-counter painkillers. Both the Cary 630 FTIR and Cary 635 FTIR referenced the same independent commercial library of substances and were evaluated on how well the measured spectrum matched the reference spectrum. The similarity was indicated by the hit quality index (HQI), where an HQI of 1 indicates a perfect match. Custom libraries formed using spectra collected with the Cary 630 FTIR can also be used directly for compound identification with the Cary 635 FTIR while maintaining reliability and accuracy of the matches. The spectrum method and HQI parameters are outlined in Tables 4 and 5, respectively.

Table 4. Experimental spectral parameters for qualitative search using the Agilent Cary 630 FTIR-ATR and Cary 635 FTIR-ATR spectrometers.

Parameter	Value
Method	Qualitative search
Mode	Absorbance
Spectral Range	650–4,000 cm^{-1}
Number of Background/Sample Scans	32
Spectral Resolution	4 cm^{-1}

Table 5. Search parameters for qualitative search results for both the Agilent Cary 630 FTIR-ATR and 635 FTIR-ATR spectrometers.

Library Identification Parameter	Value
Library	Agilent FTIR starter library: Pharmaceuticals*
Minimum Hit Quality	80%
Maximum Hits Displayed	6 items
Quality Hit Threshold	90%
Quality Marginal Threshold	95%

* Spectra from the independent library were not measured on either the Cary 630 FTIR or the Cary 635 FTIR.

Both the Cary 630 FTIR and Cary 635 FTIR successfully identified the pure ibuprofen and acetaminophen using a reference library (Figure 6). Both spectrometers were able to match the known reference sample with a high degree of confidence, surpassing the typical quality marginal threshold of 0.95, demonstrated by the green highlight. For further application-based requirements, MicroLab software also allows users to specify a custom quality threshold for each qualitative search.

Table 6 compares the HQIs of both spectrometers for both acetaminophen and ibuprofen and confirms the comparisons made in Figure 6—that the Cary 635 FTIR and the Cary 630 FTIR demonstrate HQIs within 0.05 and 0.1% of each other. The streamlined workflow and color-coded results from both spectrometers enables efficient and effective analysis; therefore, for rapid substance identification, the Cary 635 FTIR is a seamless replacement for its predecessor.

Table 6. HQIs for pharamcetical samples by the Agilent Cary 630 FTIR and Cary 635 FTIR spectrometers.

	Acetaminophen	Ibuprofen
Cary 630 FTIR	0.98662	0.97135
Cary 635 FTIR	0.98708	0.97003

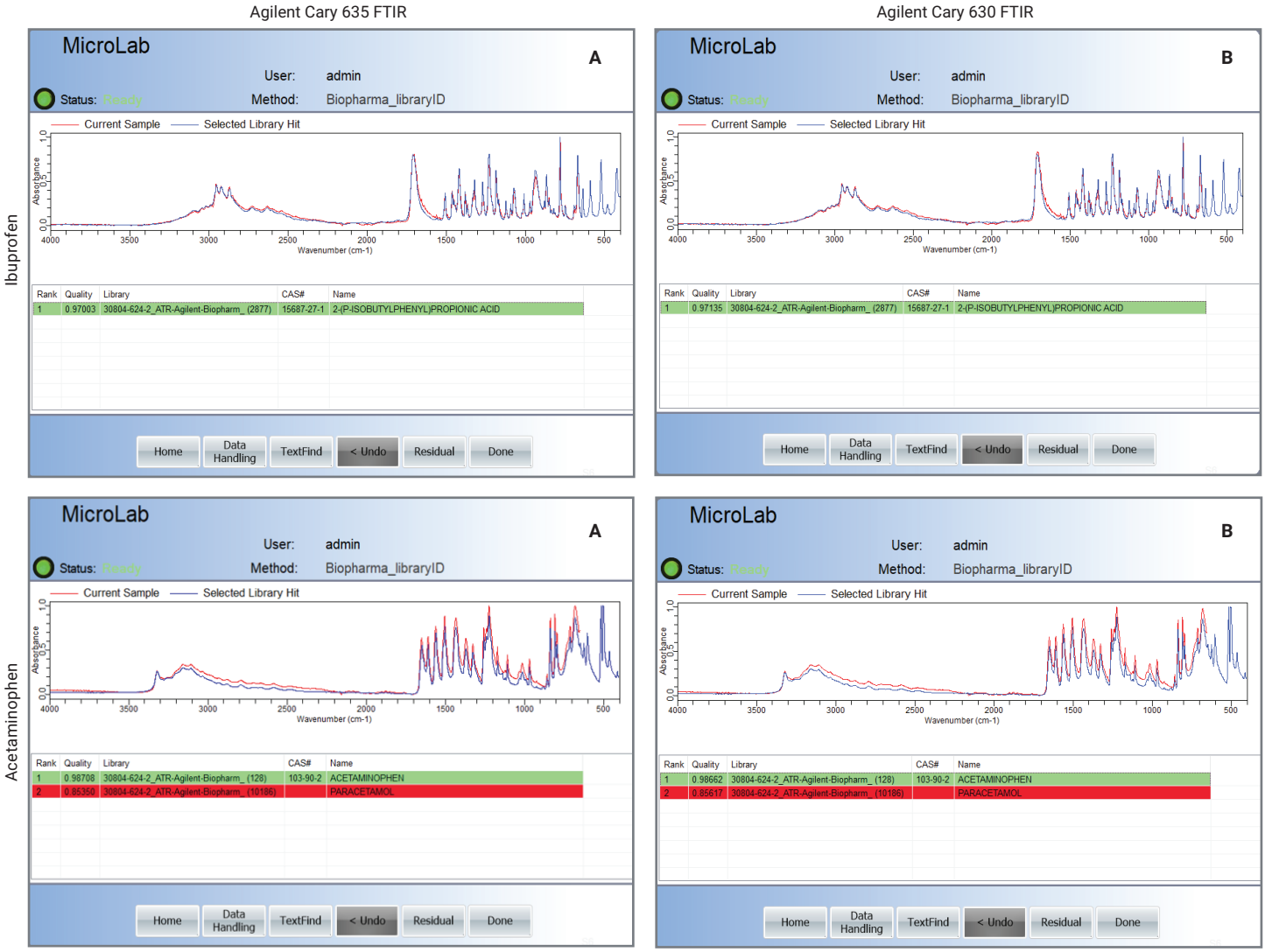

Figure 6. Identification results of ibuprofen (top) and acetaminophen (bottom) from the Agilent Cary 635 FTIR (A) and Cary 630 FTIR (B) spectrometers.

Quantification

The quantification abilities of the Cary 630 FTIR and the Cary 635 FTIR were evaluated by determining the ethanol concentration within hand sanitizer. Calibration curves were formed using the spectra of standard solutions measured with both instruments and quantifying the concentration of ethanol using the characteristic C-O stretch band found between 1,000 and 1,120 cm^{-1} within Agilent MicroLab Quant software (Figure 7). The method parameters are outlined in Table 7.

Hand sanitizer standards were made up according to the World Health Organization's recommended formulation for ethanol-based hand sanitizers (Table 7), with a range of ethanol concentrations (Table 8).

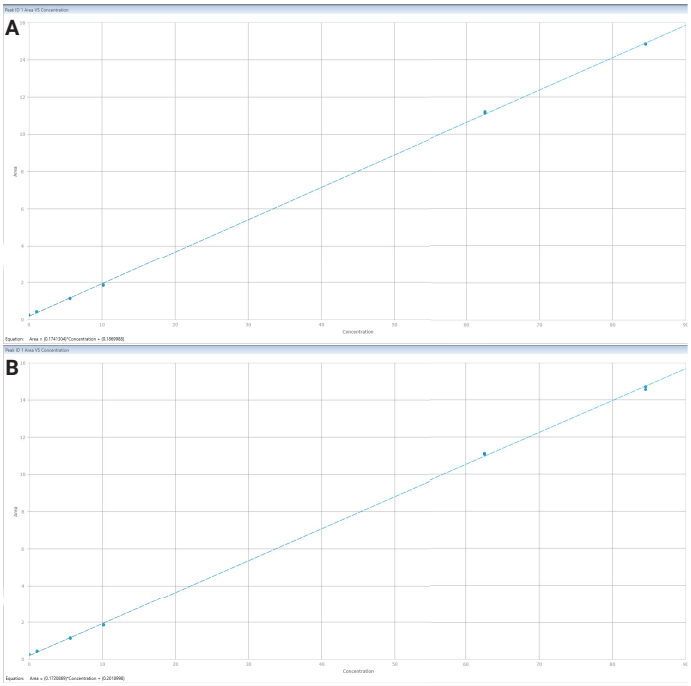

Figure 7. Calibration curves of ethanol-based hand sanitizer. The ethanol concentration was in % w/w and each standard had three replicate measurements. The calibration curves from both the Agilent Cary 630 FTIR spectrometer (A) and the Agilent Cary 635 FTIR spectrometer (B) have an R^2 value ≥ 0.999.

Both the Cary 635 FTIR and the Cary 630 FTIR produced comparable calibration curves using parallel workflows. The spectrometers utilized the accompanying MicroLab Quant software in the same way to process collected spectra of the standard solutions. Generating an analytical method—from measuring the standard solutions to peak area selection with the MicroLab software—takes less than 10 minutes using either spectrometer. After that, it takes under a minute to obtain a color-coded result from each sample measurement, as shown in Figure 8, which demonstrates that both spectrometers quantified the ethanol concentration within a commercial hand-sanitizer sample to be 79% w/w.

Table 7. Ethanol-based hand sanitizer formulation recommended by the WHO. Sterile water makes up the remainder of the volume.

Ingredients	Percentage (% v/v)
Ethanol	80
Hydrogen Peroxide	0.125
Glycerol	1.45

Table 8. Hand sanitizer standard solution ethanol concentrations.

Ethanol Concentration (% w/w)
0
1.07
5.62
10.17
62.54
84.51

Table 9. Experimental parameters for component quantification using the Agilent Cary 630 FTIR-ATR and 635 FTIR-ATR spectrometers.

Parameter	Value
Method	Components
Mode	Absorbance
Spectral Range	650–4,000 cm^{-1}
Number of Background/Sample Scans	32
Spectral Resolution	4 cm^{-1}

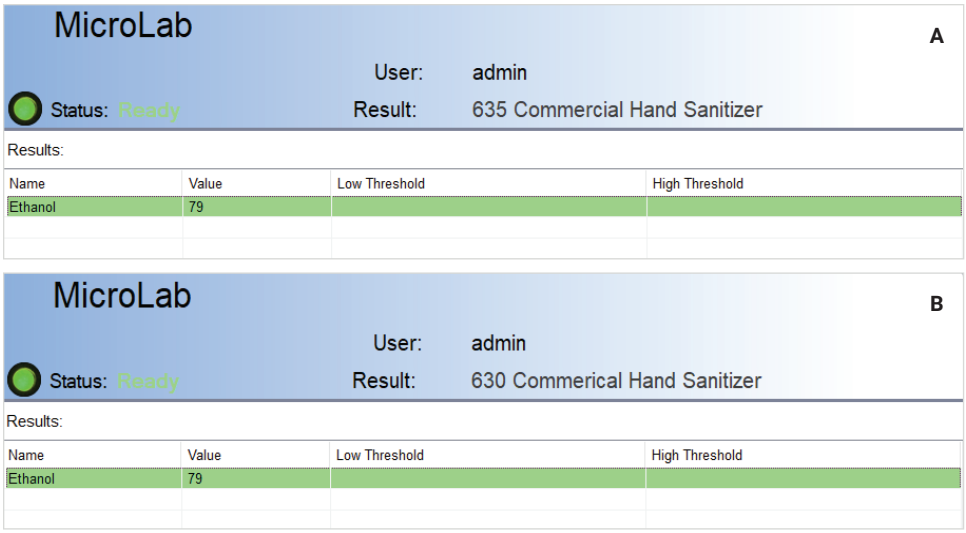

Figure 8. Ethanol quantification result within the commercial hand sanitizer sample from the Agilent Cary 635 FTIR spectrometer (A) and the Agilent Cary 630 FTIR spectrometer (B).

Conclusion

The comparison presented here of both the Agilent Cary 635 FTIR and Cary 630 FTIR spectrometers demonstrated shared methodologies that produced consistent results across key applications within pharmacopoeia, including spectrum production, compound identification, and substance quantification.

Featuring the same modularity, robustness, and ease of use as the Cary 630 FTIR, the Cary 635 FTIR also offers greater sensitivity and signal-to-noise ratio, resulting from an enhanced IR source intensity. Therefore, users operating in regulated environments can confidently upgrade to the Cary 635 FTIR with the understanding that the workflow from the Cary 630 FTIR is directly transferrable, and that their routine analyses will remain consistent and reliable.

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