

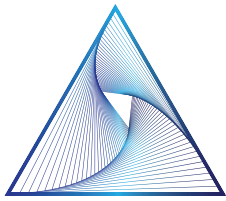
## APPLICATION NOTE 048

# Illustration of Fentanyl Analog Analysis Utilizing Gas Chromatography Coupled with the DiscovIR Solid Phase Infrared Detector

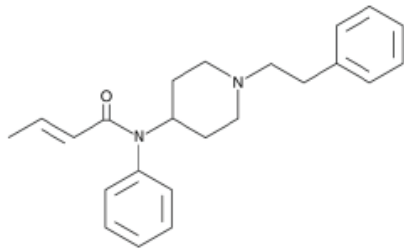
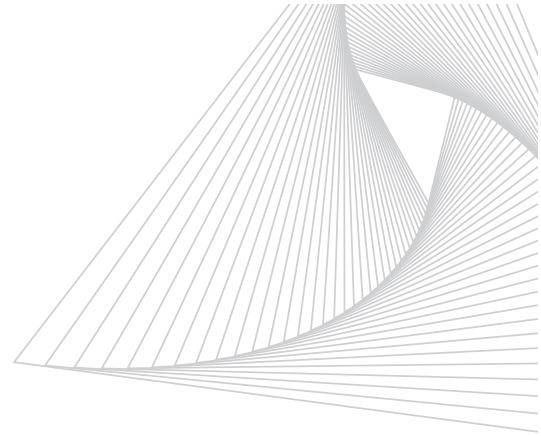
The recent influx of numerous novel synthetic opioids and fentanyl analogs to the forensic laboratory has been problematic for forensic chemists around the globe. The motivations for use of these new compounds include their legal status, ready availability, low cost, users' curiosity or preference for their particular pharmacological properties and the intention to avoid detection. According to the National Institute on Drug Abuse there were 70,237 overdose deaths in 2017. The largest increase were deaths related to fentanyl and fentanyl analogs with more than 28,400. With numbers like this, and the increasing risk to the public, it's become imperative that these compounds can be identified with confidence.

This application note will examine the analysis of some common fentanyl analogs. These compounds also have isomers that have very similar mass spectrum patterns. This can prove to be difficult for a conclusive identification, especially if the retention times are also very close. Infrared spectrometry can be used to conclusively identify these compounds. However, these compounds frequently are mixed with other compounds. This will require extractions that may or may not isolate each compound. Therefore, bench top IRs may not be able to provide the data needed. The DiscovIR-GC can provide the separation needed to isolate each compound and provide a spectrum for each component within a sample.

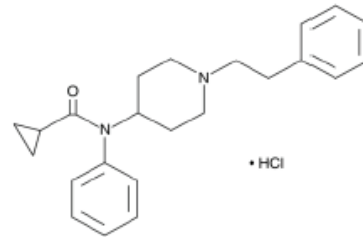
Below are the molecules examined for this application note to demonstrate DiscovIR's ability to differentiate between isomers pairs.



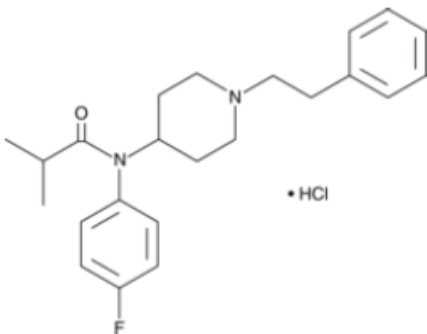
**SPECTRA**  
ANALYSIS



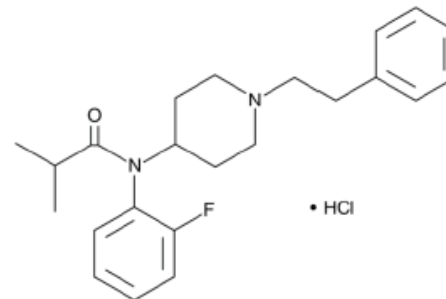
**Crotonyl Fentanyl**



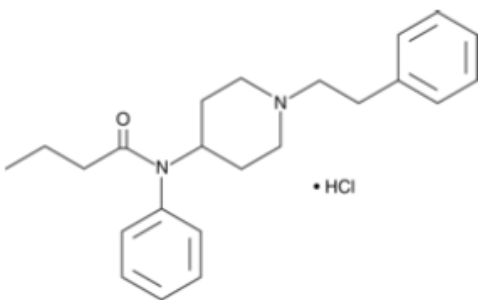
**Cyclopropyl Fentanyl**



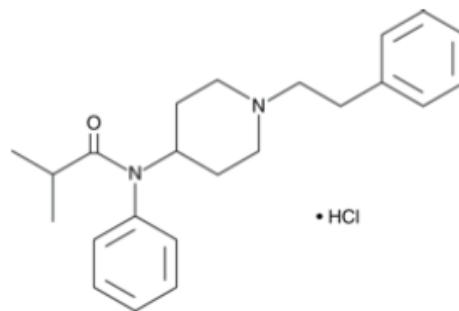
**4-Fluoroisobutyryl Fentanyl (FIBF)**



**2-Fluoroisobutyryl Fentanyl (2-FIBF)**



**Butyryl Fentanyl**



**Isobutyryl Fentanyl**

All compounds were purchased from Cayman Chemical. Powders were dissolved in MeOH to 1mg/mL solution. Each compound was analyzed utilizing the DiscovIR coupled with a Dani GC. The GC program for this analysis was as follows: 90.00° C for 1 min then 30.00°C for 4.00 min, injector temperature 250.00°C, injection volume 1mL, split of 5:1 and a flow of 4.00 mL/min. Collection occurred onto a ZnSe disc super-cooled to -40°C with LN2. Thus, separation of any mixture is achieved with the GC, with the resulting IR collected as a solid phase. Solid phase collection results in improved resolution when compared to gas phase or light pipe technology.

The results were high quality spectra with differentiation between the isomer pairs.

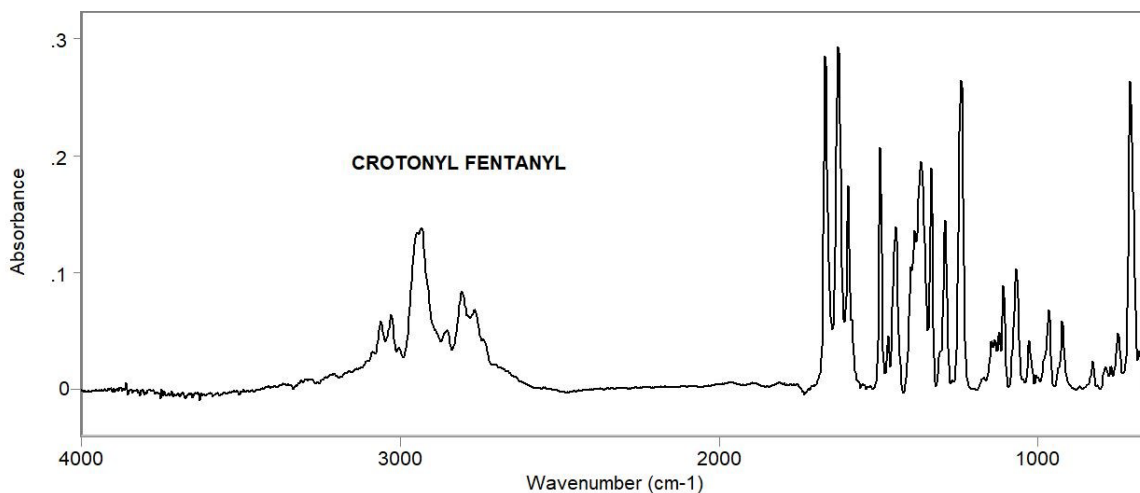


Figure 1. Crotonyl Fentanyl IR spectrum 4000-700 wavenumbers

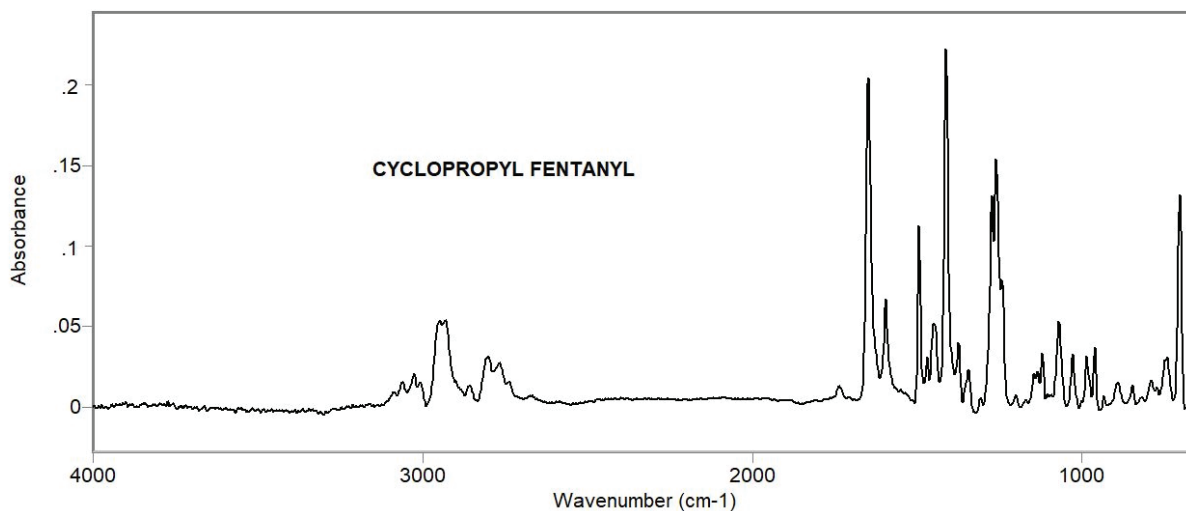


Figure 2. Cyclopropyl Fentanyl IR spectrum 4000-700 wavenumbers

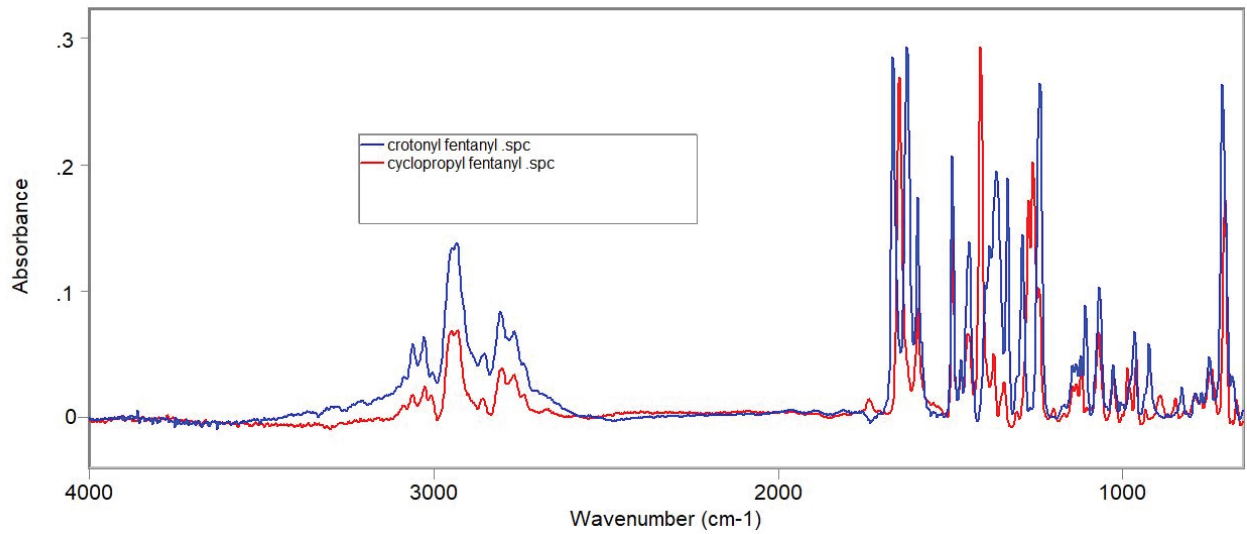
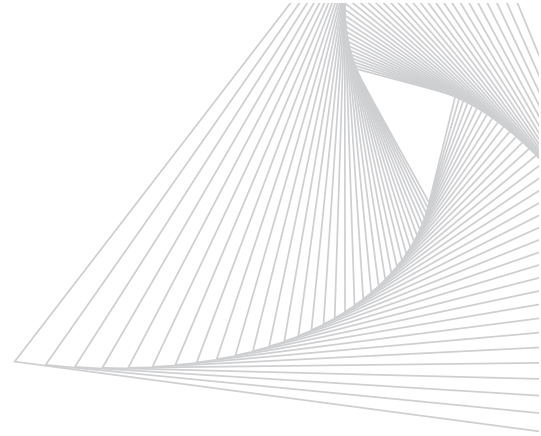
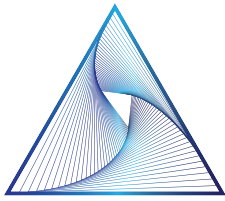


Figure 3. Overlay of Crotonyl Fentanyl and Cyclopropyl Fentanyl

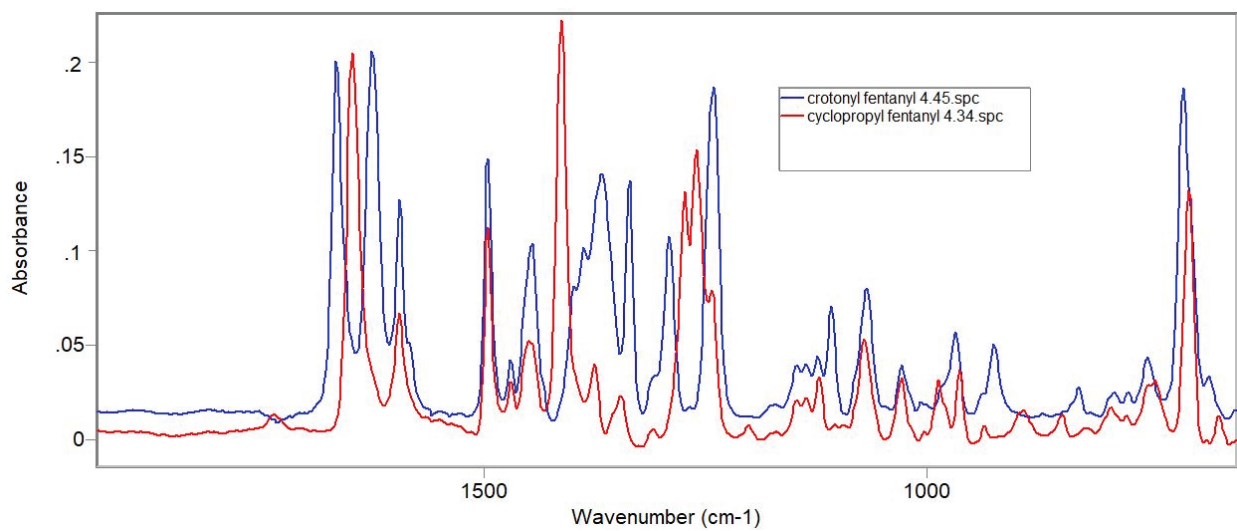


Figure 4. Overlay of Crotonyl Fentanyl and Cyclopropyl Fentanyl Fingerprint Region

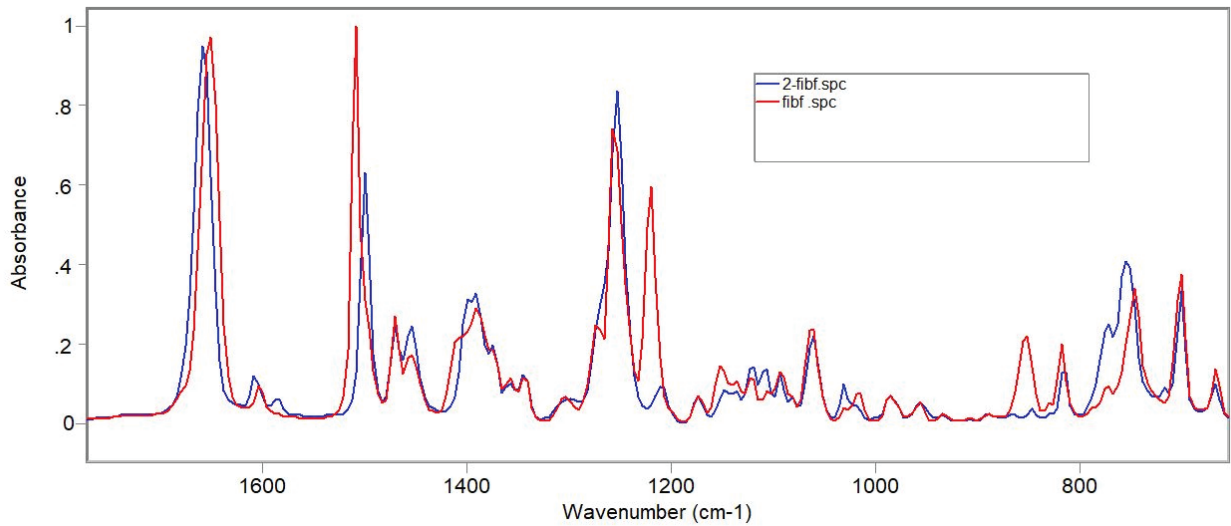
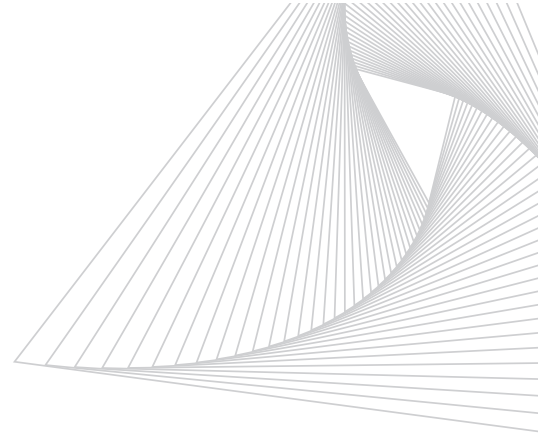
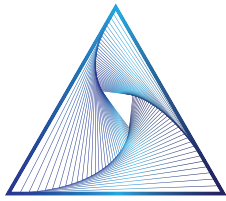


Figure 5. Overlay of Fluoroisobutyryl Fentanyl and 2-Fluoroisobutyryl Fentanyl Fingerprint Region

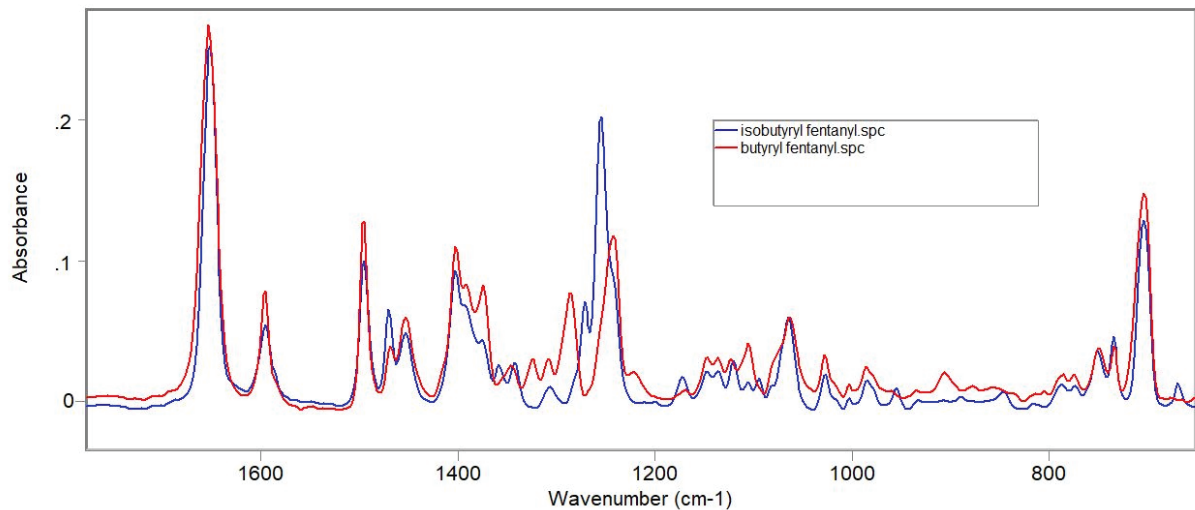


Figure 6. Overlay of Butyryl Fentanyl and Isobutyryl Fentanyl Fingerprint Region

## Advantages of Utilizing Solid Phase DiscovIR-GC

1. Spectral Resolution True 4cm<sup>-1</sup>
2. Sensitivity – ng level of nonadecane, <100ng level of most controlled substances
3. Compatible with most existing solid phase (ATR) IR libraries
4. Compatible with existing GC-MS columns and methods, no need for operator to change to unknown columns or methods

DiscovIR-GC <sup>®</sup> Specifications	
Infrared Spectrum Range	4000-700 cm <sup>-1</sup>
Resolution	4 cm <sup>-1</sup>
Spectrum Type	Transmittance
Re-Usable ZnSe Sample Disc Capacity	20 hours

## References

1. The Fentanyl Epidemic and Evolution of Fentanyl Analogs in the United States and the European Union, Paul J. Jannetto, Anders Helander, Uttam Garg, Gregory C. Janis, Bruce Goldberger, Hemamalini Ketha, DOI: 10.1373/clinchem.2017.281626 Published January 2019
2. National Institute for Drug Abuse (2019 January). Overdose Death Rates, retrieved from <https://www.drugabuse.gov/related-topics/trends-statistics/overdose-death-rates>

## Acknowledgements

1. Cayman Chemicals – Supplying Reference Standards and their outstanding support
2. National Forensic Laboratory (NFL) of Slovenia for use of their NFL DiscovIR library
3. US Army Crime Lab (USACIL) for use of their USACIL 2018 library