IRD 3 Application Note

Fentanyl Analogues

Introduction

Fentanyl is an opioid and a Schedule II controlled substance used primarily as a pain medication. The biological effects of fentanyl are similar to those of heroin. Some fentanyl analogues are thousands of times more potent than street heroin and produce more respiratory depression making them much more dangerous to users. In 2016, fentanyl and its analogues caused over 20,000 deaths in the US, a rise of 540% over the previous 3 years.
The DEA has classified illicit versions of the synthetic opioid at the same level as heroin, allowing criminal prosecution of anyone who possesses, distributes or manufactures these versions of the drug. Although some of these analogues have been banned, manufacturers have created new variations that differ enough to evade current legal restrictions.
Fentanyl and its analogues present a unique challenge for forensic labs. Identifying the exact compound with certainty can be difficult when the molecular weights, chemical structures and GC retention times are nearly identical. GC-FTIR is a powerful analytical technique that allows for the rapid differentiation of compounds with minute differences including isomers and analogues. This example analyzes two fentanyl analogues, acetyl fentanyl and *p*-fluoroisobutyryl fentanyl and demonstrates the ability of the IRD 3 to easily differentiate these compounds.

Product Overview

The IRD 3 is designed from the chromatographer's point-of-view and is the only analytical infrared instrument that seamlessly combines the separating power of the Gas Chromatograph with the molecular identification of FTIR.

- Dedicated FTIR for use with GC
- Low maintenance and easy to use
- Small footprint
- Software interfaces with GC control software
- Seamless integration with MS
- SWGDRUG category A detector

The IRD 3 is the perfect tool for the chromatographer looking to obtain more information about unknown samples. Using a heated light pipe flow cell, the sample is kept in the vapor phase while interacting with IR light. This allows molecules to freely rotate in a low energy environment. Keeping the molecular geometry intact during analysis provides unique and highly reproducible spectra.

Results

Figure 1 shows the IR spectra for acetyl fentanyl and *p*-fluoroisobutyryl fentanyl collected on the IRD 3. The compounds are structurally similar but there are many discernable differences in their IR spectra. The spectra for *p*-fluoroisobutyryl fentanyl has a larger absorption band at 1200 cm^{-1} that correspond to the branching isobutyryl's C-C vibrations and the C-F stretching in the fluorinated benzene ring. This spectra also contains a larger band at 1500 cm^{-1} due to the C-C stretching and bending of the in-plane benzene ring. The spectra for acetyl fentanyl has a sharper single absorption band at 700 cm^{-1} due to its two monosubstituted benzene rings.

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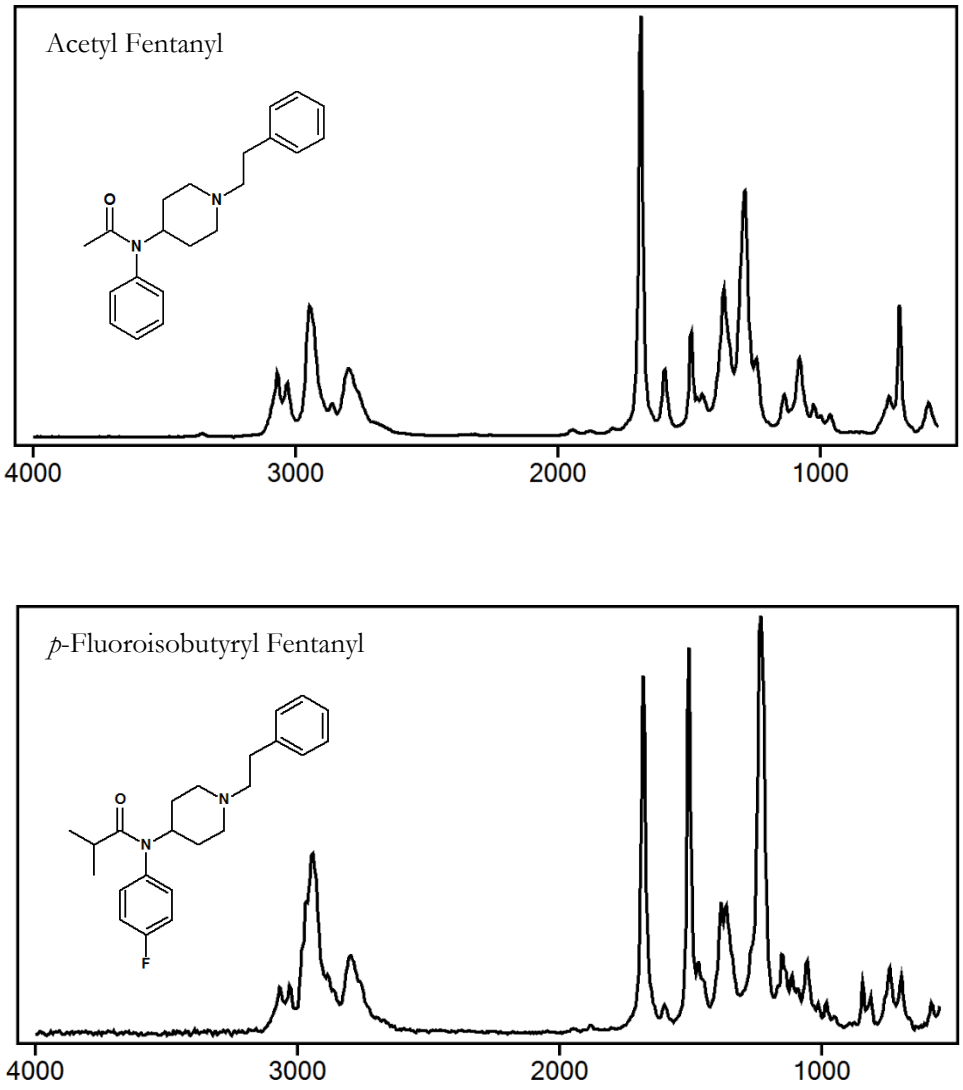
Figure 1.



Conclusion

Fentanyl and its analogues can be difficult to differentiate using GC-MS alone because of their similarities in molecular weight, chemical structure and GC retention time. Figure 1 shows that acetyl fentanyl and *p*-fluoroisobutyryl fentanyl are easily identifiable using the IRD 3. It is a powerful tool that assists the chromatographer in making a positive ID of compounds with similar chemical structures or identical molecular weights. The IRD 3 allows molecules to freely rotate in a low energy environment, keeping the molecular geometry intact during analysis. Therefore providing a unique and highly reproducible spectra.