B189 The Analytical Profile of Fluorobutyryl Fentanyl Isomers

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After attending this presentation, attendees will be familiar with approaches for effectively differentiating positional and structural isomers of fluorobutyryl fentanyl. Attendees will better understand the challenges that forensic laboratories may encounter with new fentanyl-related compounds.

This presentation will impact the forensic science community by providing analytical techniques for differentiating fluorobutyryl fentanyl isomers efficiently and effectively. This presentation will also impact the forensic science community by providing different approaches for other similar fentanyl substances forensic drug laboratories may encounter.

Fentanyl, a Schedule II synthetic opioid, was first synthesized in the late 1950s by Paul Janssen and is used licitly to treat severe pain. Presently, there are numerous fentanyl-related compounds.[1] Examples of such compounds include acetyl fentanyl, butyryl fentanyl, furanyl fentanyl, and acryl fentanyl. The identification of isomers of substances presents a challenge to the forensic drug analyst; new compounds are constantly being illicitly synthesized, such as fluorobutyryl fentanyl. The molecular formula of fentanyl is $C_{22}H_{28}N_2O$, whereas fluorobutyryl fentanyl is $C_{23}H_{29}FN_2O$. With an addition of a fluorine and a methyl group, the structure changes from fentanyl to fluorobutyryl fentanyl. Moving the position of the fluorine on the benzene ring allows for three different positional isomers of this compound. Furthermore, substituting the butanamide with isobutanamide allows for a different structural isomer. This study focuses on the identification of various isomers of fluorobutyryl fentanyl (meta-fluorobutyryl fentanyl, ortho-fluorobutyryl fentanyl, para-fluorobutyryl fentanyl, and para-fluoroisobutyryl fentanyl).

Techniques used in the identification of controlled substances must be both selective and sensitive. Sometimes, confirmatory techniques are not selective between isomers; hence, other approaches must be explored. In this study, various instruments were used to analyze four isomers of fluorobutyryl fentanyl, including Gas Chromatograph/Mass Spectrometry-Low Thermal Mass (GC/MS-LTM), Gas Chromatograph/Flame Ionization Detector (GC/FID), Gas Chromatograph/Flame Ionization Detector-Low Thermal Mass (GC/FID-LTM), Fourier Transform Infrared Spectroscopy with an Attenuated Total Reflectance (FTIR/ATR), ion trap (Tandem Mass Spectrometer or MS/MS), and Direct Analysis in Real-Time Mass Spectrometer (/ART®-MS).

Preliminary results demonstrated that GC-FID is an effective instrument in differentiating the two structural isomers of fluorobutyryl fentanyl. Depending on purity, FTIR/ATR can also be a suitable technique in differentiating the four isomers. Due to their very similar structures, these compounds fragment similarly; therefore, the use of GC/MS, DART®-MS, and MS/MS alone has proven to be insufficient in distinguishing isomers of fluorobutyryl fentanyl.

Reference(s):

1. Vardanyan, R., Victor J. Hruby. Fentanyl-related compounds and derivatives: current status and future prospects for pharmaceutical applications. *Future Med Chem.* 6(4). (2014): 385-412. www.ncbi.nlm.nih.gov. Web 19 July 2017.

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