B18 Structural Elucidation of Synthetic Opioids

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After attending this presentation, attendees will better understand the analytical strategy employed by the Contraband Drug Analysis Section of the Canada Border Services Agency for identifying new substances.

This presentation will impact the forensic science community by providing an overview of analytical challenges encountered during casework involving fentanyl analogues and related drugs. The impact of salt forms and mixtures on the analytical approach as well as the use of Nuclear Magnetic Resonance (NMR) methods for structural elucidation will be discussed. These challenges will be communicated with the drug analysis community in the hopes of spreading awareness and providing others with the ability to apply caution when presented with analysis of these substances and gaining confidence in structural determination.

With the emergence of powerful new opioid agonists (such as W-18 and U-47700) and a resurgence of fentanyl and its analogues, it is increasingly important for drug chemists to share analytical data and strategies for the identification of these compounds. The number of sites on the fentanyl structure that are easily substituted has led to a vast number of potential analogues. Identifying where substitutions have occurred on the molecule by structure elucidation can be challenging. As a result, NMR techniques are often required.

There has been a steady increase in both the number and diversity of synthetic opioid shipments intercepted by the Canada Border Services Agency (both importations and exportations). As of the beginning of 2017, the Contraband Drug Analysis Section has identified an average of one new fentanyl analogue per month. According to a recent United Nations Report, Canada consumes more prescription opioids per capita than any other country in the world. As a consequence, many users look to the illicit market to support their addictions. The emergence of fentanyl, its analogues, and other low-dose drugs in the illicit market has developed new concerns for public safety professionals and new challenges for forensic drug analysis.

When encountering a new drug substance, database references are not always available and literature references can be difficult to find. In these cases, full structural elucidation allows for the identification of the compound. The Contraband Drug Analysis Section is fortunate to have a number of instruments to assist in substance identification: Attenuated Total Reflectance/Fourier Transform Infrared (ATR/FTIR), FT-Raman, Gas Chromatography/Mass Spectrometry (GC/MS), Liquid Chromatography/Tandem Mass Spectrometry (LC/MS/MS), Gas Chromatography/ Infrared Spectroscopy (GC/IR), and Nuclear Magnetic Resonance (NMR), among others. Upon analysis of fentanyl analogues, there have been circumstances in which typical analysis methods were not enough to confidently identify the compound. As an example, NMR methods beyond the routine ^{1}H, ^{13}C, ^{1}H-^{1}H COSY, ^{1}H-^{13}C HSQC, ^{1}H-^{13}C HBMC, and Distortionless Enhancement by Polarization Transfer (DEPT) experiments were employed, including ^{1}H-^{15}N HMBC and Two-Dimensional Incredible Natural-Abundance Double-Quantum Transfer Experiment (2D INADEQUATE) in order to identify 2-methoxy-furanylfentanyl and rule out 3-methoxy-furanylfentanyl. Details of this case as well as structural elucidation of other compounds will be discussed.

Fentanyl, NMR, Elucidation

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