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Direct-Infusion Electrospray Ionization-Mass Spectrometry Profiling of Fentanyl and Acetylfentanyl Reaction Mixtures

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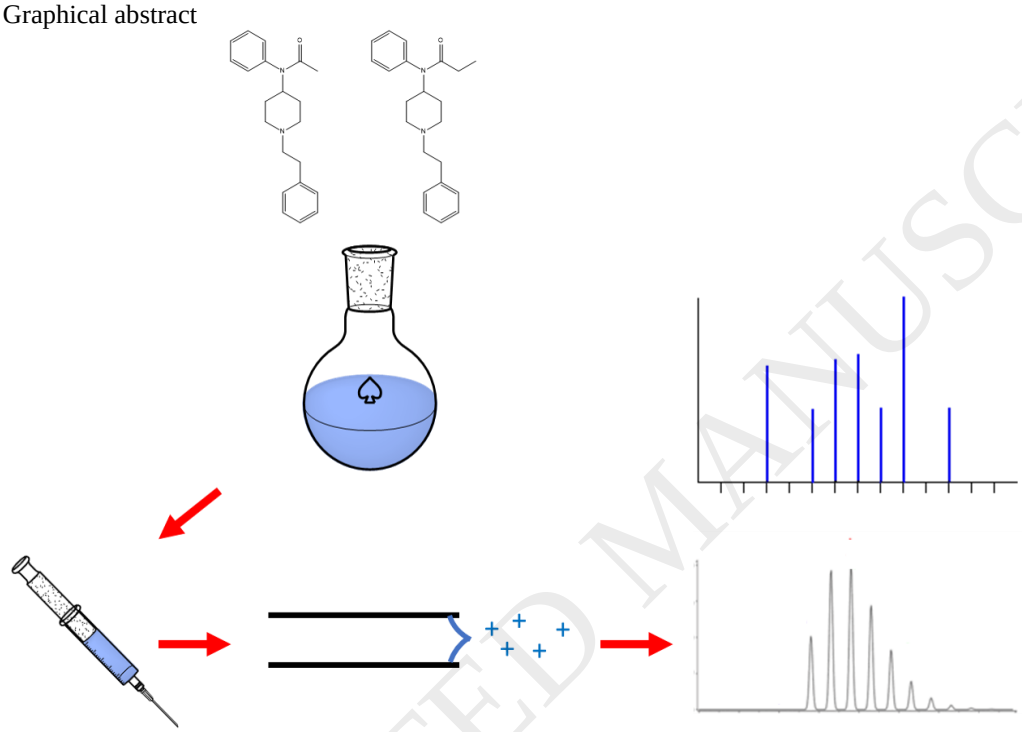
Graphical abstract



Highlights

- Syntheses of fentanyl and acetylfentanyl were performed.
- These syntheses were subjected to DI-ESI-MS and HRMS analysis.
- Amine oxide and O-acetylated byproducts were detected in both reactions.

Abstract

The widespread distribution and variety of fentanyl-related opioids has prompted many forensic researchers to begin exploring new techniques to carefully process and identify the many components of these seized exhibits. While these analyses typically consist of chromatographic separation, this can be a tedious and time-consuming process. To improve upon the accurate detection and structural elucidation of the components of these complex samples, a direct-infusion technique was utilized with ESI-MS on both a triple quadrupole and Orbitrap mass spectrometer to both structurally identify and propose reaction mechanisms for minor, unknown components. Results from these direct-infusion experiments suggest amine oxide formation and O-acetylation within crude reaction mixtures of both fentanyl and acetylfentanyl producing ions at *m/z* 395 and 353, respectively. Other previously detected components, including both byproducts and degradation products, of these samples have also been identified by their exact masses and fragmentation. Complementary fragmentation and exact mass data