B173 The Development of an *In Silico* Mass Spectral Library

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Learning Overview: The goal of this presentation is to provide forensic practitioners with a tool for rapidly and inexpensively down-selecting novel fentalog standards for synthesis and purchase.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by providing forensic practitioners with a tool for rapidly and inexpensively down-selecting novel fentalog standards for synthesis and purchase.

The abuse of opiates, in particular those in the fentanyl family, is a growing epidemic. Because fentanyl and its derivatives (fentalogs) are readily synthesized, a serious analytical challenge has developed. Much like bath salts and other synthetic cannabinoids, small changes in the structure can make the producers of these compounds more difficult to prosecute. Furthermore, these changes can hinder the efforts of forensic drug chemists and toxicologists to identify samples. A major challenge with identifying emerging fentalogs and other novel psychoactive substances (NPS) is the lack of available standards and their associated mass spectra.

To address this challenge, the authors developed a proof-of-concept, *in silico* mass spectral library for fentalogs. This library contains simulated spectra of as-yet uncharacterized fentanyl derivatives, which facilitates rapid identification of emerging fentalogs. The library contains mass spectra generated using ACD/Labs Spectrus Processor and MS Fragmenter software packages. The resulting theoretical fragmentation patterns were used to create a searchable database based in Microsoft Excel. The process began by drawing chemical structures for reasonable, but uncharacterized, fentalogs. The software package then generated mass spectra by fragmenting the structure according to all allowable fragmentation pathways based on mass spectral fragmentation rules. These fragments comprise the *in silico* spectrum for a compound and are included in the library database.

As an initial test, mass spectra were generated for 15 commercially available fentalogs using the software. Experimental mass spectra were obtained for these compounds by analyzing chemical standards with GC/MS. The experimentally obtained spectra were used as challenge spectra for the database. To evaluate the library, the ten most dominant mass fragments from the GC/MS spectrum were searched against the database. The total number of mass spectral fragments that corresponded with the theoretical mass spectrum in the *in silico* library were recorded, and candidate library matches were determined. The candidate matches were placed into tiers according to the number of theoretical fragments found to match the experimental fragments. The candidates with the largest number of matching fragments were placed into Tier 1. Among the 15 challenge compounds, 12 appeared in Tier 1. Additionally, 12 of the challenge compounds had fragment matches to nine or more theoretical ions.

Library compounds with the highest number of matching fragments can be considered structural candidates for the analysis of unknowns. This can enable a laboratory to acquire novel fentalog standards using a simple selection process. In addition, this allows an analyst to rapidly evaluate candidate structures without the need for time-intensive structural elucidation studies.

Fentalogs, GC/MS, Library