OUTCOMES

What were the major goals of the project?

The original proposal was separated into two main aims, each with four major goals or objectives.

Aim 1: Understand the mechanisms of fragmentation of odd-electron and even-electron cathinone analogs. One specific deliverable was to understand the mechanism of formation of the tropylium ion and the methylenedioxy analog of synthetic cathinones; these fragments are abundant and important, yet their formation mechanism remained elusive until our study. Aim 1 was accomplished through the following tasks:

1. Synthesized and/or acquired synthetic cathinones with the ^{13}C isotope label at the alpha or carbonyl position.
2. Synthesized and/or acquired deuterated synthetic cathinones with the D isotope labels on the pyrrolidine, benzyl, or alkyl moieties.
3. Synthesized and/or acquired synthetic cathinones with an ^{18}O isotope label in the carbonyl position.
3. Comparison of the fragmentation patterns of each synthetic cathinone using EI-MS, DART-MS/MS and ESI-MS/MS, Infrared ion spectroscopy, molecular modeling, and high-resolution mass spectrometry (HRMS).
4. Proposed fragmentation mechanisms for each compound and confirmed with MSn analyses of additional analogs.

Aim 2: Understand the mechanisms of fragmentation of odd-electron and even-electron fentanyl analogs. Aim 2 was accomplished through the following tasks:

1. Synthesized and/or acquired fentanyl analogs with the ^{13}C isotope label in various positions.
2. Synthesized and/or acquired fentanyl analogs with D or ^{18}O labels in various positions.
3. Comparison of the fragmentation patterns of each synthetic fentanyl analog using EI-MS, DART-MS/MS and ESI-MS/MS, and HRMS.
4. Proposed fragmentation mechanisms for each compound and confirmed with MSn analyses of additional analogs.

Activities/Accomplishments

The following paragraphs summarize the findings in seven different publications that resulted from this work.