## B115 Improving Qualitative Synthetic Cathinone Identification by Gas Chromatography/ Mass Spectrometry (GC/MS) Using Cold Electron Ionization (Cold-EI)

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After attending this presentation, attendees will understand the merits of Cold-EI in comparison to those of classical Electron Ionization (EI) in the analysis of synthetic cathinones. Attendees will be shown that better identification of synthetic cathinones is possible with Cold EI due to the presence of molecular ion in the mass spectra compared to no molecular ion in the EI spectra.

This presentation will impact the forensic science community by suggesting an alternative avenue for improved identification of forensic drugs using MS. Examples include analyses of emerging drugs, such as synthetic cathinones that yield inconclusive mass spectra due to the lack of molecular ions under classical EI.

Synthetic cathinones are emerging drugs with molecular structures similar to that of cathinone, the active ingredient in the khat plant. They are specifically designed to avoid legal prosecution of the manufacturers and dealers. Synthetic cathinones, which are beta keto-amphetamines, produce amphetamine-like effects when abused. Many synthetic cathinones are scheduled in the United States to protect the public interest. They became known as bath salts, mainly because they are typically misbranded when sold.

Synthetic cathinones are notoriously labile compounds that undergo extensive fragmentation when analyzed using classical EI. As a result, the resulting mass spectra contain little to no molecular ion peak, making the identification uncertain. The interpretation of the spectra is further complicated because synthetic cathinones produce relatively few fragments. Cold-EI relies on vibrational cooling of the analytes prior to ionization, thus reducing thermally induced fragmentation. This technique has been shown to increase the relative abundance of the molecular ion for thermally labile compounds and maintain the integrity of the fragments obtained by classical EI, thus improving the confidence in their identification. The confidence can be further improved by performing Tandem Mass Spectrometry (MS/MS) analyses.

This study subjected a total of 35 controlled synthetic cathinones and positional isomers to analyses by two GC/MS instruments; one equipped with a classical EI ion source and a quadrupole analyzer and another equipped with a cold-EI ion source and a quadropole Time-Of-Flight (qTOF) analyzer. Both instruments used 30m x 0.25mm, 0.25µm Elite-5MS columns for the GC separation.

As expected, all the classical EI mass spectra of synthetic cathinones contained molecular ion with relative intensity of less than 1%. In most cases, more of the molecular ions survived when the analysis was conducted by cold-EI ionization, with some analytes reaching molecular ion relative intensities of more than 25%. MS/MS analyses were performed on analytes that provided molecular ion with more than 5% relative intensity.

To reveal the additional discrimination that the presence of the molecular ion in the mass spectra brings to the spectra, the MS data obtained by the two methods was subjected to Principal Component Analysis (PCA).

**Cold Electron Ionization, Synthetic Cathinones, Molecular Ion**