A119 New Gas Chromatography-Positive Chemical Ionization Tandem Mass Spectrometric Method for the Detection of Methylenedioxypyrovalerone (MDPV), 4-Methylmethcathinone (Mephedrone), and 4-Methoxymethcathinone (Methedrone)

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After attending this presentation, attendees will be familiar with a new approach for the analysis and identification of common "bath salts" ingredients utilizing GC-MS/MS with chemical ionization.

This presentation will impact the forensic science community by providing a definitive method for the identification of synthetic cathinones which are becoming increasingly popular among recreational drug users and are rapidly being regulated by state and national governments.

MDPV, mephedrone, and methedrone are some of the most common compounds currently seen in products being marketed as "bath salts." They are structurally similar to the scheduled stimulants cathinone, and methcathinone. Therefore, the synthetic cathinones, including mephedrone, methedrone, and MDPV, are also structurally similar to each other. As a result, they have similar fragmentation patterns, often with poor molecular ions, when characterized by traditional GC-MS methods utilizing electron ionization. In this study, different GC-MS techniques, including electron and chemical ionization and single and triple quadrupole (QQQ) mass spectrometry, were evaluated in order to determine the most definitive method for identification of synthetic cathinones. Here, it is proposed that GC-MS/MS with chemical ionization in multiple reaction monitoring (MRM) mode can unequivocally detect the presence of and identify the studied compounds.

The method was also developed with the designer drug market in mind. As has been demonstrated recently with the synthetic cannabinoids, "bath salts" have also shown the tendency to have variable contents as bans on certain compounds are enacted. Most often, "bath salts" are marketed as a "legal high," so changing the active compounds in accordance to the new laws is common. As these new compounds arrive on the market, and are also likely regulated, forensic analysis will need to be able to detect them in addition to those currently controlled. This method was developed so that any synthetic cathinones can be run, responses can be optimized, and the appropriate MRM ions can be added to the method with minimal adjustments to facilitate rapid analysis.

Electron ionization, with both single and triple quadrupole analysis, gave very similar spectra for mephedrone and methedrone. Chromatographic peaks also had poor shapes. MDPV exhibited a low-detail fragmentation pattern, but a characteristic peak at *m/z* 126 was detected, due to the presence of the pyrrolidinyl group on the alkyl chain of the compound, that helped distinguish it from the other investigated compounds. Because of similar fragments in single quadrupole analysis for the other two drugs, fragments chosen for tandem mass spectrometry also produced similar patterns. Chemical ionization significantly increased the intensity of the protonated molecular ion relative to the nearly nonexistent molecular ion produced with electron ionization. When triple quadrupole analysis was paired with chemical ionization, unique mass spectra were also observed through the selection of the protonated molecular ion as the precursor ion at Q1. Additionally, chromatographic peaks were clean and lacking the shoulder present in electron ionization analyses.

Compounds that could potentially interfere with the compounds of interest were also subjected to the method. Compounds studied for possible interference included amphetamine, caffeine, cathine, ephedrine, ketamine, phentermine, alprazolam, benzylpiperazine (BZP), clonazepam, cocaine, codeine, diazepam, heroin, hydrocodone, methamphetamine, 3,4-methylenedioxyamphetamine (MDA), 3,4-methylenedioxymethamphetamine (MDMA), oxycodone, pseudoephedrine, trifluoromethylphenylpiperazine (TFMPP), cathinone, inositol, and phenethylamine. No interference was observed, though peaks were occasionally present in the chromatogram. Future studies should be performed to optimize compound-specific conditions for the analysis of other synthetic cathinones in order to confirm the broad application to this class of drugs.

Bath Salts, Designer Drug Analysis, Cathinones

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