



A138 Separation and Identification of Synthetic Cathinones Using GC/MS, GC-QQQ/MS, and ESI-IMS/MS

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After attending this presentation, attendees will learn the use of ion mobility as a separation technique coupled to a mass spectrometer for the analysis of synthetic cathinone and the differences in ionization (ESI vs CI vs EI) in fragmentation and identification of these analytes of interest.

This presentation will impact the forensic science community by making it possible to unambiguously separate the cathinones with IMS faster than with GC/MS, while also preserving the molecular ion due to the soft ionization using ESI.

Cathinone is the main component of the *khat* plant which produces a stimulating effect similar to amphetamines.¹ The ease of online availability of a number of the *synthetic cathinones*, also known as legal highs or bath salts, have led to increased use and abuse over the past few years.² In this study, six synthetic cathinones, recently scheduled as Schedule I controlled substances in Florida as of July 2012, 4-methylmethcathinone (mephedrone or 4MMC), 3-fluoromethcathinone (flephedrone or 3FMC), 4-methylethcathinone (4MEC), 4-methoxymethcathinone (methedrone or bkPMMA), 3,4-methylenedioxyethcathinone (methylone or bkMDMA), and 3,4-methylenedioxypropylvalerone (MDPV), were analyzed using a commercially available electrospray ionization-ion mobility spectrometer-mass spectrometer (ESI-IMS-MS), a gas chromatograph-mass spectrometer (GC/MS) using electron ionization (EI), and a GC/MS Triple Quadrupole (QQQ) with both EI and chemical ionization (CI) modes. One of the advantages of using the softer CI and ESI ionization sources is the creation of molecular ions of the easily fragmented compounds and, in the case of ESI, the ability to analyze nonvolatile compounds and ionize compounds in the liquid phase.³ A fast and selective method is reported that can be used to unambiguously identify this increasingly important class of drugs. A high-resolution IMS was used to separate mixtures of these synthetic cathinones within less than 20ms. The limits of detection were determined and good separations from two-compound mixtures were achieved with typical concentrations of MDPV and other compounds (20:100ppm), and methylone and other compounds (20:100ppm) using ESI-IMS-MS. The analysis of these cathinones was also carried out using GC/MS, which is currently the standard technique used in forensic laboratories, to compare with ESI-IMS-MS. In addition, GC-QQQ-MS with EI and CI modes was used to determine the identification of fragmented ions from these cathinones. The analysis of several actual seized police case samples was also performed using the same instruments to illustrate the utility of the developed IMS-MS and GC-QQQ-MS methods.

These methods, reported for the first time for the drugs listed, make it possible to unambiguously separate the cathinones with IMS faster than with GC/MS while also preserving the molecular ion due to the soft ionization using ESI.

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References:

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