K6 Identification of Synthetic Cathinones From Electron Impact Mass Spectra

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After attending this presentation, attendees will be able to describe characteristic fragmentation pathways for existing synthetic cathinones and predict new fragments for novel analogs as they arise.

This presentation will impact the forensic science community by highlighting the importance of mass spectral properties, the specificity of ion selection during analysis, and the practical limitations associated with some drugs within this class.

The popularity of synthetic cathinones and the diverse number of drugs within this relatively new class has increased considerably in recent years. Gas Chromatography/Mass Spectrometry (GC/MS) is still the most widely used technique in routine forensic toxicology investigations. Due to the proliferation of structural analogs and limited cross-reactivity toward the entire class of drugs, chromatographic-based screening is of great importance for the synthetic cathinones. Chromatographic separation of analytes can be readily achieved using multi-component mixtures; however, the Electron Impact (EI) mass spectral properties of some of the forensically important synthetic cathinones can present a challenge due to the limited number of diagnostic ions.

The characteristic fragmentation pathways synthetic cathinones are described and discussed for nineteen secondary and tertiary amines within this class. These include buphedrone, ethcathinone, methcathinone, pentedrone, 4-EMC, 4-MEC, flephedrone, mephedrone, methedrone, α-PVP, MPBP, naphyrone, pyrovalerone, butlyone, ethylone, methylone, pentylone, MDPBP, and MDPV. Although protonated molecular ions are readily observed using hyphenated Electrospray Ionization (ESI) techniques, parent ions are hard to obtain using EI/GC/MS. Molecular ions when they are present are odd, due to the "nitrogen rule." The mass spectra of synthetic cathinones are dominated by two characteristic cleavages to form iminium and acylium ions that are associated with the side chain and the core benzene ring (which is often substituted). The presence of the carbonyl bond on the α-carbon and the lone pair of electrons on the oxygen of the ketone moiety plays an important role in EI ionization. In addition to the rationalization of non-derivatized cathinones, acylation, silylation, and two-step reductive silylation and reductive acylation methods will also be presented and discussed in terms of their mass spectral properties. Although fragmentation is largely predictable, it presents some practical limitations in terms of the specificity of some diagnostic ions, necessitating careful attention to chromatographic separation and identification criteria.

Cathinones, Mass Spectra, Electron Impact