K34 Stability of the Synthetic Cathinones: Implications for Forensic Toxicology

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After attending this presentation, attendees will understand the challenges associated with the stability of the synthetic cathinones and the implications for forensic toxicology analysis and interpretation.

This presentation will impact the forensic community by increasing awareness pertaining to the stability of the synthetic cathinones and the need to consider this factor during analytical and interpretive deliberations.

Synthetic cathinones are an important class of designer drug. The widespread attention and publicity associated with these psychostimulants have resulted in numerous legislative actions at the state and federal level throughout the United States and elsewhere. These amphetamine-like drugs are characterized by a beto-keto functional group. Although the synthetic cathinones share many properties of their phenethylamine counterparts, the presence of the ketone moiety is responsible for a number of unique and distinct differences in terms of chemical behavior and in particular, stability.

A series of synthetic cathinones were evaluated as part of a study to investigate novel derivatives by Gas Chromatography/Mass Spectrometry (GC/MS). During the course of this work, it was evident that several drugs within the class were unstable. Degradation of first-generation cathinones was first documented more than 30 years ago in drug chemistry. More recently, forensic toxicology reports have highlighted apparent instability for some of the newer drugs within this class, but more research is needed.

Degradation was most often characterized by a second peak, or shoulder, on the principal analyte yielding a molecular ion 2 mass units lower than the major analyte peak. Corresponding mass losses on the highly characteristic and often dominant iminium ion were also observed. Earlier studies with methcathinone showed that this minor component arose through thermal oxidation of the 2,3-carbon-carbon bond to yield the 2,3-enamine.[1] Oxidative degradation of these arylaminoketones was observed *in situ*. Even tertiary amines, which are reported to be the most stable of the cathinone species, were subject to degradation. GC conditions were optimized to allow for baseline separation for many of the degradation products. Degradation data and spectra illustrating the characteristic fragmentations and proposed structures will be discussed for 3,4-methylenedioxypyrovalerone (MDPV), 4-methyl-α-pyrrolidinobutiophenone (MPBP), pyrovalerone, 3,4-methylenedioxy-α-pyrrolidinobutiophenone (MDPBP), naphyrone, ethylone, mephedrone, 4-Ethylmethcathinone (4-EMC), methcathinone, methedrone, flephedrone, and methylone.

Stability of the arylaminoketones is an important consideration for forensic toxicology. Stability data and mass spectra for the cathinone degradation products will be presented and discussed within the context of forensic toxicological analysis, selection of appropriate instrumental methods, and implications for the interpretation of results.

Reference:

1. J DeRuiter, L Hayes, A Valaer, CR Clark and FT Noggle. Methcathinone and designer analogues: synthesis, stereochemical analysis and analytical properties. Journal of Chromatographic Science, 32: 552-564 (1994).

Cathinone, Stability, GC/MS

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