B190 Analysis of Phenethylamine Street Drugs for Psychoactive Compounds and Impurities

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After attending this presentation, attendees will understand details concerning the challenges of separation and analysis of the various phenethylamine compounds and how the analysis of the reference materials differs from what is observed in actual street samples. Separation utilizing Ultra-High Performance Liquid Chromatography, coupled with Time-Of-Flight/Mass Spectrometry (UHPLC-TOF/MS) will be demonstrated along with a direct sample analysis approach utilizing Direct Sample Analysis (DSA)-TOF/MS.

This presentation will impact the forensic science community by discussing how discovering the impurities within these compounds and raising awareness of the dangers of consuming drugs from incompetent synthesis may prevent future overdoses and health complications and diminish the market for unsafe illegal drugs.

The purpose of this study is to determine not only the identity of the psychoactive compound(s) and their concentrations in the various street samples but also to determine impurities which may exist from less-than-ideal synthetic procedures likely employed by potential users/manufacturers of "2C-type" drugs. Serious health complications and fatal overdoses have brought phenethylamine designer drug use to the public's attention. The phenethylamine compounds alone are not believed to be causing the health complications but rather the cause may be impurities within the sample. These impurities may result from the improper technique and inadequate equipment used during illegal synthesis. The substituents on these emerging drugs are constantly changed in order to avoid legal ramifications; however, many of these compounds are Schedule I drugs and, therefore, their analogs are also illegal according the Federal Analog Act. These compounds are 2C-X-series analogs of mescaline. The name "2C" results from the two carbons in the ethyl chain. These synthetic drugs are marketed as having affects similar to LSD and are typically consumed sublingually via blotter paper. The compounds have psychedelic affects on the $5HT^{2A}$ receptor in the brain. The compounds have a variety of street names including "N-BOMB," "Smiles," and "Bromo-DragonFLY."

The objective of this research is to qualitatively and quantitatively identify the drugs and potential impurities. Street samples were compared to known standards in order to determine if impurities exist that may be resulting in health complications. The analysis was done using a variety of UHPLC instruments. Liquid chromatography was utilized rather than gas chromatography because the 2C compounds are considerably more reactive than many other recreational drugs. Analysis by gas chromatography has proven troublesome, at best. Additionally, using gas chromatography would require derivatization, which generally utilizes aprotic solvents, which do not allow for dissolution of the 2C compounds. Following UHPLC separation, TOF/MS was employed for compound identification and subsequent quantification. Finally, a separate sample introduction technique (DSA) was coupled with TOF/MS, thus providing various methods of analysis and identification of the targeted drugs and impurities, which will all be compared and contrasted in this presentation.

MS/MS spectra were used to determine the fragmentation patterns; these fragmentation patterns were observed for 28 standards. The first fragment for every 2C compound was a loss of 17amu, representing the loss of the -NH2 substituent. Compounds belonging to the NBOMe subgroup fragmented into a 121 peak. Halogenated compounds displayed the loss of a halogen group. The mass spectrum for every 2C compound includes a peak at 77m/z, which represents the phenyl ion, and a peak at 91m/z, which represents the tropylium ion. While all the MS/MS spectra for the compounds were similar in fragmentation patterns, they displayed differences that allow the analyst to distinguish which compound is present. Using a high-resolution MS instrument enables an analyst to determine the molecular formula of unknown compounds. The mass spectra generated after UHPLC separation and DSA of a blotter paper street sample were compared with the spectra of the 19 standards. Upon comparison, 25C NBOMe and 25B NBOMe were identified on the blotter paper. This identification was confirmed by comparing mass spectra fragmentation patterns and isotope ratios for chlorine and bromine from the street sample and the standards. Discovering the impurities within these compounds and raising awareness of the dangers of consuming drugs from incompetent synthesis may prevent future overdoses and health complications and diminish the market for unsafe illegal drugs. Because these drugs are emerging substances of abuse, there are no accepted protocols for analysis. DSA allows for a quick screening of seized compounds that can then be analyzed and identified using UHPLC-TOF/MS.

2C, Phenethylamines, DSA-TOF/MS