K7 Investigation of Unknown Designer Drugs and Metabolites in Urine Collected From Electronic Dance Music (EDM) Attendees

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After attending this presentation, attendees will understand the process of structure elucidation and compound identification when unknown analytes are encountered using chromatographic and spectrometric techniques for the analysis of urine samples. This presentation may also give rise to the determination of novel compounds identified in the attendees of EDM festivals by allowing meeting attendees to contribute their input regarding similar peaks they may have encountered.

This presentation will impact the forensic science community by presenting the identification of several metabolites discovered in authentic urine samples that have not been thoroughly explored in the literature.

The designer drug market has continued to expand over the last several years with structural modifications continually being introduced in an attempt to skirt legal rulings. Blood, urine, and oral fluid samples were collected from volunteers attending an EDM festival in addition to asking the volunteers to answer questions regarding recent drug use, effects, and dosage. This group was targeted in an effort to attain authentic specimens from a population suspected to have a high likelihood of using designer drugs. The urine samples were analyzed via a battery of analytical methods in order to fully investigate the compounds present as well as the anticipation of detecting unknown analytes or metabolites. Results produced by the analysis on both Gas Chromatography/Mass Spectrometry (GC/MS) and Liquid Chromatography/Time-Of-Flight (LC/TOF) were key in the determination of unknown compounds. Samples were extracted using a solid phase extraction which targeted basic drugs to optimize the detection of designer stimulant and hallucinogen related compounds.

The GC/MS results were very promising with a quantity of designer drugs being detected including methylone, ethylone, butylone, dimethylone, 5-APB, fluoroamphetamine, and alpha-PVP. This presentation will describe the process to elucidate unknown peaks, several of which were minor metabolites of common compounds including cocaine, quetiapine, and dextromethorphan or were endogenous in nature. The most interesting unknown peaks were present in combination with alpha-PVP. The mass spectra of each of the two peaks displayed a prominent 126 ion, although the two peaks had separate retention times than all the other designer drugs present in the extensive in-house library. The samples were also analyzed on the LC/TOF and produced peaks with accurate masses and retention times that were unique to these unknown compounds as compared to the instrument database.

These two peaks of interest have yet to be identified and it is the goal of this presentation to allow the scientific community to comment and collaborate to aid in the identification of unpublished metabolites or novel compounds. The combination of structure prediction software, comparison of results from various analytical methods, and investigation of fragments using elemental composition serve as great tools in the elucidation of unknown compounds.

Metabolite Elucidation, Designer Drugs, LC-TOF