A177 High Throughput Analysis of Street-Quality Drug Mixtures by DART® GSX Analysis and MassWorks™ Post Acquisition Characterization

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After attending this presentation, attendees will have an understanding of the analytical capabilities of the Direct Analysis in Real Time (DART®) GSX™ instrumental platform from IonSense® for the rapid analysis of street-quality drug mixtures. The inherent, high throughput capabilities of this technique will be compared to current Gas Chromatography/Mass Spectrometry (GC/MS) analytical methods.

This presentation will impact the forensic science community by demonstrating the qualitative high throughput analysis of street-quality controlled substances by DART® ionization which allows for the rapid characterization of unknown evidence samples by decreasing laboratory time and costs of instrumental operation compared to current GC/MS platforms.

The new DART® GSX™ platform allows for the ambient ionization of solid and liquid samples. Ionized species are then detected and analyzed by an Agilent® Gas Chromatography/Mass Selective Detector (GC/MSD) quadrupole mass analyzer. Protonation of molecules for mass analysis is achieved by the formation of metastable helium species which then react with atmospheric water and create protonated water clusters. These protonated water clusters interact with the analytes of interest, creating protonated species, which enter the mass analyzer and are separated from neutrals through the use of ion optics. Simulated street quality drug mixtures were created in increasing complexity and concentration with the addition of common adulterants and diluents in order to mimic unknown evidence samples commonly encountered in the analysis of controlled substances. Common adulterants and diluents including, but not limited, to lidocaine, benzocaine, procaine, levamisole, caffeine, creatinine, mannitol, inositol, and boric acid were utilized in the creation of street-quality cocaine mixtures. A continually developing mass spectral library for common adulterants and diluents by DART® ionization was created in order to aid in the post-acquisition analysis of cocaine mixtures. Further confirmation of mass spectral data created by the DART® GSX™ platform was performed on an equivalent DART® ionization source interfaced to a Thermo LCQ™ Classic with an ion trap mass analyzer.

Post-acquisition processing of mass spectral data for cocaine mixtures were performed through Agilent® ChemStation® analysis software. The stepwise subtraction of suspected adulterants/diluents contained within cocaine mixtures was performed to enable rapid and simple mass differentiation and analyte confirmation of cocaine. Further analysis by Selective Ion Monitoring (SIM) enabled the successful identification of cocaine and its fragments within samples where the concentration of adulterants and diluents present were greater than 500 times the concentration of the amount of cocaine present within the same sample. Several sampling methods and substrate types, such as stainless steel wire mesh, cotton swabs, polyester swabs, and glass capillaries, were examined to enable rapid automated sample introduction.

MassWorks™ post-acquisition analysis software from Cerno Bioscience was used for accurate mass assignment and chemical formula determination. Using known calibration standards along with the MSIntegrity calibration technology, Calibrated Line-shape Isotope Profile Search (CLIPS) was performed to increase spectral accuracy on the unit resolution GSX quadrupole system and to identify molecular formulas for known mixtures.

Comparative analysis of the DART® GSX™ instrumental platform versus current GC/MS platforms demonstrated the characterization of complex cocaine mixtures in a fraction of the time required by equivalent GC/MS methods. With a decrease in the use of consumables, time spent on sample preparation/introduction, and cost of operation, DART® ionization eliminates several drawbacks of current GC/MS methodologies for the characterization of controlled substances in forensic laboratories.

DART®, Cocaine, High Throughput

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